A Complete Bibliography of Publications in *Computer Physics Communications*: 2010–2019

Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: `beebe@math.utah.edu`, `beebe@acm.org`, `beebe@computer.org` (Internet)
WWW URL: `https://www.math.utah.edu/~beebe/`

08 November 2023
Version 1.95

Title word cross-reference

D

[WG12]. **TaylUR** [vH10]. **TD** [HM17]. **TD-DFT** [HM17]. **TDDFT** [PVK^{+}18, PUO14]. **TDDS** [GLHR19]. **TDF** [SGDS16]. **TDHF** [MRSU14, SRS^{+}18]. **TDSE** [FZY17, ÓN14]. **TE** [LS17b, LSSW14]. **tearing** [HSK^{+}12]. **Technical** [DNP^{+}12, DPW16, LS15a]. **technique** [BALV16, BCDP18, CS10, DG10a, DG10b, DM17, Eba13, EKDGG15, GHvdL11, GGG16, GTS14, Hon10, JAS17, KN13, Koh15, KR16, LLX14b, NPAD11, NDSH18, NVAFO18, QZ19, Ram10, SK14, TH17, VDB14, WLS13, WDR16, MAIVAH14]. **techniques** [BCS10, BD12, BJM15, BVSG19, BSW12, GSB^{+}14, JZJ18, KHKR14, LAG^{+}17, MIW^{+}13, MC12, MHWH19, OBH10, PLF^{+}17, RGH10, RWKS15, WMI19, ZWC^{+}19]. **technological** [CMdB11]. **technology** [DM12, MSI^{+}10, MRL19, RB18]. **telegraph** [PKT15, XYK12]. **telescope** [ECD^{+}10]. **tell** [KSL^{+}11]. **TEM** [KQYH17]. **Temperature** [HST^{+}11, HEF^{+}11, OBM19, BM16, CM10a, GB14, HvWT17, Hin11, KST14a, KCT15, KA17, KGNS10, Liu13, LK15, Liu15a, LJD^{+}19, Mil16, RF16, SLK19, SLC11, SC15, SC16b, SPSP18, VdLF14]. **Temperature-controlled** [HST^{+}11]. **temperature-dependent** [SLC11]. **temperatures** [Wai12]. **tempering** [Boe14, FFT^{+}14, JJ15, VdLF14, VDF15]. **Template** [LHL11, BJ14]. **TemplateTagger** [BJ14]. **Temporal** [MDF11, SCB^{+}17a, YHCS11, IBP^{+}15, KEH12]. **TENO** [Fu19a, Fu19b]. **tensile** [SCM^{+}18]. **Tension** [RM10a, DIR^{+}19]. **Tensor** [SPS18, BK12, Bre10, DKOS14, DLW^{+}18, GCH^{+}18, HR11, KAK12, KK14b, KK14a, KCA^{+}15, Lya15, MK19, NKS15, Nie18, PGO17]. **Tensors** [Dep17, Ara14a, Ara14b]. **term** [Pla16]. **terms** [ACMM10, ACML11, ACM12, Deg15, HMU10, LNP^{+}17, MSR10]. **ternary** [Sza16]. **terrain** [OAKS11]. **TERS** [Nat10, Nat09]. **Tersoff** [Ngu17]. **Tesla** [Lya15, AAA^{+}16]. **Tessellation** [CMSN18]. **tessellations** [SOJ14]. **Test** [LNSD15, PBE14, SISW10, TdAdSS11, VEM12, ZZG^{+}16]. **test-kinetic** [VEM12]. **TESTER** [DGPW11]. **Testing** [ES11, FMRP16, Pit10, Liu11, MGFRG12, TVT^{+}16, Zlo14]. **Tests** [SMJ17, Gag12b, Gag12a, GH18]. **tetrahedral** [JG16]. **tetrahedron** [GJ18b, Kap12a]. **tetrahedron-based** [GJ18b]. **Tevatron** [BBH^{+}10, BBH^{+}11a]. **TFmix** [SLK19]. **Th** [CHW^{+}15, GJ14]. **th-order** [GJ14]. **their** [BDJS18, GSMK17, GCVA14b, KAR^{+}15]. **theoretic** [SSBS15]. **Theoretical** [HCC14, LQZ^{+}13, NS11b, NVW^{+}13, Sit18]. **theories** [ADF^{+}15, CJ12, Cip11, Fri14a, LM19, LSSW14, SA14]. **Theory** [GS17a, VCMS^{+}13, ZZH^{+}16, ASA18, ADT^{+}19, BPC12, BB13a, BW12a, BG11, BO12, BRH^{+}16, CXH^{+}15, CKhN11, Chr18, CZ19, Cri18, DF13, FK15, GWL^{+}17, GTK^{+}19a, GBR^{+}14, HAH13, Hsu11b, HHS^{+}10, JCW^{+}13, KBB^{+}17, KVW11, KBSP19, KPST15, Kra17, Kra18a, LA13, LSDD14, LWES18, LSK^{+}14, MGRB11, MBF^{+}10, MOB12, MSS^{+}16, MG10a, Mül11a, MC17, Naz12, NRSVW12, Nut14, OOK^{+}12, OT11, Pre18, QJF16, RWKS15, San15, SD15, SCRS17, SSH16, SBH^{+}12, SÜ18, TVGB15, VBS^{+}17, WHG^{+}19, Wan10b, WM13, YZWR14, YLYL17, ZAHA10, BK13b, BC10, DBB12, GS17b, LT15]. **thermal** [CCXC15, DS13b, FSH13, Fow18, FM15, GM14, TKP12, Wan16,

References

Aaij:2016:TAR

[AAA+16] R. Aaij, S. Amato, L. Anderlini, S. Benson, M. Cattaneo, M. Clemencic, B. Couturier, M. Frank, V. V. Gligorov, T. Head, C. Jones, I. Komarov, O. Lupton, R. Matev, G. Raven, B. Sciascia, T. Skwarnicki, P. Spradlin, S. Stahl, B. Storaci, M. Vesterinen, et al. Tesla: an application for real-time data analysis in high energy physics. *Computer Physics Communications*, 208(??):35–42, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302107`.

Andonov:2010:SSM

[AAB+10a] A. Andonov, A. Arbuzov, D. Bardin, S. Bondarenko, P. Christova, L. Kalinovskaya, V. Kolesnikov, and R. Sadykov. Standard SANC modules. *Computer Physics Communications*, 181(2):305–312, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003154`.

Ask:2010:REV

[AAB+10b] S. Ask, I. V. Akin, L. Benucci, A. De Roeck, M. Goebel, and J. Haller. Real emission and virtual exchange of gravitons and unparticles in Pythia8. *Computer Physics Communications*, 181(9):1593–1604, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001670`.

Arbona:2013:SGP

[AABC+13] A. Arbona, A. Artigues, C. Bona-Casas, J. Massó, B. Miñano, A. Rigo, M. Trias, and C. Bona. Simflowny: a general-purpose platform for the management of physical models and simulation problems. *Computer Physics Communications*, 184(10):2321–2331, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001471`.

Abedian:2013:HOW

[AAD13] Rooholah Abedian, Hojatollah Adibi, and Mehdi Dehghan. A high-order weighted essentially non-oscillatory (WENO) finite difference scheme for nonlinear degenerate parabolic equations. *Computer Physics Communications*, 184(8):1874–1888, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001094.

Abedian:2014:HOS

[AAD14] Rooholah Abedian, Hojatollah Adibi, and Mehdi Dehghan. A high-order symmetrical weighted hybrid ENO-flux limiter scheme for hyperbolic conservation laws. *Computer Physics Communications*, 185(1):106–127, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300283X.

Azooz:2014:LPR

[AAJA14] A. A. Azooz, Y. A. Al-Jawaady, and Z. T. Ali. Langmuir probe RF plasma compensation using a simulation method. *Computer Physics Communications*, 185(1):350–356, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003044.

Azooz:2012:PNT

[AANAJ12] A. A. Azooz, S. H. Al-Nia'emi, and M. A. Al-Jubbori. A parameterization of nuclear track profiles in CR-39 detector. *Computer Physics Communications*, 183(11):2470–2479, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002238.

Allanach:2014:NMS

[AAT+14] B. C. Allanach, P. Athron, Lewis C. Tunstall, A. Voigt, and A. G. Williams. Next-to-minimal SOFTSUSY. *Computer Physics Communications*, 185(9):2322–2339, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001386. See corrigendum [AAT+20].

Aslanyan:2017:ECD

[AAT17] V. Aslanyan, A. G. Aslanyan, and G. J. Tallents. Efficient calculation of degenerate atomic rates by numerical quadrature on GPUs. *Computer Physics Communications*, 219(??):261–268, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301856.

Allanach:2020:CNM

[AAT+20] B. C. Allanach, P. Athron, Lewis C. Tunstall, A. Voigt, and A. G. Williams. Corrigendum to “Next-to-Minimal SOFTSUSY” [Comput. Phys. Comm. **185** (2014) 2322–2339] (New Version Announcement). *Computer Physics Communications*, 250(??):Article 107044, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519303753. See [AAT+14].

Allanach:2010:IPV

[AB10] B. C. Allanach and M. A. Bernhard. Including R-parity violation in the numerical computation of the spectrum of the Minimal Supersymmetric Standard Model: SOFTSUSY3.0. *Computer Physics Communications*, 181(1):232–245, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003051.

Antoine:2013a:CMD

[ABB13] Xavier Antoine, Weizhu Bao, and Christophe Besse. Computational methods for the dynamics of the nonlinear Schrödinger/Gross–Pitaevskii equations. *Computer Physics Communications*, 184(12):2621–2633, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002403.

Alioli:2014:UBH

[ABB+14] S. Alioli, S. Badger, J. Bellm, B. Biedermann, F. Boudjema, G. Cullen, A. Denner, H. van Deurzen, S. Dittmaier, R. Frederix, S. Frixione, M. V. Garzelli, S. Gieseke, E. W. N. Glover, N. Greiner, G. Heinrich, V. Hirschi, S. Höche, J. Huston,

H. Ita, N. Kauer, F. Krauss, G. Luisoni, D. Maître, F. Maltoni, P. Nason, C. Oleari, R. Pittau, S. Plätzer, S. Pozzorini, L. Reina, C. Reuschle, T. Robens, J. Schlenk, M. Schönherr, F. Siegert, J. F. von Soden-Fraunhofen, F. Tackmann, F. Tramontano, P. Uwer, G. Salam, P. Skands, S. Weinzierl, J. Winter, V. Yundin, G. Zanderighi, and M. Zaro. Update of the Binoth Les Houches Accord for a standard interface between Monte Carlo tools and one-loop programs. *Computer Physics Communications*, 185(2):560–571, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003482.

Ablinger:2016:CTL

[ABB+16] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, and C. Schneider. Calculating three loop ladder and V-topologies for massive operator matrix elements by computer algebra. *Computer Physics Communications*, 202(??):33–112, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000175.

Athron:2019:BFF

[ABB+19] Peter Athron, Csaba Balázs, Michael Bardsley, Andrew Fowlie, Dylan Harries, and Graham White. Bubbleprofiler: Finding the field profile and action for cosmological phase transitions. *Computer Physics Communications*, 244(??):448–468, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301754.

Aebischer:2018:WEF

[ABC+18] Jason Aebischer, Ilaria Brivio, Alejandro Celis, Jared A. Evans, Yun Jiang, Jacky Kumar, Xuanyou Pan, Werner Porod, Janusz Rosiek, David Shih, Florian Staub, David M. Straub, Danny van Dyk, and Avelino Vicente. WCxf: an exchange format for Wilson coefficients beyond the Standard Model. *Computer Physics Communications*, 232(??):71–83, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302054.

Antuono:2014:MSD

[ABCM14] M. Antuono, B. Bouscasse, A. Colagrossi, and S. Marrone. A measure of spatial disorder in particle methods. *Computer Physics Communications*, 185(10):2609–2621, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002124.

Allanach:2015:HOC

[ABdA15] B. C. Allanach, A. Bednyakov, and R. Ruiz de Austri. Higher order corrections and unification in the minimal supersymmetric standard model: SOFTSUSY3.5. *Computer Physics Communications*, 189(??):192–206, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004135.

Antoine:2017:AIT

[ABDR17] Xavier Antoine, Christophe Besse, Romain Duboscq, and Vittorio Rispoli. Acceleration of the imaginary time method for spectrally computing the stationary states of Gross–Pitaevskii equations. *Computer Physics Communications*, 219(??):70–78, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301388.

Alexandrou:2019:MAS

[ABF19] Constantia Alexandrou, Simone Bacchio, and Jacob Finkenrath. Multigrid approach in shifted linear systems for the non-degenerated twisted mass operator. *Computer Physics Communications*, 236(??):51–64, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303618.

Athron:2018:FEI

[ABH+18] Peter Athron, Markus Bach, Dylan Harries, Thomas Kwasnitza, Jae hyeon Park, Dominik Stöckinger, Alexander Voigt, and Jobst Ziebell. FlexibleSUSY 2.0: Extensions to investigate the phenomenology of SUSY and non-SUSY models. *Computer Physics Communications*, 230(??):145–217, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301322.

Auzinger:2019:PSM

[ABH+19] Winfried Auzinger, Iva Brezinová, Harald Hofstätter, Othmar Koch, and Michael Quell. Practical splitting methods for the adaptive integration of nonlinear evolution equations. Part II: Comparisons of local error estimation and step-selection strategies for nonlinear Schrödinger and wave equations. *Computer Physics Communications*, 234(??):55–71, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302984.

Awile:2012:FNL

[ABRS12] Omar Awile, Ferit Büyükkeçeci, Sylvain Reboux, and Ivo F. Sbalzarini. Fast neighbor lists for adaptive-resolution particle simulations. *Computer Physics Communications*, 183(5):1073–1081, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000057.

Ablinger:2019:NIH

[ABRS19] J. Ablinger, J. Blümlein, M. Round, and C. Schneider. Numerical implementation of harmonic polylogarithms to weight $w = 8$. *Computer Physics Communications*, 240(??):189–201, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300578.

Angeli:2013:AEM

[AC13] C. Angeli and R. Cimiraglia. Automated evaluation of matrix elements between contracted wavefunctions: a Mathematica version of the FRODO program. *Computer Physics Communications*, 184(2):443–444, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003323.

Ayala:2015:AMP

[AC15] César Ayala and Gorazd Cvetic. anQCD: a Mathematica package for calculations in general analytic QCD models. *Computer Physics Communications*, 190(??):182–199, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000120.

Ayala:2016:AFP

[AC16] César Ayala and Gorazd Cvetic. anQCD: Fortran programs for couplings at complex momenta in various analytic QCD models. *Computer Physics Communications*, 199(??):114–117, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003719.

Allanach:2017:CSH

[AC17] B. C. Allanach and T. Cridge. The calculation of sparticle and Higgs decays in the minimal and next-to-minimal supersymmetric standard models: SOFTSUSY4.0. *Computer Physics Communications*, 220(??):417–502, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302412.

Ayala:2018:AMP

[AC18] César Ayala and Gorazd Cvetic. anQCD: a Mathematica package for calculations in general analytic QCD models (new version announcement). *Computer Physics Communications*, 222(??):413, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302928.

Arnal:2017:SCS

[ACC17] Ana Arnal, Fernando Casas, and Cristina Chiralt. On the structure and convergence of the symmetric Zassenhaus formula. *Computer Physics Communications*, 217(??):58–65, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301182.

Alvaro:2013:NMK

[ACCB13] M. Alvaro, E. Cebrián, M. Carretero, and L. L. Bonilla. Numerical methods for kinetic equations in semiconductor superlattices. *Computer Physics Communications*, 184(3):720–731, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003815.

Alexandrou:2014:EDQ

[ACD+14a] C. Alexandrou, M. Constantinou, V. Drach, K. Hadjiyiannakou, K. Jansen, G. Koutsou, A. Strelchenko, and A. Vaquero. Evaluation of disconnected quark loops for hadron structure using GPUs. *Computer Physics Communications*, 185(5):1370–1382, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000228.

Alloul:2014:FCT

[ACD+14b] Adam Alloul, Neil D. Christensen, Céline Degrande, Claude Duhr, and Benjamin Fuks. FeynRules 2.0: A complete toolbox for tree-level phenomenology. *Computer Physics Communications*, 185(8):2250–2300, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001350.

Avellar:2014:DLF

[ACDdM14] J. Avellar, M. S. Cardoso, L. G. S. Duarte, and L. A. C. P. da Mota. Determining Liouvillian first integrals for dynamical systems in the plane and an integrability analysis. *Computer Physics Communications*, 185(5):1496–1497, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000290.

Avellar:2015:FHO

[ACDdM15] J. Avellar, A. L. G. C. Claudino, L. G. S. Duarte, and L. A. C. P. da Mota. Finding higher order Darboux polynomials for a family of rational first order ordinary differential equations. *Computer Physics Communications*, 195(??):216–217, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001745.

Avellar:2019:DRS

[ACDdM19] J. Avellar, M. S. Cardoso, L. G. S. Duarte, and L. A. C. P. da Mota. Dealing with rational second order ordinary differential equations where both Darboux and Lie find it difficult: the S-function method. *Computer Physics Communications*, 234(??):302–314, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301620.

Alves:2013:GED

[ACdS13] Victor G. L. Alves, Simone C. Cardoso, and Ademir X. da Silva. Gafchromic EBT2 dosimetry via robust optimization. *Computer Physics Communications*, 184(7):1708–1716, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000805.

Antuono:2012:NDT

[ACM12] M. Antuono, A. Colagrossi, and S. Marrone. Numerical diffusive terms in weakly-compressible SPH schemes. *Computer Physics Communications*, 183(12):2570–2580, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002342.

Antuono:2011:PGW

[ACML11] M. Antuono, A. Colagrossi, S. Marrone, and C. Lugni. Propagation of gravity waves through an SPH scheme with numerical diffusive terms. *Computer Physics Communications*, 182(4):866–877, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004911.

Antuono:2010:FSF

[ACMM10] M. Antuono, A. Colagrossi, S. Marrone, and D. Molteni. Free-surface flows solved by means of SPH schemes with numerical diffusive terms. *Computer Physics Communications*, 181(3):532–549, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003506.

Adams:2019:CMC

[ACMM19] Mark F. Adams, Stephen L. Cornford, Daniel F. Martin, and Peter McCorquodale. Composite matrix construction for structured grid adaptive mesh refinement. *Computer Physics Communications*, 244(??):35–39, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302176.

Arsoski:2015:EFD

[ACTP15] V. V. Arsoski, N. A. Cukarić, M. Z. Tadić, and F. M. Peeters. An efficient finite-difference scheme for computation of electron states in free-standing and core-shell quantum wires. *Computer Physics Communications*, 197(??):17–26, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002866.

Angelani:2011:NMB

[AD11] L. Angelani and R. Di Leonardo. Numerical modeling of bacteria propelled micromotors. *Computer Physics Communications*, 182(9):1970–1973, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000828.

Antoine:2014:GMT

[AD14] Xavier Antoine and Romain Duboscq. GPELab, a Matlab toolbox to solve Gross–Pitaevskii equations I: Computation of stationary solutions. *Computer Physics Communications*, 185(11):2969–2991, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002318.

Antoine:2015:GMT

[AD15] Xavier Antoine and Romain Duboscq. GPELab, a Matlab toolbox to solve Gross–Pitaevskii equations II: Dynamics and stochastic simulations. *Computer Physics Communications*, 193(??):95–117, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001113`.

Ackland:2011:MSR

[ADD+11] G. J. Ackland, K. D'Mellow, S. L. Daraszewicz, D. J. Hepburn, M. Uhrin, and K. Stratford. The MOLDY short-range molecular dynamics package. *Computer Physics Communications*, 182(12):2587–2604, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551100261X`.

Avellar:2012:PMI

[ADdM12a] J. Avellar, L. G. S. Duarte, and L. A. C. P. da Mota. PSsolver: a Maple implementation to solve first order ordinary differential equations with Liouvillian solutions. *Computer Physics Communications*, 183(10):2313–2314, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001518`.

Avellar:2012:NPN

[ADdM+12b] J. Avellar, L. G. S. Duarte, L. A. C. P. da Mota, N. de Melo, and J. E. F. Skea. The Ndynamics package — numerical analysis of dynamical systems and the fractal dimension of boundaries. *Computer Physics Communications*, 183(9):2019–2020, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001294`.

Avellar:2014:MPF

[ADdM14] J. Avellar, L. G. S. Duarte, and L. A. C. P. da Mota. A Maple package to find first order differential invariants of 2ODEs via a Darboux approach. *Computer Physics Communications*, 185(1):307–316, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002762`.

Avellar:2015:IFD

[ADdM15] J. Avellar, L. G. S. Duarte, and L. A. C. P. da Mota. Improving a family of Darboux methods for rational second order ordinary differential equations. *Computer Physics Communications*, 195(??):221–223, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001927.

Alves:2016:IGF

[ADdM16a] P. R. L. Alves, L. G. S. Duarte, and L. A. C. P. da Mota. Improvement in global forecast for chaotic time series. *Computer Physics Communications*, 207(??):325–340, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301278.

Alves:2016:NMI

[ADdM16b] P. R. L. Alves, L. G. S. Duarte, and L. A. C. P. da Mota. A new method for improved global mapping forecast. *Computer Physics Communications*, 207(??):539–541, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301734.

Alves:2017:APC

[ADdM17] P. R. L. Alves, L. G. S. Duarte, and L. A. C. P. da Mota. Alternative predictors in chaotic time series. *Computer Physics Communications*, 215(??):265–268, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300656.

Alwall:2015:CDR

[ADF+15] Johan Alwall, Claude Duhr, Benjamin Fuks, Olivier Mattelaer, Deniz Gizem Öztürk, and Chia-Hsien Shen. Computing decay rates for new physics theories with FeynRules and MadGraph $5_{\mathrm{aMC@NLO}}$. *Computer Physics Communications*, 197(??):312–323, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003306.

Actis:2017:RCO

[ADH+17] Stefano Actis, Ansgar Denner, Lars Hofer, Jean-Nicolas Lang, Andreas Scharf, and Sandro Uccirati. R E C O L L A — REcursive Computation of One-Loop Amplitudes. *Computer Physics Communications*, 214(??):140–173, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300048`.

Arthuis:2019:AAG

[ADT+19] P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasseri, and J.-P. Ebran. ADG: Automated generation and evaluation of many-body diagrams I. Bogoliubov many-body perturbation theory. *Computer Physics Communications*, 240(??):202–227, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518304156`.

Auer:2018:MIM

[AEKO18] N. Auer, L. Einkemmer, P. Kandolf, and A. Ostermann. Magnus integrators on multicore CPUs and GPUs. *Computer Physics Communications*, 228(??):115–122, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300584`.

Akushevich:2012:MCG

[AFIS12] I. Akushevich, O. F. Filoti, A. Ilyichev, and N. Shumeiko. Monte Carlo generator ELRADGEN 2.0 for simulation of radiative events in elastic *ep*-scattering of polarized particles. *Computer Physics Communications*, 183(7):1448–1467, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000306`.

Avery:2017:XNV

[AFZ17] Patrick Avery, Zackary Falls, and Eva Zurek. XtalOpt Version r10: an open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 217(??):210–211, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301005`.

Avery:2018:XNV

[AFZ18] Patrick Avery, Zackary Falls, and Eva Zurek. XtalOpt version r11: an open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 222(??):418–419, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302989.

Arioli:2012:LRM

[AG12a] M. Arioli and S. Gratton. Linear regression models, least-squares problems, normal equations, and stopping criteria for the conjugate gradient method. *Computer Physics Communications*, 183(11):2322–2336, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002019.

Asadchev:2012:MPE

[AG12b] Andrey Asadchev and Mark S. Gordon. Mixed-precision evaluation of two-electron integrals by Rys quadrature. *Computer Physics Communications*, 183(8):1563–1567, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000823.

Alves:2014:CAP

[AG14] Danilo T. Alves and Edney R. Granhen. A computer algebra package for calculation of the energy density produced via the dynamical Casimir effect in one-dimensional cavities. *Computer Physics Communications*, 185(7):2101–2114, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001003.

Asunta:2015:MNB

[AGB+15] O. Asunta, J. Govenius, R. Budny, M. Gorelenkova, G. Tardini, T. Kurki-Suonio, A. Salmi, S. Sipilä, the ASDEX Upgrade Team, and the JET EFDA Contributors. Modelling neutral beams in fusion devices: Beamlet-based model for fast particle simulations. *Computer Physics Communications*, 188(??):33–46, March 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003701.

Ammon:2016:ENS

[AGH+16] A. Ammon, A. Genz, T. Hartung, K. Jansen, H. Leövey, and J. Volmer. On the efficient numerical solution of lattice systems with low-order couplings. *Computer Physics Communications*, 198(??):71–81, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003422.

Attig:2011:TSE

[AGL11] N. Attig, P. Gibbon, and Th. Lippert. Trends in supercomputing: The European path to exascale. *Computer Physics Communications*, 182(9):2041–2046, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004571.

Alpers:2015:PTV

[AGMS15] Andreas Alpers, Peter Gritzmann, Dmitry Moseev, and Mirko Salewski. 3D particle tracking velocimetry using dynamic discrete tomography. *Computer Physics Communications*, 187(??):130–136, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003683.

Ambia-Garrido:2010:MST

[AGVP10] J. Ambia-Garrido, Arnold Vainrub, and B. Montgomery Pettitt. A model for structure and thermodynamics of ssDNA and dsDNA near a surface: a coarse grained approach. *Computer Physics Communications*, 181(12):2001–2007, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003358.

Asgari:2013:NST

[AH13] Zohreh Asgari and S. M. Hosseini. Numerical solution of two-dimensional sine-Gordon and MBE models using Fourier spectral and high order explicit time stepping methods. *Computer Physics Communications*, 184(3):565–572, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003426`.

Andersen:2019:HHE

[AHH+19] Jeppe R. Andersen, Tuomas Hapola, Marian Heil, Andreas Maier, and Jennifer Smillie. HEJ 2: High energy resummation for hadron colliders. *Computer Physics Communications*, 245(??):Article 106832, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302097`.

Alexandrou:2012:EFL

[AHK+12] C. Alexandrou, K. Hadjiyiannakou, G. Koutsou, A. O'Cais, and A. Strelchenko. Evaluation of fermion loops applied to the calculation of the η' mass and the nucleon scalar and electromagnetic form factors. *Computer Physics Communications*, 183(6):1215–1224, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000380`.

Athron:2015:FSG

[AhPSV15] Peter Athron, Jae hyeon Park, Dominik Stöckinger, and Alexander Voigt. FlexibleSUSY — a spectrum generator generator for supersymmetric models. *Computer Physics Communications*, 190(??):139–172, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000065`.

Anderson:2016:SMM

[AIG16] Joshua A. Anderson, M. Eric Irrgang, and Sharon C. Glotzer. Scalable Metropolis Monte Carlo for simulation of hard shapes. *Computer Physics Communications*, 204(??):21–30, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551630039X`.

Arthur:2013:MCI

[AK13a] Rudy Arthur and A. D. Kennedy. Monte Carlo integration with subtraction. *Computer Physics Communications*, 184(12):2794–2802, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002646.

Augustinsky:2013:IGF

[AK13b] Pavel Augustinský and Jan Kunes. Improved Green's function measurement for hybridization expansion quantum Monte Carlo. *Computer Physics Communications*, 184(9):2119–2126, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001409.

Aldegunde:2015:ECS

[AK15] M. Aldegunde and K. Kalna. Energy conserving, self-force free Monte Carlo simulations of semiconductor devices on unstructured meshes. *Computer Physics Communications*, 189(??):31–36, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004032.

Allanach:2012:CNM

[AKH12] B. C. Allanach, C. H. Kom, and M. Hanussek. Computation of neutrino masses in R-parity violating supersymmetry: SOFTSUSY3.2. *Computer Physics Communications*, 183(3):785–793, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003924.

Adler:2018:VIS

[AKH$^+$18] Joan Adler, Sampo Kulju, Jari Hyväluoma, Keijo Mattila, Kit Choi, Ioannis Tziakos, Didrik Pinte, G. A. García, Y. Makushok, V. Makushok, J. Lama, G. Román-Pérez, Adham Hashibon, Mehdi Sadeghi, Nathan Franklin, and Amihai Silverman. Visualization in the integrated SimPhoNy multiscale simulation framework. *Computer Physics Communications*, 231(??):45–61, October 2018. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301589.

Ambrogi:2018:SVU

[AKK+18] Federico Ambrogi, Sabine Kraml, Suchita Kulkarni, Ursula Laa, Andre Lessa, Veronika Magerl, Jory Sonneveld, Michael Traub, and Wolfgang Waltenberger. SModelS v1.1 user manual: Improving simplified model constraints with efficiency maps. *Computer Physics Communications*, 227(??):72–98, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300353.

Atay:2016:TNA

[AKKK16] T. Atay, M. Kaplan, Y. Kilic, and N. Karapinar. A-Track: a new approach for detection of moving objects in FITS images. *Computer Physics Communications*, 207(??):524–530, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302119.

Aksenova:2015:SMS

[AKR15] E. V. Aksenova, D. I. Kokorin, and V. P. Romanov. Simulation of multiple scattering in the systems with complicated phase function. *Computer Physics Communications*, 196(??):384–389, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002829.

Aurentz:2017:CGI

[AKS17] Jared L. Aurentz, Vassilis Kalantzis, and Yousef Saad. Cucheb: a GPU implementation of the filtered Lanczos procedure. *Computer Physics Communications*, 220(??):332–340, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301984.

Azarov:2018:IPV

[AKV18] V. I. Azarov, A. Kramida, and M. Ya. Vokhmentsev. IDEN2 — a program for visual identification of spectral lines and energy levels in optical spectra of atoms and simple molecules.

Computer Physics Communications, 225(??):149–153, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304174.

Ahmed:2013:BSS

[AKZ+13] S. J. Ahmed, J. Kivinen, B. Zaporzan, L. Curiel, S. Pichardo, and O. Rubel. BerryPI: a software for studying polarization of crystalline solids with WIEN2k density functional all-electron package. *Computer Physics Communications*, 184(3):647–651, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003712.

Antoine:2017:CPS

[AL17] X. Antoine and E. Lorin. Computational performance of simple and efficient sequential and parallel Dirac equation solvers. *Computer Physics Communications*, 220(??):150–172, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302084.

Asensio:2019:GEI

[ALA+19] Isaac Alonso Asensio, Alejandro Alvarez Laguna, Mohamed Hassanine Aissa, Stefaan Poedts, Nataly Ozak, and Andrea Lani. A GPU-enabled implicit finite volume solver for the ideal two-fluid plasma model on unstructured grids. *Computer Physics Communications*, 239(??):16–32, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300372.

Appel:2018:ERI

[ALC18] L. C. Appel, I. Lupelli, and JET Contributors. Equilibrium reconstruction in an iron core tokamak using a deterministic magnetisation model. *Computer Physics Communications*, 223(??):1–17, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730303X.

Aliev:2011:HHT

[ALL+11] M. Aliev, H. Lacker, U. Langenfeld, S. Moch, P. Uwer, and M. Wiedermann. HATHOR — HAdronic Top and Heavy quarks crOss section calculatoR. *Computer Physics Communications*, 182(4):1034–1046, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005333.

Adelmann:2016:DKS

[ALS16] Andreas Adelmann, Uldis Locans, and Andreas Suter. The dynamic kernel scheduler — part 1. *Computer Physics Communications*, 207(??):83–90, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301370.

Amodio:2014:NSW

[ALSW14] P. Amodio, T. Levitina, G. Settanni, and E. B. Weinmüller. Numerical simulation of the whispering gallery modes in prolate spheroids. *Computer Physics Communications*, 185(4):1200–1206, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004244.

Alvarez:2012:IHS

[Alv12] Gonzalo Alvarez. Implementation of the SU(2) Hamiltonian symmetry for the DMRG algorithm. *Computer Physics Communications*, 183(10):2226–2232, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001646.

Arbey:2010:SRP

[AM10] A. Arbey and F. Mahmoudi. SuperIso Relic: a program for calculating relic density and flavor physics observables in supersymmetry. *Computer Physics Communications*, 181(7):1277–1292, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000901.

Arbey:2011:SRV

[AM11] A. Arbey and F. Mahmoudi. SuperIso Relic v3.0: a program for calculating relic density and flavour physics observables: Extension to NMSSM. *Computer Physics Communications*, 182(7):1582–1583, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001123.

Abdul:2014:MGK

[AM14a] R. F. Abdul and R. L. Mace. A method to generate kappa distributed random deviates for particle-in-cell simulations. *Computer Physics Communications*, 185(10):2383–2386, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400160X.

Ahmad:2014:IOP

[AM14b] Iftikhar Ahmad and Muhammad Maqbool. Investigation of the optical properties of P, As and Sb incorporated AlGaX alloys using full potential linearized augmented plane wave method. *Computer Physics Communications*, 185(11):2829–2833, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400229X.

Atisattapong:2017:ADT

[AM17] Wanyok Atisattapong and Pasin Marupanthorn. A $1/t$ algorithm with the density of two states for estimating multidimensional integrals. *Computer Physics Communications*, 220(??):122–128, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302060.

Aleynikov:2019:FWC

[AM19] Pavel Aleynikov and Nikolai B. Marushchenko. 3D full-wave computation of RF modes in magnetised plasmas. *Computer Physics Communications*, 241(??):40–47, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300980.

Austin:2018:EJN

[AMJ18] Kieran S. Austin, Martin Marenz, and Wolfhard Janke. Efficiencies of joint non-local update moves in Monte Carlo simulations of coarse-grained polymers. *Computer Physics Communications*, 224(??):222–229, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465517303545`.

Alhama:2011:ERM

[AMM11] F. Alhama, F. Marín, and J. A. Moreno. An efficient and reliable model to simulate microscopic mechanical friction in the Frenkel–Kontorova-Tomlinson model. *Computer Physics Communications*, 182(11):2314–2325, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002165`.

Alves:2015:MTA

[AMR15] Nelson A. Alves, Lucas D. Morero, and Leandro G. Rizzi. Microcanonical thermostatistics analysis without histograms: Cumulative distribution and Bayesian approaches. *Computer Physics Communications*, 191(??):125–131, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000557`.

Arbona:2018:SUP

[AMR+18] A. Arbona, B. Miñano, A. Rigo, C. Bona, C. Palenzuela, A. Artigues, C. Bona-Casas, and J. Massó. Simflowny 2: An upgraded platform for scientific modelling and simulation. *Computer Physics Communications*, 229(??):170–181, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300870`.

Arbey:2019:SRV

[AMR19] A. Arbey, F. Mahmoudi, and G. Robbins. SuperIso Relic v4: a program for calculating dark matter and flavour physics observables in supersymmetry. *Computer Physics Communications*, 239(??):238–264, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465519300207.

Allanach:2017:ITL

[AMRdA17] B. C. Allanach, Stephen P. Martin, David G. Robertson, and Roberto Ruiz de Austri. The inclusion of two-loop SUSYQCD corrections to gluino and squark pole masses in the minimal and next-to-minimal supersymmetric standard model: SOFTSUSY3.7. *Computer Physics Communications*, 219(??):339–345, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301364.

Anonymous:2010:CPC

[Ano10a] Anonymous. Computer Physics Communications — list of editors. *Computer Physics Communications*, 181(1):iv–vi, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003609.

Anonymous:2010:EBa

[Ano10b] Anonymous. Editorial Board. *Computer Physics Communications*, 181(1):??, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003567.

Anonymous:2010:EBb

[Ano10c] Anonymous. Editorial Board. *Computer Physics Communications*, 181(2):??, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003725.

Anonymous:2010:EBc

[Ano10d] Anonymous. Editorial Board. *Computer Physics Communications*, 181(3):??, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000032.

Anonymous:2010:EBd

[Ano10e] Anonymous. Editorial Board. *Computer Physics Communications*, 181(4):??, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000024X.

Anonymous:2010:EBe

[Ano10f] Anonymous. Editorial Board. *Computer Physics Communications*, 181(5):??, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000627.

Anonymous:2010:EBf

[Ano10g] Anonymous. Editorial Board. *Computer Physics Communications*, 181(6):??, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001013.

Anonymous:2010:EBg

[Ano10h] Anonymous. Editorial Board. *Computer Physics Communications*, 181(7):??, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001268.

Anonymous:2010:EBh

[Ano10i] Anonymous. Editorial Board. *Computer Physics Communications*, 181(8):??, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001499.

Anonymous:2010:EBi

[Ano10j] Anonymous. Editorial Board. *Computer Physics Communications*, 181(9):??, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002110.

Anonymous:2010:EBj

[Ano10k] Anonymous. Editorial Board. *Computer Physics Communications*, 181(10):??, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002730.

Anonymous:2010:EBk

[Ano10l] Anonymous. Editorial Board. *Computer Physics Communications*, 181(11):??, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003243.

Anonymous:2010:EBl

[Ano10m] Anonymous. Editorial Board. *Computer Physics Communications*, 181(12):??, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003644.

Anonymous:2010:GDS

[Ano10n] Anonymous. A generic data structure for integrated modelling of tokamak physics and subsystems. *Computer Physics Communications*, 181(6):987–998, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000214.

Anonymous:2010:PSI

[Ano10o] Anonymous. A proposal for a standard interface between Monte Carlo tools and one-loop programs. *Computer Physics Communications*, 181(9):1612–1622, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001700.

Anonymous:2011:ADS

[Ano11a] Anonymous. The advanced data searching system with AMGA at the Belle II experiment. *Computer Physics Communications*, 182(1):270–273, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465510002705.

Anonymous:2011:CPC

[Ano11b] Anonymous. Computer Physics Communications — list of editors. *Computer Physics Communications*, 182(1):iv–vi, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003930.

Anonymous:2011:EBa

[Ano11c] Anonymous. Editorial Board. *Computer Physics Communications*, 182(1):??, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003899.

Anonymous:2011:EBb

[Ano11d] Anonymous. Editorial Board. *Computer Physics Communications*, 182(2):??, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004352.

Anonymous:2011:EBc

[Ano11e] Anonymous. Editorial Board. *Computer Physics Communications*, 182(3):??, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004996.

Anonymous:2011:EBd

[Ano11f] Anonymous. Editorial Board. *Computer Physics Communications*, 182(4):??, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000154.

Anonymous:2011:EBe

[Ano11g] Anonymous. Editorial Board. *Computer Physics Communications*, 182(5):??, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000506.

Anonymous:2011:EBf

[Ano11h] Anonymous. Editorial Board. *Computer Physics Communications*, 182(6):??, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000956.

Anonymous:2011:EBg

[Ano11i] Anonymous. Editorial Board. *Computer Physics Communications*, 182(7):??, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001317.

Anonymous:2011:EBh

[Ano11j] Anonymous. Editorial Board. *Computer Physics Communications*, 182(8):??, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001706.

Anonymous:2011:EBi

[Ano11k] Anonymous. Editorial Board. *Computer Physics Communications*, 182(9):??, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001858.

Anonymous:2011:EBj

[Ano11l] Anonymous. Editorial Board. *Computer Physics Communications*, 182(10):??, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002232.

Anonymous:2011:EBk

[Ano11m] Anonymous. Editorial Board. *Computer Physics Communications*, 182(11):??, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002517.

Anonymous:2011:EBl

[Ano11n] Anonymous. Editorial Board. *Computer Physics Communications*, 182(12):??, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002888.

Anonymous:2011:RCF

[Ano11o] Anonymous. ROOT — a C++ framework for petabyte data storage, statistical analysis and visualization. *Computer Physics Communications*, 182(6):1384–1385, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000701.

Anonymous:2012:CPC

[Ano12a] Anonymous. Computer Physics Communications — list of editors. *Computer Physics Communications*, 183(1):iv–vi, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003171.

Anonymous:2012:EBa

[Ano12b] Anonymous. Editorial Board. *Computer Physics Communications*, 183(1):??, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003134.

Anonymous:2012:EBb

[Ano12c] Anonymous. Editorial Board. *Computer Physics Communications*, 183(2):??, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003535.

Anonymous:2012:EBc

[Ano12d] Anonymous. Editorial Board. *Computer Physics Communications*, 183(3):??, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004140.

Anonymous:2012:EBd

[Ano12e] Anonymous. Editorial Board. *Computer Physics Communications*, 183(4):??, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200015X.

Anonymous:2012:EBe

[Ano12f] Anonymous. Editorial Board. *Computer Physics Communications*, 183(5):??, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000409.

Anonymous:2012:EBf

[Ano12g] Anonymous. Editorial Board. *Computer Physics Communications*, 183(6):??, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000720.

Anonymous:2012:EBg

[Ano12h] Anonymous. Editorial Board. *Computer Physics Communications*, 183(7):??, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000951.

Anonymous:2012:EBh

[Ano12i] Anonymous. Editorial Board. *Computer Physics Communications*, 183(8):??, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001373.

Anonymous:2012:EBi

[Ano12j] Anonymous. Editorial Board. *Computer Physics Communications*, 183(9):??, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001920.

Anonymous:2012:EBj

[Ano12k] Anonymous. Editorial Board. *Computer Physics Communications*, 183(10):??, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002135.

Anonymous:2012:EBk

[Ano12l] Anonymous. Editorial Board. *Computer Physics Communications*, 183(11):??, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002408.

Anonymous:2012:EBl

[Ano12m] Anonymous. Editorial Board. *Computer Physics Communications*, 183(12):??, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002688.

Anonymous:2013:CPC

[Ano13a] Anonymous. Computer Physics Communications — list of Editors. *Computer Physics Communications*, 184(1):iv–v, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003219.

Anonymous:2013:EBa

[Ano13b] Anonymous. Editorial Board. *Computer Physics Communications*, 184(1):??, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003177.

Anonymous:2013:EBb

[Ano13c] Anonymous. Editorial Board. *Computer Physics Communications*, 184(2):??, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003487.

Anonymous:2013:EBc

[Ano13d] Anonymous. Editorial Board. *Computer Physics Communications*, 184(3):??, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004134.

Anonymous:2013:EBd

[Ano13e] Anonymous. Editorial Board. *Computer Physics Communications*, 184(4):??, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000143.

Anonymous:2013:EBe

[Ano13f] Anonymous. Editorial Board. *Computer Physics Communications*, 184(5):??, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000416.

Anonymous:2013:EBf

[Ano13g] Anonymous. Editorial Board. *Computer Physics Communications*, 184(6):??, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000842.

Anonymous:2013:EBg

[Ano13h] Anonymous. Editorial Board. *Computer Physics Communications*, 184(7):??, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001173.

Anonymous:2013:EBh

[Ano13i] Anonymous. Editorial Board. *Computer Physics Communications*, 184(8):??, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001495.

Anonymous:2013:EBi

[Ano13j] Anonymous. Editorial Board. *Computer Physics Communications*, 184(9):??, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001811.

Anonymous:2013:EBj

[Ano13k] Anonymous. Editorial Board. *Computer Physics Communications*, 184(10):??, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002142.

Anonymous:2013:EBk

[Ano13l] Anonymous. Editorial Board. *Computer Physics Communications*, 184(11):??, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002543.

Anonymous:2014:EBa

[Ano14a] Anonymous. Editorial Board. *Computer Physics Communications*, 185(9):ifc, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400191X.

Anonymous:2014:EBb

[Ano14b] Anonymous. Editorial Board. *Computer Physics Communications*, 185(10):ifc, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002331.

Anonymous:2014:EBc

[Ano14c] Anonymous. Editorial Board. *Computer Physics Communications*, 185(11):ifc, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002859.

Anonymous:2014:EBd

[Ano14d] Anonymous. Editorial Board. *Computer Physics Communications*, 185(12):ifc, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003270.

Anonymous:2015:BPC

[Ano15a] Anonymous. *Computer Physics Communications* — list of Editors. *Computer Physics Communications*, 186(??):iv–v, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003609.

Anonymous:2015:EBa

[Ano15b] Anonymous. Editorial Board. *Computer Physics Communications*, 186(??):ifc, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003567.

Anonymous:2015:EBb

[Ano15c] Anonymous. Editorial Board. *Computer Physics Communications*, 187(??):ifc, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003877.

Anonymous:2015:EBc

[Ano15d] Anonymous. Editorial Board. *Computer Physics Communications*, 188(??):ifc, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004226.

Anonymous:2015:EBd

[Ano15e] Anonymous. Editorial Board. *Computer Physics Communications*, 189(??):ifc, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000235.

Anonymous:2015:EBe

[Ano15f] Anonymous. Editorial Board. *Computer Physics Communications*, 190(??):ifc, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000624.

Anonymous:2015:EBf

[Ano15g] Anonymous. Editorial Board. *Computer Physics Communications*, 191(??):ifc, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000995.

Anonymous:2015:EBg

[Ano15h] Anonymous. Editorial Board. *Computer Physics Communications*, 192(??):ifc, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001289.

Anonymous:2015:EBh

[Ano15i] Anonymous. Editorial Board. *Computer Physics Communications*, 193(??):ifc, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001563.

Anonymous:2015:EBi

[Ano15j] Anonymous. Editorial Board. *Computer Physics Communications*, 194(??):ifc, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001782.

Anonymous:2015:EBj

[Ano15k] Anonymous. Editorial Board. *Computer Physics Communications*, 195(??):ifc, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002386.

Anonymous:2015:EBk

[Ano15l] Anonymous. Editorial Board. *Computer Physics Communications*, 196(??):ifc, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003124.

Anonymous:2015:EBl

[Ano15m] Anonymous. Editorial Board. *Computer Physics Communications*, 197(??):ifc, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003562.

Anonymous:2016:CPC

[Ano16a] Anonymous. Computer physics communications — list of Editors. *Computer Physics Communications*, 198(??):iv–v, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500380X.

Anonymous:2016:EBa

[Ano16b] Anonymous. Editorial Board. *Computer Physics Communications*, 198(??):ifc, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003768.

Anonymous:2016:EBb

[Ano16c] Anonymous. Editorial Board. *Computer Physics Communications*, 199(??):ifc, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004257.

Anonymous:2016:EBc

[Ano16d] Anonymous. Editorial Board. *Computer Physics Communications*, 200(??):ifc, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000096.

Anonymous:2016:EBd

[Ano16e] Anonymous. Editorial Board. *Computer Physics Communications*, 201(??):ifc, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300091.

Anonymous:2016:EBe

[Ano16f] Anonymous. Editorial Board. *Computer Physics Communications*, 202(??):ifc, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300510.

Anonymous:2016:EBf

[Ano16g] Anonymous. Editorial Board. *Computer Physics Communications*, 203(??):ifc, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300820.

Anonymous:2016:EBg

[Ano16h] Anonymous. Editorial Board. *Computer Physics Communications*, 204(??):ifc, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301126.

Anonymous:2016:EBh

[Ano16i] Anonymous. Editorial Board. *Computer Physics Communications*, 205(??):ifc, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301321.

Anonymous:2016:EBi

[Ano16j] Anonymous. Editorial Board. *Computer Physics Communications*, 206(??):ifc, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301540.

Anonymous:2016:EBj

[Ano16k] Anonymous. Editorial Board. *Computer Physics Communications*, 207(??):ifc, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302223.

Anonymous:2016:EBk

[Ano16l] Anonymous. Editorial Board. *Computer Physics Communications*, 208(??):ifc, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302594.

Anonymous:2016:IFC

[Ano16m] Anonymous. Inside front cover. *Computer Physics Communications*, 209(??):ifc, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302922.

Anonymous:2017:EBa

[Ano17a] Anonymous. Editorial Board. *Computer Physics Communications*, 210(??):ifc, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303241.

Anonymous:2017:EBb

[Ano17b] Anonymous. Editorial Board. *Computer Physics Communications*, 211(??):ifc, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303514.

Anonymous:2017:EBc

[Ano17c] Anonymous. Editorial Board. *Computer Physics Communications*, 212(??):ifc, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303769.

Anonymous:2017:EBd

[Ano17d] Anonymous. Editorial Board. *Computer Physics Communications*, 213(??):ifc, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300140.

Anonymous:2017:EBe

[Ano17e] Anonymous. Editorial Board. *Computer Physics Communications*, 214(??):ifc, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300541.

Anonymous:2017:EBf

[Ano17f] Anonymous. Editorial Board. *Computer Physics Communications*, 215(??):ifc, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300863.

Anonymous:2017:EBg

[Ano17g] Anonymous. Editorial Board. *Computer Physics Communications*, 216(??):ifc, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301108.

Anonymous:2017:EBh

[Ano17h] Anonymous. Editorial Board. *Computer Physics Communications*, 217(??):ifc, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301455.

Anonymous:2017:EBi

[Ano17i] Anonymous. Editorial Board. *Computer Physics Communications*, 218(??):ifc, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301716.

Anonymous:2017:EBj

[Ano17j] Anonymous. Editorial Board. *Computer Physics Communications*, 219(??):ifc, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302199.

Anonymous:2017:EBk

[Ano17k] Anonymous. Editorial Board. *Computer Physics Communications*, 220(??):ifc, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302709.

Anonymous:2017:EBl

[Ano17l] Anonymous. Editorial Board. *Computer Physics Communications*, 221(??):ifc, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303077.

Anonymous:2018:EBa

[Ano18a] Anonymous. Editorial Board. *Computer Physics Communications*, 222(??):ifc, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303594.

Anonymous:2018:EBb

[Ano18b] Anonymous. Editorial Board. *Computer Physics Communications*, 223(??):ifc, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303740.

Anonymous:2018:EBc

[Ano18c] Anonymous. Editorial Board. *Computer Physics Communications*, 224(??):ii, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304289.

Anonymous:2018:EBd

[Ano18d] Anonymous. Editorial Board. *Computer Physics Communications*, 225(??):ii, April 2018. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300195.

Anonymous:2018:EBe

[Ano18e] Anonymous. Editorial board. *Computer Physics Communications*, 226(??):ii, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300511.

Anonymous:2018:EBf

[Ano18f] Anonymous. Editorial Board. *Computer Physics Communications*, 227(??):ii, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300699.

Anonymous:2018:EBg

[Ano18g] Anonymous. Editorial Board. *Computer Physics Communications*, 228(??):ii, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301103.

Anonymous:2018:EBh

[Ano18h] Anonymous. Editorial Board. *Computer Physics Communications*, 229(??):ii, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830167X.

Anonymous:2018:EBi

[Ano18i] Anonymous. Editorial board. *Computer Physics Communications*, 230(??):ii, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301875.

Anonymous:2018:EBj

[Ano18j] Anonymous. Editorial board. *Computer Physics Communications*, 231(??):ii, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301966.

Anonymous:2018:EBk

[Ano18k] Anonymous. Editorial Board. *Computer Physics Communications*, 232(??):ii, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302352.

Anonymous:2018:EBl

[Ano18l] Anonymous. Editorial Board. *Computer Physics Communications*, 233(??):ii, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830287X.

Anonymous:2019:B

[Ano19a] Anonymous. Board. *Computer Physics Communications*, 240(??):ii, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301067.

Anonymous:2019:EBa

[Ano19b] Anonymous. Editorial Board. *Computer Physics Communications*, 234(??):ii, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303357.

Anonymous:2019:EBb

[Ano19c] Anonymous. Editorial Board. *Computer Physics Communications*, 235(??):ii, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303813.

Anonymous:2019:EBc

[Ano19d] Anonymous. Editorial Board. *Computer Physics Communications*, 236(??):ii, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304351.

Anonymous:2019:EBd

[Ano19e] Anonymous. Editorial Board. *Computer Physics Communications*, 237(??):ii, April 2019. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300244.

Anonymous:2019:EBe

[Ano19f] Anonymous. Editorial Board. *Computer Physics Communications*, 238(??):ii, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300517.

Anonymous:2019:EBf

[Ano19g] Anonymous. Editorial Board. *Computer Physics Communications*, 239(??):ii, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930075X.

Anonymous:2019:EBg

[Ano19h] Anonymous. Editorial Board. *Computer Physics Communications*, 241(??):ii, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301419.

Anonymous:2019:EBh

[Ano19i] Anonymous. Editorial Board. *Computer Physics Communications*, 242(??):ii, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301651.

Anonymous:2019:EBi

[Ano19j] Anonymous. Editorial Board. *Computer Physics Communications*, 243(??):ii, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301894.

Anonymous:2019:EBj

[Ano19k] Anonymous. Editorial Board. *Computer Physics Communications*, 244(??):ii, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302450.

Anonymous:2019:EBk

[Ano19l] Anonymous. Editorial Board. *Computer Physics Communications*, 245(??):Article 106887, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302747`.

Anonymous:2019:RTD

[Ano19m] Anonymous. Real-time data processing in the ALICE High Level Trigger at the LHC. *Computer Physics Communications*, 242(??):25–48, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301250`.

Anonymous:2020:CBP

[Ano20] Anonymous. Corrigendum to "Bratu's problem: a novel approach using fixed-point iterations and Green's function" [Comput. Phys. Comm. **198** (2016) 97–104]. *Computer Physics Communications*, 252(??):Article 107132, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304382`. See [KK16a].

Aldecoa:2015:HGG

[AOK15] Rodrigo Aldecoa, Chiara Orsini, and Dmitri Krioukov. Hyperbolic graph generator. *Computer Physics Communications*, 196(??):492–496, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002088`.

Ayala:2014:DHI

[APC+14] Orlando Ayala, Hossein Parishani, Liu Chen, Bogdan Rosa, and Lian-Ping Wang. DNS of hydrodynamically interacting droplets in turbulent clouds: Parallel implementation and scalability analysis using 2D domain decomposition. *Computer Physics Communications*, 185(12):3269–3290, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003105`.

Alcaraz-Pelegrina:2011:SPP

[APRG11] J. M. Alcaraz-Pelegrina and P. Rodríguez-García. Simulations of pulse propagation in optical fibers using graphics processor units. *Computer Physics Communications*, 182(7):1414–1420, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000853.

Aichhorn:2016:TDT

[APS+16] Markus Aichhorn, Leonid Pourovskii, Priyanka Seth, Veronica Vildosola, Manuel Zingl, Oleg E. Peil, Xiaoyu Deng, Jernej Mravlje, Gernot J. Kraberger, Cyril Martins, Michel Ferrero, and Olivier Parcollet. TRIQS/DFTTools: a TRIQS application for ab initio calculations of correlated materials. *Computer Physics Communications*, 204(??):200–208, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300728.

Amaku:2010:DCD

[APV10] M. Amaku, P. R. Pascholati, and V. R. Vanin. Decay chain differential equations: Solution through matrix algebra. *Computer Physics Communications*, 181(1):21–23, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002628.

Abrarov:2010:HAA

[AQJ10] S. M. Abrarov, B. M. Quine, and R. K. Jagpal. High-accuracy approximation of the complex probability function by Fourier expansion of exponential multiplier. *Computer Physics Communications*, 181(5):876–882, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004160.

Aragon:2014:CIAa

[Ara14a] Alejandro M. Aragón. A C++11 implementation of arbitrary-rank tensors for high-performance computing. *Computer Physics Communications*, 185(6):1681–1696, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000186.

Aragon:2014:CIAb

[Ara14b] Alejandro M. Aragón. A C++11 implementation of arbitrary-rank tensors for high-performance computing. *Computer Physics Communications*, 185(11):3065–3066, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002586.

Abdel-Rehim:2017:IEM

[ARAB+17] Abdou Abdel-Rehim, Constantia Alexandrou, Joshua Berlin, Mattia Dalla Brida, Jacob Finkenrath, and Marc Wagner. Investigating efficient methods for computing four-quark correlation functions. *Computer Physics Communications*, 220(??):97–121, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302035.

Arbey:2012:APC

[Arb12] A. Arbey. AlterBBN: a program for calculating the BBN abundances of the elements in alternative cosmologies. *Computer Physics Communications*, 183(8):1822–1831, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001233.

Al-Refaie:2017:PAH

[ART17] Ahmed F. Al-Refaie and Jonathan Tennyson. A parallel algorithm for Hamiltonian matrix construction in electron-molecule collision calculations: MPI–SCATCI. *Computer Physics Communications*, 221(??):53–62, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302436.

Al-Refaie:2017:PCT

[ARYT17] Ahmed F. Al-Refaie, Sergei N. Yurchenko, and Jonathan Tennyson. **G**PU **A**ccelerated **IN**tensities MPI (GAIN-MPI): a new method of computing Einstein-A coefficients. *Computer Physics Communications*, 214(??):216–224, May 2017.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300255.

Ahmed:2011:RSM

[AS11a] Jahir Abbas Ahmed and S. B. Santra. Rotational sandpile models: a finite size scaling study. *Computer Physics Communications*, 182(9):1851–1855, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004625.

Alexandrescu:2011:ENM

[AS11b] Adrian Alexandrescu and José R. Salgueiro. Efficient numerical method for linear stability analysis of solitary waves. *Computer Physics Communications*, 182(12):2479–2485, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100244X.

Agarwal:2016:GCA

[AS16] Animesh Agarwal and Luigi Delle Site. Grand-canonical adaptive resolution centroid molecular dynamics: Implementation and application. *Computer Physics Communications*, 206(??):26–34, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301175.

Afibuzzaman:2018:SND

[ASA18] Md Afibuzzaman, Bastian Schuetrumpf, and Hasan Metin Aktulga. Scalable nuclear density functional theory with Sky3D. *Computer Physics Communications*, 223(??):34–44, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303491.

Ascasibar:2010:EMP

[Asc10] Yago Ascasibar. Estimating multidimensional probability fields using the Field Estimator for Arbitrary Spaces (FiEstAS) with applications to astrophysics. *Computer Physics Communications*, 181(8):1438–1443, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465510001220.

Akhmatskaya:2014:NRP

[ASEA14] E. Akhmatskaya, D. Sokolovski, and C. Echeverría-Arrondo. Numerical Regge pole analysis of resonance structures in elastic, inelastic and reactive state-to-state integral cross sections. *Computer Physics Communications*, 185(7):2127–2137, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001106.

Aldegunde:2010:RSF

[ASGLK10] M. Aldegunde, Natalia Seoane, A. J. García-Loureiro, and K. Kalna. Reduction of the self-forces in Monte Carlo simulations of semiconductor devices on unstructured meshes. *Computer Physics Communications*, 181(1):24–34, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900277X.

Asinari:2010:NBE

[Asi10] Pietro Asinari. Nonlinear Boltzmann equation for the homogeneous isotropic case: Minimal deterministic Matlab program. *Computer Physics Communications*, 181(10):1776–1788, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002420.

Aslanyan:2014:OOO

[Asl14] Grigor Aslanyan. Cosmo++: an object-oriented C++ library for cosmology. *Computer Physics Communications*, 185(12):3215–3227, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003026.

Almansa:2016:PGP

[ASPDL+16] Julio Almansa, Francesc Salvat-Pujol, Gloria Díaz-Londoño, Artur Carnicer, Antonio M. Lallena, and Francesc Salvat. PENGEOM — a general-purpose geometry package for Monte Carlo simulation of radiation transport in material systems defined by quadric surfaces. *Computer Physics*

Communications, 199(??):102–113, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003707.

Afshar:2013:ESR

[ASPW13] Y. Afshar, F. Schmid, A. Pishevar, and S. Worley. Exploiting seeding of random number generators for efficient domain decomposition parallelization of dissipative particle dynamics. *Computer Physics Communications*, 184(4):1119–1128, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003992.

Andrienko:2013:SHM

[ASS13] Daniil A. Andrienko, Sergey T. Surzhikov, and Joseph S. Shang. Spherical harmonics method applied to the multi-dimensional radiation transfer. *Computer Physics Communications*, 184(10):2287–2298, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001756.

Acs:2018:CAS

[ÁSS18] Bernadett Ács, Gergely Szlobodnyik, and Gábor Szederkényi. A computational approach to the structural analysis of uncertain kinetic systems. *Computer Physics Communications*, 228(??):83–95, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830064X.

Acs:2016:CAP

[ÁSTT16] Bernadett Ács, Gábor Szederkényi, Zsolt Tuza, and Zoltán A. Tuza. Computing all possible graph structures describing linearly conjugate realizations of kinetic systems. *Computer Physics Communications*, 204(??):11–20, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300352.

Adachi:2019:SCM

[ATA+19] Daiki Adachi, Naoto Tsujimoto, Ryosuke Akashi, Synge Todo, and Shinji Tsuneyuki. Search for common minima in joint optimization of multiple cost functions. *Computer Physics Communications*, 241(??):92–97, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300475`.

Avery:2019:XNV

[ATCZ19] Patrick Avery, Cormac Toher, Stefano Curtarolo, and Eva Zurek. XtalOpt Version r12: an open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 237(??):274–275, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518304089`.

Avidor:2019:PPI

[ATW+19] N. Avidor, P. S. M. Townsend, D. J. Ward, A. P. Jardine, J. Ellis, and W. Allison. PIGLE — Particles Interacting in Generalized Langevin Equation simulator. *Computer Physics Communications*, 242(??):145–152, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301274`.

Adhikari:2013:CWP

[AV13] Satrajit Adhikari and António J. C. Varandas. The coupled 3D wave packet approach for triatomic reactive scattering in hyperspherical coordinates. *Computer Physics Communications*, 184(2):270–283, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002871`.

Assmann:2016:WOC

[AWK+16] E. Assmann, P. Wissgott, J. Kunes, A. Toschi, P. Blaha, and K. Held. `woptic`: Optical conductivity with Wannier functions and adaptive k-mesh refinement. *Computer Physics Communications*, 202(??):1–11, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465515004488.

An:2011:SCM

[AYDY11] Xizhong An, Runyu Yang, Kejun Dong, and Aibing Yu. DEM study of crystallization of monosized spheres under mechanical vibrations. *Computer Physics Communications*, 182(9):1989–1994, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000658.

Avery:2017:CRO

[AZ17a] Patrick Avery and Eva Zurek. Corrigendum to "RandSpg: an open-source program for generating atomistic crystal structures with specific spacegroups" [comput. phys. comm. **213** (2017) 208–216]. *Computer Physics Communications*, 220(??):509, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301595. See [AZ17b].

Avery:2017:ROS

[AZ17b] Patrick Avery and Eva Zurek. RandSpg: an open-source program for generating atomistic crystal structures with specific spacegroups. *Computer Physics Communications*, 213(??):208–216, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303848. See corrigendum [AZ17a].

Azadegan:2013:MPC

[Aza13] B. Azadegan. A Mathematica package for calculation of planar channeling radiation spectra of relativistic electrons channeled in a diamond-structure single crystal (quantum approach). *Computer Physics Communications*, 184(3):1064–1069, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200389X.

Arshi:2014:MOS

[AZM14] S. Safaei Arshi, A. Zolfaghari, and S. M. Mirvakili. A multi-objective shuffled frog leaping algorithm for in-core fuel management optimization. *Computer Physics Communications*, 185(10):2622–2628, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002185.

Adler:2011:SVN

[AZS+11] Joan Adler, Jeremie Zaffran, Amihai Silverman, Anastassia Sorkin, Or Cohen, and Rafi Kalish. Simulation and visualization of nanodiamond and nanographite. *Computer Physics Communications*, 182(9):2009–2012, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004807.

Babaev:2014:PCN

[Bab14] A. A. Babaev. Parallel code NSBC: Simulations of relativistic nuclei scattering by a bent crystal. *Computer Physics Communications*, 185(1):368–379, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300307X.

Blyth:2019:PEB

[BABC19] D. Blyth, J. Alcaraz, S. Binet, and S. V. Chekanov. ProIO: an event-based I/O stream format for protobuf messages. *Computer Physics Communications*, 241(??):98–112, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300992.

Badnell:2011:BPD

[Bad11] N. R. Badnell. A Breit–Pauli distorted wave implementation for autostructure. *Computer Physics Communications*, 182(7):1528–1535, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001160.

Boyd:2018:SAM

[BAF18] John P. Boyd, Paolo Amore, and Francisco M. Fernández. Spectral algorithms for multiple scale localized eigenfunctions in infinitely long, slightly bent quantum waveguides. *Computer Physics Communications*, 224(??):209–221, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303557.

Bray:2015:SCC

[BAK+15] A. W. Bray, I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray. Solving close-coupling equations in momentum space without singularities. *Computer Physics Communications*, 196(??):276–279, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500260X.

Bray:2016:SCC

[BAK+16] A. W. Bray, I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray. Solving close-coupling equations in momentum space without singularities II. *Computer Physics Communications*, 203(??):147–151, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300431.

Bray:2017:SCC

[BAK+17] A. W. Bray, I. B. Abdurakhmanov, A. S. Kadyrov, D. V. Fursa, and I. Bray. Solving close-coupling equations in momentum space without singularities for charged targets. *Computer Physics Communications*, 212(??):55–58, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303149.

Balac:2019:WMT

[Bal19] Stéphane Balac. WGMode: a Matlab toolbox for whispering gallery modes volume computation in spherical optical micro-resonators. *Computer Physics Communications*, 243(??):121–134, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465519301511.

Berardi:2016:NDA

[BALV16] Marco Berardi, Andrea Andrisani, Luciano Lopez, and Michele Vurro. A new data assimilation technique based on ensemble Kalman filter and Brownian bridges: an application to Richards' equation. *Computer Physics Communications*, 208(??):43–53, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302132.

Barletta:2011:CCD

[Bar11a] Paolo Barletta. COOL: a code for dynamic Monte Carlo simulation of molecular dynamics. *Computer Physics Communications*, 182(2):388–399, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003607.

Barnard:2011:UEM

[Bar11b] A. S. Barnard. Useful equations for modeling the relative stability of common nanoparticle morphologies. *Computer Physics Communications*, 182(1):11–13, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002675.

Barletta:2012:CCD

[Bar12a] Paolo Barletta. COOL: a code for dynamic Monte Carlo simulation of molecular dynamics. *Computer Physics Communications*, 183(2):438–439, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003250.

Bigaouette:2012:NGM

[BAR12b] Nicolas Bigaouette, Edward Ackad, and Lora Ramunno. Nonlinear grid mapping applied to an FDTD-based, multicenter 3D Schrödinger equation solver. *Computer Physics Communications*, 183(1):38–45, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465511002839.

Bourchtein:2010:ICN

[BB10] Andrei Bourchtein and Ludmila Bourchtein. On iterated Crank–Nicolson methods for hyperbolic and parabolic equations. *Computer Physics Communications*, 181(7):1242–1250, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000913.

Bourchtein:2012:SIT

[BB12] Andrei Bourchtein and Ludmila Bourchtein. A semi-implicit time-splitting scheme for a regional nonhydrostatic atmospheric model. *Computer Physics Communications*, 183(3):570–587, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003869.

Bazavov:2013:PPM

[BB13a] Alexei Bazavov and Bernd A. Berg. Program package for multicanonical simulations of U(1) lattice gauge theory — second version. *Computer Physics Communications*, 184(3):1075–1076, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003700.

Brambilla:2013:EIB

[BB13b] M. Brambilla and R. Bilato. An efficient interface between the solvers of Maxwell's equations and of the quasilinear kinetic equation for simulations of ion cyclotron heating in tokamak plasmas. *Computer Physics Communications*, 184(9):2053–2060, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001331.

Beerwerth:2015:KSM

[BB15] Randolf Beerwerth and Heiko Bauke. Krylov subspace methods for the Dirac equation. *Computer Physics Communications*, 188(??):189–197, March 2015. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003804.

Belanger:2011:ISD

[BBB+11] G. Bélanger, F. Boudjema, P. Brun, A. Pukhov, S. Rosier-Lees, P. Salati, and A. Semenov. Indirect search for dark matter with micrOMEGAs_2.4. *Computer Physics Communications*, 182(3):842–856, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004881.

Barducci:2015:XEQ

[BBB+15] D. Barducci, A. Belyaev, M. Buchkremer, J. Marrouche, S. Moretti, and L. Panizzi. XQCAT: eXtra Quark Combined Analysis Tool. *Computer Physics Communications*, 197(??):263–275, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003021.

Basagaoglu:2017:CPS

[BBB+17a] Hakan Basagaoglu, Justin Blount, Jarred Blount, Bryant Nelson, Sauro Succi, Phil M. Westhart, and John R. Harwell. Computational performance of SequenceL coding of the lattice Boltzmann method for multi-particle flow simulations. *Computer Physics Communications*, 213(??):92–99, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303915.

Bazan:2017:SDP

[BBB17b] Fermín S. V. Bazán, Luciano Bedin, and Leonardo S. Borges. Space-dependent perfusion coefficient estimation in a 2D bioheat transfer problem. *Computer Physics Communications*, 214(??):18–30, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300024.

Barducci:2018:CLN

[BBB+18] D. Barducci, G. Bélanger, J. Bernon, F. Boudjema, J. Da Silva, S. Kraml, U. Laa, and A. Pukhov. Collider limits on new physics within micrOMEGAs_4.3. *Computer Physics Communications*, 222(??):327–338, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303235.

Bethune:2019:MSE

[BBB+19] Iain Bethune, Ralf Banisch, Elena Breitmoser, Antonia B. K. Collis, Gordon Gibb, Gianpaolo Gobbo, Charles Matthews, Graeme J. Ackland, and Benedict J. Leimkuhler. MIST: a simple and efficient molecular dynamics abstraction library for integrator development. *Computer Physics Communications*, 236(??):224–236, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303540.

Baron:2011:CKD

[BBC+11] Remi Baron, Philippe Boucaud, Jaume Carbonell, Vincent Drach, Federico Farchioni, Gregorio Herdoiza, Karl Jansen, Chris Michael, Istvan Montvay, Elisabetta Pallante, Olivier Pène, Siebren Reker, Carsten Urbach, Marc Wagner, and Urs Wenger. Computing K and D meson masses with $Nf = 2+1+1$ twisted mass lattice QCD. *Computer Physics Communications*, 182(2):299–316, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003838.

Basso:2013:PGS

[BBC+13a] L. Basso, A. Belyaev, D. Chowdhury, M. Hirsch, S. Khalil, S. Moretti, B. O'Leary, W. Porod, and F. Staub. Proposal for generalised supersymmetry Les Houches Accord for see-saw models and PDG numbering scheme. *Computer Physics Communications*, 184(3):698–719, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003803.

Bogneri:2013:CNQ

[BBC+13b] S. Bogneri, A. Bulgacx, J. Carlsonf, J. Engelt, G. Fannj, R. J. Furnstahlm, S. Gandolfif, G. Hagenl, M. Horoid, C. Johnsonq, M. Kortelainenu, E. Luska, P. Marise, H. Namk,

P. Navratilh, W. Nazarewiczu, E. Ngg, G. P. A. Nobrec, E. Ormandh, T. Papenbrockl, J. Peiu, S. C. Pieperb, S. Quaglionih, K. J. Rocheo, J. Saricha, N. Schunckh, M. Sosonkinan, J. Terasakiv, I. Thompsonh, J. P. Varye, and S. M. Wilda. Computational nuclear quantum many-body problem: the UNEDF project. *Computer Physics Communications*, 184(10):2235–2250, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001902.

Bloch:2010:SRK

[BBF+10] Jacques C. R. Bloch, Tobias Breu, Andreas Frommer, Simon Heybrock, Katrin Schäfer, and Tilo Wettig. Short-recurrence Krylov subspace methods for the overlap Dirac operator at nonzero chemical potential. *Computer Physics Communications*, 181(8):1378–1387, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001153.

Bernaschi:2013:PHS

[BBF+13] M. Bernaschi, M. Bisson, M. Fatica, S. Melchionna, and S. Succi. Petaflop hydrokinetic simulations of complex flows on massive GPU clusters. *Computer Physics Communications*, 184(2):329–341, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003025.

Buckley:2013:RUM

[BBG+13] Andy Buckley, Jonathan Butterworth, David Grellscheid, Hendrik Hoeth, Leif Lönnblad, James Monk, Holger Schulz, and Frank Siegert. Rivet user manual. *Computer Physics Communications*, 184(12):2803–2819, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001914.

Belanger:2018:MF

[BBG+18] G. Bélanger, F. Boudjema, A. Goudelis, A. Pukhov, and B. Zaldívar. micrOMEGAs5.0: Freeze-in. *Computer Physics Communications*, 231(??):173–186, October 2018. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301437.

Bechtle:2010:HCA

[BBH+10] P. Bechtle, O. Brein, S. Heinemeyer, G. Weiglein, and K. E. Williams. HiggsBounds: Confronting arbitrary Higgs sectors with exclusion bounds from LEP and the Tevatron. *Computer Physics Communications*, 181(1):138–167, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002823.

Bechtle:2011:HCN

[BBH+11a] P. Bechtle, O. Brein, S. Heinemeyer, G. Weiglein, and K. E. Williams. HiggsBounds 2.0.0: Confronting neutral and charged Higgs sector predictions with exclusion bounds from LEP and the Tevatron. *Computer Physics Communications*, 182(12):2605–2631, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002621.

Berland:2011:VWD

[BBH11b] Kristian Berland, Øyvind Borck, and Per Hyldgaard. Van der Waals density functional calculations of binding in molecular crystals. *Computer Physics Communications*, 182(9):1800–1804, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005187.

Busa:2015:CCO

[BBH+15] Ján Busa, Jr., Ján Busa, Shura Hayryan, Chin-Kun Hu, and Ming-Chya Wu. CAVE-CL: an OpenCL version of the package for detection and quantitative analysis of internal cavities in a system of overlapping balls: Application to proteins. *Computer Physics Communications*, 190(??):224–227, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004378.

Bogner:2018:LDL

[BBH^{+}18] C. Bogner, S. Borowka, T. Hahn, G. Heinrich, S. P. Jones, M. Kerner, A. von Manteuffel, M. Michel, E. Panzer, and V. Papara. Loopedia, a database for loop integrals. *Computer Physics Communications*, 225(??):1–9, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517304228`.

Baker:2013:IOM

[BBL^{+}13] Katherine Baker, Andrij Baumketner, Yuchun Lin, Shaozhong Deng, Donald Jacobs, and Wei Cai. ICSM: an order N method for calculating electrostatic interactions added to TINKER. *Computer Physics Communications*, 184(1):19–26, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002561`.

Bushlanov:2019:TBC

[BBO19] Pavel V. Bushlanov, Vladislav A. Blatov, and Artem R. Oganov. Topology-based crystal structure generator. *Computer Physics Communications*, 236(??):1–7, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303308`.

Belanger:2014:MPC

[BBPS14] G. Bélanger, F. Boudjema, A. Pukhov, and A. Semenov. micrOMEGAs_3: a program for calculating dark matter observables. *Computer Physics Communications*, 185(3):960–985, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003445`.

Belanger:2015:MTD

[BBPS15] G. Bélanger, F. Boudjema, A. Pukhov, and A. Semenov. micrOMEGAs4.1: Two dark matter candidates. *Computer Physics Communications*, 192(??):322–329, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000922`.

Bozek:2019:GGI

[BBRS19] Piotr Bozek, Wojciech Broniowski, Maciej Rybczyński, and Grzegorz Stefanek. GLISSANDO 3: GLauber Initial-State Simulation AND mOre, ver. 403. *Computer Physics Communications*, 245(??):Article 106850, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302279.

Bernaschi:2014:MKG

[BBS14] M. Bernaschi, M. Bisson, and F. Salvadore. Multi-Kepler GPU vs. multi-Intel MIC for spin systems simulations. *Computer Physics Communications*, 185(10):2495–2503, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002008.

Badger:2011:NPC

[BBU11] S. Badger, B. Biedermann, and P. Uwer. NGluon: a package to calculate one-loop multi-gluon amplitudes. *Computer Physics Communications*, 182(8):1674–1692, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001263.

Badger:2013:NEV

[BBUY13] Simon Badger, Benedikt Biedermann, Peter Uwer, and Valery Yundin. Numerical evaluation of virtual corrections to multi-jet production in massless QCD. *Computer Physics Communications*, 184(8):1981–1998, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300115X.

Blumlein:2010:MZV

[BBV10] J. Blümlein, D. J. Broadhurst, and J. A. M. Vermaseren. The Multiple Zeta Value data mine. *Computer Physics Communications*, 181(3):582–625, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003701.

Burkoff:2016:EMD

[BBV+16] Nikolas S. Burkoff, Robert J. N. Baldock, Csilla Várnai, David L. Wild, and Gábor Csányi. Exploiting molecular dynamics in nested sampling simulations of small peptides. *Computer Physics Communications*, 201(??):8–18, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004439.

Berry:2011:QVQ

[BBW11] Scott D. Berry, Paul Bourke, and Jingbo B. Wang. qwViz: Visualisation of quantum walks on graphs. *Computer Physics Communications*, 182(10):2295–2302, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002128.

Bekas:2010:VLS

[BC10] C. Bekas and A. Curioni. Very large scale wavefunction orthogonalization in Density Functional Theory electronic structure calculations. *Computer Physics Communications*, 181(6):1057–1068, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000524.

Budiardja:2011:PFB

[BC11] Reuben D. Budiardja and Christian Y. Cardall. Parallel FFT-based Poisson solver for isolated three-dimensional systems. *Computer Physics Communications*, 182(10):2265–2275, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001809.

Budiardja:2019:GBO

[BC19] Reuben D. Budiardja and Christian Y. Cardall. GenASiS basics: Object-oriented utilitarian functionality for large-scale physics simulations (version 3). *Computer Physics Communications*, 244(??):483–486, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301729.

Bakhta:2018:CWF

[BCC+18] Athmane Bakhta, Eric Cancès, Paul Cazeaux, Shiang Fang, and Efthimios Kaxiras. Compression of Wannier functions into Gaussian-type orbitals. *Computer Physics Communications*, 230(??):27–37, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301231.

Bonati:2012:QSS

[BCDI12] C. Bonati, G. Cossu, M. D'Elia, and P. Incardona. QCD simulations with staggered fermions on GPUs. *Computer Physics Communications*, 183(4):853–863, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003997.

Boella:2018:GPT

[BCDP18] E. Boella, G. Coppa, A. D'Angola, and B. Peiretti Paradisi. Gridless particle technique for the Vlasov–Poisson system in problems with high degree of symmetry. *Computer Physics Communications*, 224(??):136–143, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303879.

Bishop:2015:OAM

[BCFR15] Kevin P. Bishop, Steve Constable, Nabil F. Faruk, and Pierre-Nicholas Roy. OpenMM accelerated MMTK. *Computer Physics Communications*, 191(??):203–208, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500048X.

Bevilacqua:2013:HN

[BCG+13] G. Bevilacqua, M. Czakon, M. V. Garzelli, A. van Hameren, A. Kardos, C. G. Papadopoulos, R. Pittau, and M. Worek. HELAC-NLO. *Computer Physics Communications*, 184(3):986–997, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003761.

Brown:2015:OLM

[BCG+15] W. Michael Brown, Jan-Michael Y. Carrillo, Nitin Gavhane, Foram M. Thakkar, and Steven J. Plimpton. Optimizing legacy molecular dynamics software with directive-based offload. *Computer Physics Communications*, 195(??):95–101, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500171X.

Ballenegger:2011:RSS

[BCH11] V. Ballenegger, J. J. Cerdà, and C. Holm. Removal of spurious self-interactions in particle-mesh methods. *Computer Physics Communications*, 182(9):1919–1923, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000464.

Borowka:2013:NEM

[BCH13] Sophia Borowka, Jonathon Carter, and Gudrun Heinrich. Numerical evaluation of multi-loop integrals for arbitrary kinematics with SecDec 2.0. *Computer Physics Communications*, 184(2):396–408, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003062.

Bertone:2017:AHP

[BCH17] Valerio Bertone, Stefano Carrazza, and Nathan P. Hartland. APFELgrid: a high performance tool for parton density determinations. *Computer Physics Communications*, 212(??):205–209, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303125.

Beckett:2011:BIL

[BCJ+11] Mark G. Beckett, Paul Coddington, Bálint Joó, Chris M. Maynard, Dirk Pleiter, Osamu Tatebe, and Tomoteru Yoshie. Building the International Lattice Data Grid. *Computer Physics Communications*, 182(6):1208–1214, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000476.

Beliakov:2013:EIBb

[BCJW13] G. Beliakov, D. Creighton, M. Johnstone, and T. Wilkin. Efficient implementation of Bailey and Borwein pseudo-random number generator based on normal numbers. *Computer Physics Communications*, 184(8):1999–2004, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001276. See also [BJCW13].

Bolis:2016:APA

[BCM+16] A. Bolis, C. D. Cantwell, D. Moxey, D. Serson, and S. J. Sherwin. An adaptable parallel algorithm for the direct numerical simulation of incompressible turbulent flows using a Fourier spectral/*hp* element method and MPI virtual topologies. *Computer Physics Communications*, 206(??):17–25, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630100X.

Bazzotti:2010:UGA

[BCMS10] M. Bazzotti, G. Carminati, A. Margiotta, and M. Spurio. An update of the generator of atmospheric muons from parametric formulas (MUPAGE). *Computer Physics Communications*, 181(4):835–836, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004093.

Belyaev:2013:CCP

[BCP13] Alexander Belyaev, Neil D. Christensen, and Alexander Pukhov. CalcHEP 3.4 for collider physics within and beyond the Standard Model. *Computer Physics Communications*, 184(7):1729–1769, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000313.

Beale:2016:OSC

[BCP+16] Steven B. Beale, Hae-Won Choi, Jon G. Pharoah, Helmut K. Roth, Hrvoje Jasak, and Dong Hyup Jeon. Open-source computational model of a solid oxide fuel cell. *Computer*

Physics Communications, 200(??):15–26, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003872.

Belanger:2011:SLI

[BCPS11] G. Bélanger, Neil D. Christensen, A. Pukhov, and A. Semenov. SLHAplus: a library for implementing extensions of the Standard Model. *Computer Physics Communications*, 182(3):763–774, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004261.

Bertone:2014:APE

[BCR14] Valerio Bertone, Stefano Carrazza, and Juan Rojo. APFEL: a PDF evolution library with QED corrections. *Computer Physics Communications*, 185(6):1647–1668, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000873.

Bali:2010:ENR

[BCS10] Gunnar S. Bali, Sara Collins, and Andreas Schäfer. Effective noise reduction techniques for disconnected loops in Lattice QCD. *Computer Physics Communications*, 181(9):1570–1583, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001621.

Blanes:2017:HOC

[BCT17] Sergio Blanes, Fernando Casas, and Mechthild Thalhammer. High-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear evolution equations. *Computer Physics Communications*, 220(??):243–262, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302357.

Busato:2018:OOT

[BCTP18] Emmanuel Busato, David Calvet, and Timothée Theveneaux-Pelzer. OpTHyLiC: An Optimised Tool for Hybrid Limits Computation. *Computer Physics Communications*, 226

(??):136–150, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300134.

Bianchi:2010:RTO

[BD10] S. Bianchi and R. Di Leonardo. Real-time optical micromanipulation using optimized holograms generated on the GPU. *Computer Physics Communications*, 181(8):1444–1448, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001232.

Barka:2012:ASH

[BD12] André Barka and Nicolas Douchin. Asymptotic simplifications for hybrid BEM/GO/PO/PTD techniques based on a Generalized Scattering Matrix approach. *Computer Physics Communications*, 183(9):1928–1936, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001543.

Buehler:2014:CCH

[BD14] Stephan Buehler and Claude Duhr. CHAPLIN-Complex Harmonic Polylogarithms in Fortran. *Computer Physics Communications*, 185(10):2703–2713, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001969.

Bierwage:2012:OBR

[BDBV12] A. Bierwage, C. Di Troia, S. Briguglio, and G. Vlad. Orbit-based representation of equilibrium distribution functions for low-noise initialization of kinetic simulations of toroidal plasmas. *Computer Physics Communications*, 183(5):1107–1123, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000288.

Bern:2014:NNE

[BDC+14] Z. Bern, L. J. Dixon, F. Febres Cordero, S. Höche, H. Ita, D. A. Kosower, and D. Maître. Ntuples for NLO events at hadron colliders. *Computer Physics Communications*, 185(5):1443–1460, May 2014. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000241.

Beuria:2018:LCP

[BDDM18] Jyotiranjan Beuria, Asesh Krishna Datta, Dipsikha Debnath, and Konstantin T. Matchev. LHC collider phenomenology of minimal universal extra dimensions. *Computer Physics Communications*, 226(??):187–205, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300031.

Bonciani:2019:NRC

[BDGG19] Roberto Bonciani, Giuseppe Degrassi, Pier Paolo Giardino, and Ramona Gröber. A numerical routine for the crossed vertex diagram with a massive-particle loop. *Computer Physics Communications*, 241(??):122–131, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930092X.

Butykai:2017:PPF

[BDGM+17] A. Butykai, P. Domínguez-García, F. M. Mor, R. Gaál, L. Forró, and S. Jeney. PFMCal: Photonic force microscopy calibration extended for its application in high-frequency microrheology. *Computer Physics Communications*, 220(??):507–508, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302394.

Barrio:2018:OLA

[BDJS18] Roberto Barrio, Peibing Du, Hao Jiang, and Sergio Serrano. ORTHOPOLY: A library for accurate evaluation of series of classical orthogonal polynomials and their derivatives. *Computer Physics Communications*, 231(??):146–162, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301577.

Barasinski:2011:QEH

[BDK11] A. Barasiński, A. Drzewiński, and G. Kamieniarz. Quantum effects and Haldane gap in magnetic chains with alternating anisotropy axes. *Computer Physics Communications*, 182(9):2013–2016, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004947.

Belov:2010:HXB

[BDKS10] S. Belov, L. Dudko, D. Kekelidze, and A. Sherstnev. HepML, an XML-based format for describing simulated data in high energy physics. *Computer Physics Communications*, 181(10):1758–1768, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002031.

Beck:2019:ASO

[BDL+19] A. Beck, J. Derouillat, M. Lobet, A. Farjallah, F. Massimo, I. Zemzemi, F. Perez, T. Vinci, and M. Grech. Adaptive SIMD optimizations in particle-in-cell codes with fine-grain particle sorting. *Computer Physics Communications*, 244(??):246–263, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301481.

Berger:2016:HWN

[BDP16] Casey E. Berger, Joaquín E. Drut, and William J. Porter. Hard-wall and non-uniform lattice Monte Carlo approaches to one-dimensional Fermi gases in a harmonic trap. *Computer Physics Communications*, 208(??):103–108, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302351.

Bell:2015:ETC

[BDPM15] Robert A. Bell, Simon M.-M. Dubois, Michael C. Payne, and Arash A. Mostofi. Electronic transport calculations in the ONETEP code: Implementation and applications. *Computer Physics Communications*, 193(??):78–88, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001241.

Barrio:2015:DRH

[BDT15] Roberto Barrio, Angeles Dena, and Warwick Tucker. A database of rigorous and high-precision periodic orbits of the Lorenz model. *Computer Physics Communications*, 194(??):76–83, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001381.

Bonciani:2011:GHP

[BDV11] R. Bonciani, G. Degrassi, and A. Vicini. On the generalized harmonic polylogarithms of one complex variable. *Computer Physics Communications*, 182(6):1253–1264, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000737.

Barros:2011:SSP

[BdVGS11] Alison Barros, Euler de Vilhena Garcia, and Rafael Morgado Silva. Simulation of stochastic processes using graphics hardware. *Computer Physics Communications*, 182(4):989–993, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005369.

Bian:2014:SIS

[BE14] Xin Bian and Marco Ellero. A splitting integration scheme for the SPH simulation of concentrated particle suspensions. *Computer Physics Communications*, 185(1):53–62, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002786.

Bierwage:2019:SMP

[BEKP19] A. Bierwage, T. Zh. Esirkepov, J. K. Koga, and A. S. Pirozhkov. Similarity of magnetized plasma wake channels behind relativistic laser pulses with different wavelengths. *Computer Physics Communications*, 244(??):49–68, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302152.

Byun:2017:DSI

[BENK+17] Hye Suk Byun, Mohamed Y. El-Naggar, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta. A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics. *Computer Physics Communications*, 219(??):246–254, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301819.

Berg:2014:DSS

[Ber14] Bernd A. Berg. Detection of a small shift in a broad distribution. *Computer Physics Communications*, 185 (12):3250–3258, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003063.

Berg:2016:CLS

[Ber16a] Bernd A. Berg. Corrigendum to "Least square fitting with one explicit parameter less" [comput. phys. comm. 200 (2016) 254–258]. *Computer Physics Communications*, 208(??):169, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302156. See [Ber16b].

Berg:2016:LSF

[Ber16b] Bernd A. Berg. Least square fitting with one explicit parameter less. *Computer Physics Communications*, 200(??):254–258, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003987. See corrigendum [Ber16a].

Beu:2011:SFA

[Beu11] Titus A. Beu. Simulation of the flow of aqueous solutions through carbon nanotubes. *Computer Physics Communications*, 182(9):2004–2008, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004601.

Breslau:2010:IIS

[BF10] J. A. Breslau and G. Y. Fu. Implementation of an implicit shear Alfvén operator in the M3D code. *Computer Physics Communications*, 181(10):1661–1670, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001803.

Balac:2016:SCP

[BF16] Stéphane Balac and Arnaud Fernandez. SPIP: a computer program implementing the interaction picture method for simulation of light-wave propagation in optical fibre. *Computer Physics Communications*, 199(??):139–152, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003926.

Boeck:2011:OOD

[BFD+11] S. Boeck, C. Freysoldt, A. Dick, L. Ismer, and J. Neugebauer. The object-oriented DFT program library S/PHI/nX. *Computer Physics Communications*, 182(3):543–554, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003619.

Blennow:2010:NOP

[BFM10] Mattias Blennow and Enrique Fernandez-Martinez. Neutrino oscillation parameter sampling with MonteCUBES. *Computer Physics Communications*, 181(1):227–231, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900304X.

Bernaschi:2012:MGC

[BFPP12] M. Bernaschi, M. Fatica, G. Parisi, and L. Parisi. Multi-GPU codes for spin systems simulations. *Computer Physics Communications*, 183(7):1416–1421, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000689.

Blumer:2011:QMC

[BG11] N. Blümer and E. V. Gorelik. Quantum Monte Carlo simulations of antiferromagnetism in ultracold fermions on optical lattices within real-space dynamical mean-field theory. *Computer Physics Communications*, 182(1):115–118, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002407.

Blau:2013:GFC

[BG13a] Christian Blau and Helmut Grubmuller. g_contacts: Fast contact search in bio-molecular ensemble data. *Computer Physics Communications*, 184(12):2856–2859, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002464.

Bonhommeau:2013:MMC

[BG13b] David A. Bonhommeau and Marie-Pierre Gaigeot. MCMC^2: a Monte Carlo code for multiply-charged clusters. *Computer Physics Communications*, 184(3):873–884, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003669.

Bonhommeau:2014:MMD

[BG14a] David A. Bonhommeau and Marie-Pierre Gaigeot. MDMC^2: a molecular dynamics code for investigating the fragmentation dynamics of multiply charged clusters. *Computer Physics Communications*, 185(2):684–694, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003433.

Bueno:2014:CIH

[BG14b] A. Bueno and A. Gascón. CORSIKA implementation of heavy quark production and propagation in extensive air showers. *Computer Physics Communications*, 185(2):638–650, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003299.

Benson:2019:NTM

[BG19a] Sean Benson and Konstantin Gizdov. NNDrone: a toolkit for the mass application of machine learning in high energy physics. *Computer Physics Communications*, 240(??):15–20, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300785.

Bingham:2019:RTD

[BG19b] Peter S. Bingham and Jimena D. Gorfinkiel. `reskit`: a toolkit to determine the poles of an S-matrix. *Computer Physics Communications*, 239(??):272–282, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930013X.

Back:2018:LDP

[BGH+18] John Back, Tim Gershon, Paul Harrison, Thomas Latham, Daniel O'Hanlon, Wenbin Qian, Pablo del Amo Sanchez, Daniel Craik, Jelena Ilic, Juan Martin Otalora Goicochea, Eugenia Puccio, Rafael Silva Coutinho, and Mark Whitehead. Laura++: a Dalitz plot fitter. *Computer Physics Communications*, 231(??):198–242, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301334.

Brill:2019:WID

[BGHN19] Dab Brill, Jason B. Giles, Ian S. Haworth, and Aiichiro Nakano. WaterAlignment: Identification of displaced water molecules in molecular docking using Jonker and Volgenant shortest path augmentation for linear assignment. *Computer Physics Communications*, 244(??):324–328, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302085.

Bowman:2014:STF

[BGL+14] Richard W. Bowman, Graham M. Gibson, Anna Linnenberger, David B. Phillips, James A. Grieve, David M. Carberry, Steven Serati, Mervyn J. Miles, and Miles J. Padgett. "Red Tweezers": Fast, customisable hologram generation for optical tweezers. *Computer Physics Communications*, 185(1):268–273, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002695.

Baglio:2014:NPP

[BGM+14] J. Baglio, R. Gröber, M. Mühlleitner, D. T. Nhung, H. Rzehak, M. Spira, J. Streicher, and K. Walz. NMSSMCALC: a program package for the calculation of loop-corrected Higgs boson masses and decay widths in the (complex) NMSSM. *Computer Physics Communications*, 185(12):3372–3391, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002720.

Bloch:2011:NKS

[BH11] Jacques C. R. Bloch and Simon Heybrock. A nested Krylov subspace method to compute the sign function of large complex matrices. *Computer Physics Communications*, 182(4):878–889, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004972.

Borowka:2013:MNP

[BH13] Sophia Borowka and Gudrun Heinrich. Massive nonplanar two-loop four-point integrals with SecDec 2.1. *Computer Physics Communications*, 184(11):2552–2561, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001926.

Benda:2014:CEHa

[BH14a] Jakub Benda and Karel Houfek. Collisions of electrons with hydrogen atoms I. Package outline and high energy code. *Computer Physics Communications*, 185(11):2893–2902, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002161.

Benda:2014:CEHb

[BH14b] Jakub Benda and Karel Houfek. Collisions of electrons with hydrogen atoms II. Low-energy program using the method of the exterior complex scaling. *Computer Physics Communications*, 185(11):2903–2912, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001866.

Benda:2016:NVH

[BH16] Jakub Benda and Karel Houfek. New version of hex-ecs, the B-spline implementation of exterior complex scaling method for solution of electron–hydrogen scattering. *Computer Physics Communications*, 204(??):216–217, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300911.

Benda:2017:RDG

[BH17] Jakub Benda and Karel Houfek. Reducing the dimensionality of grid based methods for electron-atom scattering calculations below ionization threshold. *Computer Physics Communications*, 213(??):46–51, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303654.

Busa:2010:CPD

[BHH+10] Ján Busa, Shura Hayryan, Chin-Kun Hu, Jaroslav Skrivánek, and Ming-Chya Wu. CAVE: a package for detection and quantitative analysis of internal cavities in a system of overlapping balls: Application to proteins. *Computer Physics Communications*, 181(12):2116–2125, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003395.

Borowka:2015:SNE

[BHJ+15] S. Borowka, G. Heinrich, S. P. Jones, M. Kerner, J. Schlenk, and T. Zirke. SecDec-3.0: Numerical evaluation of multi-scale integrals beyond one loop. *Computer Physics Communications*, 196(??):470–491, November 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002027.

Borowka:2018:PTN

[BHJ+18] S. Borowka, G. Heinrich, S. Jahn, S. P. Jones, M. Kerner, J. Schlenk, and T. Zirke. pySecDec: a toolbox for the numerical evaluation of multi-scale integrals. *Computer Physics Communications*, 222(??):313–326, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303028.

Borowka:2019:GCQ

[BHJ+19] S. Borowka, G. Heinrich, S. Jahn, S. P. Jones, M. Kerner, and J. Schlenk. A GPU compatible quasi-Monte Carlo integrator interfaced to pySecDec. *Computer Physics Communications*, 240(??):120–137, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300670.

Bonnivard:2016:CJA

[BHN+16] Vincent Bonnivard, Moritz Hütten, Emmanuel Nezri, Aldée Charbonnier, Céline Combet, and David Maurin. CLUMPY: Jeans analysis, γ-ray and ν fluxes from dark matter (sub-)structures. *Computer Physics Communications*, 200(??):336–349, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004348.

Bulow:2016:SPS

[BHND16] F. Bülow, P. Hamberger, H. Nirschl, and W. Dörfler. A scalable parallel Stokesian Dynamics method for the simulation of colloidal suspensions. *Computer Physics Communications*, 204(??):107–120, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300753.

Basagaoglu:2017:ECP

[BHNS17] Hakan Basagaoglu, John R. Harwell, Hoa Nguyen, and Sauro Succi. Enhanced computational performance of the lattice Boltzmann model for simulating micron- and submicron-size particle flows and non-Newtonian fluid flows. *Computer Physics Communications*, 213(??):64–71, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303873.

Bothmann:2015:IMP

[BHS15] Enrico Bothmann, Nathan Hartland, and Steffen Schumann. Introducing MCgrid 2.0: Projecting cross section calculations on grids. *Computer Physics Communications*, 196(??):617–618, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002714.

Bazow:2018:MPS

[BHS18] Dennis Bazow, Ulrich Heinz, and Michael Strickland. Massively parallel simulations of relativistic fluid dynamics on graphics processing units with CUDA. *Computer Physics Communications*, 225(??):92–113, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300279.

Bi:2019:NOB

[BHT19] Sheng Bi, Li Huang, and Ning-Hua Tong. Natural orbital-based Lanczos method for Anderson impurity models. *Computer Physics Communications*, 235(??):196–209, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303163.

Binder:2015:RCI

[BHVMH15] Sebastian C. Binder, Esteban A. Hernandez-Vargas, and Michael Meyer-Hermann. Reducing complexity: an iterative strategy for parameter determination in biological networks. *Computer Physics Communications*, 190(??):15–22, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500003X.

Busa:2012:ACO

[BHW+12] Ján Busa, Jr., Shura Hayryan, Ming-Chya Wu, Ján Busa, and Chin-Kun Hu. ARVO-CL: the OpenCL version of the ARVO package — an efficient tool for computing the accessible surface area and the excluded volume of proteins via analytical equations. *Computer Physics Communications*, 183(11):2494–2497, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001580.

Brein:2013:VHS

[BHZ13] Oliver Brein, Robert V. Harlander, and Tom J. E. Zirke. vh@nnlo-Higgs Strahlung at hadron colliders. *Computer Physics Communications*, 184(3):998–1003, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003785.

Bingemann:2013:SIS

[Bin13] Dieter Bingemann. Statistical identification of structural rearrangement events in molecular dynamics trajectories. *Computer Physics Communications*, 184(3):757–764, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200392X.

Biswas:2015:IAD

[Bis15] Katja Biswas. An iterative aggregation and disaggregation method for the steady state solution of large scale continuous systems. *Computer Physics Communications*, 191(??):25–32, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000326.

Brugnano:2012:TSF

[BIT12] Luigi Brugnano, Felice Iavernaro, and Donato Trigiante. A two-step, fourth-order method with energy preserving properties. *Computer Physics Communications*, 183(9):1860–1868, September 2012. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001324.

Blavatska:2011:PCM

[BJ11] Viktoria Blavatska and Wolfhard Janke. Θ-polymers in crowded media under stretching force. *Computer Physics Communications*, 182(9):1966–1969, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005151.

Backovic:2014:TVT

[BJ14] Mihailo Backović and José Juknevich. TemplateTagger v1.0.0: a template matching tool for jet substructure. *Computer Physics Communications*, 185(4):1322–1338, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300430X.

Baity-Jesi:2014:JIN

[BJBC+14] M. Baity-Jesi, R. A. Baños, A. Cruz, L. A. Fernandez, J. M. Gil-Narvion, A. Gordillo-Guerrero, D. Iñiguez, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, J. Monforte-Garcia, A. Muñoz Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, M. Pivanti, F. Ricci-Tersenghi, J. J. Ruiz-Lorenzo, S. F. Schifano, B. Seoane, A. Tarancond, R. Tripiccione, and D. Yllanes. Janus II: A new generation application-driven computer for spin-system simulations. *Computer Physics Communications*, 185(2):550–559, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003470.

Beliakov:2013:EIBa

[BJCW13] Gleb Beliakov, Michael Johnstone, Doug Creighton, and Tim Wilkin. An efficient implementation of Bailey and Borwein's algorithm for parallel random number generation on graphics processing units. *Computing*, 95(4):309–326, April 2013. CODEN CMPTA2. ISSN 0010-485X (print), 1436-5057 (electronic). URL http://link.springer.com/article/10.1007/s00607-012-0234-8. See also [BCJW13].

Boromand:2015:VMT

[BJM15] Arman Boromand, Safa Jamali, and Joao M. Maia. Viscosity measurement techniques in Dissipative Particle Dynamics. *Computer Physics Communications*, 196(??):149–160, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002076.

Bjorkman:2011:CGG

[Bjö11] Torbjörn Björkman. CIF2Cell: Generating geometries for electronic structure programs. *Computer Physics Communications*, 182(5):1183–1186, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000336.

Bauke:2011:AFS

[BK11a] Heiko Bauke and Christoph H. Keitel. Accelerating the Fourier split operator method via graphics processing units. *Computer Physics Communications*, 182(12):2454–2463, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002414.

Blank:2011:MAS

[BK11b] M. Blank and A. Krassnigg. Matrix algorithms for solving (in)homogeneous bound state equations. *Computer Physics Communications*, 182(7):1391–1401, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000816.

Bertoglio:2012:LRQ

[BK12] Cristóbal Bertoglio and Boris N. Khoromskij. Low-rank quadrature-based tensor approximation of the Galerkin projected Newton/Yukawa kernels. *Computer Physics Communications*, 183(4):904–912, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004048.

Bahmann:2013:EEA

[BK13a] Silvia Bahmann and Jens Kortus. EVO — evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 184(6):1618–1625, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000519.

Bakulev:2013:FMP

[BK13b] Alexander P. Bakulev and Vyacheslav L. Khandramai. FAPT: a Mathematica package for calculations in QCD Fractional Analytic Perturbation Theory. *Computer Physics Communications*, 184(1):183–193, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002809.

Bytev:2015:HHF

[BK15] Vladimir V. Bytev and Bernd A. Kniehl. HYPERDIRE HYPERgeometric functions DIfferential REduction: Mathematica-based packages for the differential reduction of generalized hypergeometric functions: Horn-type hypergeometric functions of two variables. *Computer Physics Communications*, 189(??):128–154, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004056.

Bhatt:2016:FOC

[BK16a] H. P. Bhatt and A. Q. M. Khaliq. Fourth-order compact schemes for the numerical simulation of coupled Burgers' equation. *Computer Physics Communications*, 200(??): 117–138, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500418X.

Bytev:2016:HHF

[BK16b] Vladimir V. Bytev and Bernd A. Kniehl. HYPERDIRE — HYPERgeometric functions DIfferential REduction: Mathematica-based packages for the differential reduction of generalized hypergeometric functions: Lauricella function F_c of three variables. *Computer Physics*

Communications, 206(??):78–83, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301059.

Bilal:2014:TPS

[BKA+14] M. Bilal, Banaras Khan, H. A. Rahnamaye Aliabad, M. Maqbool, S. Jalai Asadabadi, and I. Ahmad. Thermoelectric properties of $SbNCa_3$ and $BiNCa_3$ for thermoelectric devices and alternative energy applications. *Computer Physics Communications*, 185(5):1394–1398, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000332.

Barnes:2017:ITE

[BKC+17] Taylor A. Barnes, Thorsten Kurth, Pierre Carrier, Nathan Wichmann, David Prendergast, Paul R. C. Kent, and Jack Deslippe. Improved treatment of exact exchange in Quantum ESPRESSO. *Computer Physics Communications*, 214(??):52–58, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300085.

Bytev:2013:HHF

[BKK13] Vladimir V. Bytev, Mikhail Yu. Kalmykov, and Bernd A. Kniehl. HYPERDIRE, HYPERgeometric functions DIfferential REduction: Mathematica-based packages for differential reduction of generalized hypergeometric functions ${}_pF_{p-1}, F_1, F_2, F_3, F_4$. *Computer Physics Communications*, 184(10):2332–2342, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001690.

Blobel:2011:FAC

[BKM11] Volker Blobel, Claus Kleinwort, and Frank Meier. Fast alignment of a complex tracking detector using advanced track models. *Computer Physics Communications*, 182(9):1760–1763, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001093.

Bytev:2014:HFD

[BKM14] Vladimir V. Bytev, Mikhail Yu. Kalmykov, and Sven-Olaf Moch. HYPERgeometric functions DIfferential REduction (HYPERDIRE): MATHEMATICA based packages for differential reduction of generalized hypergeometric functions: F_D and F_S Horn-type hypergeometric functions of three variables. *Computer Physics Communications*, 185(11):3041–3058, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002574.

Beneke:2016:NTP

[BKMP16] M. Beneke, Y. Kiyo, A. Maier, and J. Piclum. Near-threshold production of heavy quarks with QQbar_threshold. *Computer Physics Communications*, 209(??):96–115, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302144.

Buljan:2017:GAI

[BKN+17] Maja Buljan, Marko Karlusić, Nikolina Nekić, Marko Jercinović, Iva Bogdanović-Radović, Sigrid Bernstorff, Nikola Radić, and Igor Mekterović. GISAXS analysis of ion beam modified films and surfaces. *Computer Physics Communications*, 212(??):69–81, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303174.

Bauer:2016:IVT

[BKOZ16] Petr Bauer, Vladimír Klement, Tomás Oberhuber, and Vítezslav Zabka. Implementation of the Vanka-type multigrid solver for the finite element approximation of the Navier–Stokes equations on GPU. *Computer Physics Communications*, 200(??):50–56, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004026.

Brown:2012:IMD

[BKPT12] W. Michael Brown, Axel Kohlmeyer, Steven J. Plimpton, and Arnold N. Tharrington. Implementing molecular dynamics on hybrid high performance computers — particle–particle particle–mesh. *Computer Physics Communications*, 183(3):449–459, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003444.

Biborski:2015:CSD

[BKS15] Andrzej Biborski, Andrzej P. Kadzielawa, and Józef Spalek. Combined shared and distributed memory ab-initio computations of molecular-hydrogen systems in the correlated state: Process pool solution and two-level parallelism. *Computer Physics Communications*, 197(??):7–16, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002854.

Bakx:2016:FSO

[BKV16] R. Bakx, R. H. P. Kleiss, and F. Versteegen. First- and second-order error estimates in Monte Carlo integration. *Computer Physics Communications*, 208(??):29–34, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302090.

Batistakis:2014:SGT

[BL14] C. Batistakis and A. V. Lyulin. Simulated glass transition in thin polymer films: Influence of truncating the non-bonded interaction potentials. *Computer Physics Communications*, 185(4):1223–1229, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004323.

Benedetti:2018:CM

[BL18a] Florian Benedetti and Claire Loison. Comment to: "Martini straight: Boosting performance using a shorter cut-off and GPUs" by D. H. de Jong, S. Baoukina, H. I. Ingólfsson, and S. J. Marrink. *Computer Physics Communications*, 228(??):146–151, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300316. See [dJBIM16].

Bingham:2018:VAD

[BL18b] Andrew Bingham and Hyoung K. Lee. The viability of ADVANTG deterministic method for synthetic radiography generation. *Computer Physics Communications*, 228(??):5–10, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300377.

Bartholomew:2019:NHS

[BL19] Paul Bartholomew and Sylvain Laizet. A new highly scalable, high-order accurate framework for variable-density flows: Application to non-Boussinesq gravity currents. *Computer Physics Communications*, 242(??):83–94, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301006.

Blanes:2015:ESR

[Bla15] S. Blanes. Explicit symplectic RKN methods for perturbed non-autonomous oscillators: Splitting, extended and exponentially fitting methods. *Computer Physics Communications*, 193(??):10–18, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001101.

Blackburn:2019:SSE

[BLAS19] H. M. Blackburn, D. Lee, T. Albrecht, and J. Singh. Semtex: a spectral element-Fourier solver for the incompressible Navier–Stokes equations in cylindrical or Cartesian coordinates. *Computer Physics Communications*, 245 (??):Article 106804, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301730.

Bonhommeau:2014:MVM

[BLG14] David A. Bonhommeau, Marius Lewerenz, and Marie-Pierre Gaigeot. MCMC^2 (version 1.1): a Monte Carlo code for multiply-charged clusters. *Computer Physics Communications*, 185(3):1188–1191, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465513003305.

Bach:2013:LQB

[BLPP13] Matthias Bach, Volker Lindenstruth, Owe Philipsen, and Christopher Pinke. Lattice QCD based on OpenCL. *Computer Physics Communications*, 184(9):2042–2052, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001288.

Bernaschi:2017:GBD

[BLS17] M. Bernaschi, M. Lulli, and M. Sbragaglia. GPU based detection of topological changes in Voronoi diagrams. *Computer Physics Communications*, 213(??):19–28, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303599.

Bakhta:2019:MSI

[BLV+19] Athmane Bakhta, Sébastien Leclaire, David Vidal, François Bertrand, and Mohamed Cheriet. Multiscale simulation of ink seepage into paper: a mesoscopic variational model. *Computer Physics Communications*, 239(??):1–13, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300384.

Balac:2013:ERK

[BM13] Stéphane Balac and Fabrice Mahé. Embedded Runge–Kutta scheme for step-size control in the interaction picture method. *Computer Physics Communications*, 184(4):1211–1219, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004262.

Bertsch:2016:FTH

[BM16] G. F. Bertsch and J. M. Mehlhaff. A finite-temperature Hartree–Fock code for shell-model Hamiltonians. *Computer Physics Communications*, 207(??):518–523, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630203X.

Basler:2019:BBS

[BM19] Philipp Basler and Margarete Mühlleitner. BSMPT (Beyond the Standard Model Phase Transitions): a tool for the electroweak phase transition in extended Higgs sectors. *Computer Physics Communications*, 237(??):62–85, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303989.

Boukandou-Mombo:2017:NFA

[BMBC+17] Charlotte Boukandou-Mombo, Hassan Bakrim, Jonathan Claustre, Joëlle Margot, Jean-Pierre Matte, and François Vidal. New fast accurately conservative scheme for solving numerically the time-dependent isotropic Fokker–Planck equation. *Computer Physics Communications*, 220(??):173–180, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302114.

Badia:2011:LSL

[BMC+11a] J. M. Badia, J. L. Movilla, J. I. Climente, M. Castillo, M. Marqués, R. Mayo, E. S. Quintana-Ortí, and J. Planelles. Large-scale linear system solver using secondary storage: Self-energy in hybrid nanostructures. *Computer Physics Communications*, 182(2):533–539, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004224.

Badia:2011:PSH

[BMC+11b] J. M. Badia, J. L. Movilla, J. I. Climente, M. Castillo, M. Marqués, R. Mayo, E. S. Quintana-Ortí, and J. Planelles. A parallel solver for huge dense linear systems. *Computer Physics Communications*, 182(11):2441–2442, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002207.

Bussone:2019:THM

[BMDP19] A. Bussone, M. Della Morte, V. Drach, and C. Pica. Tuning the hybrid Monte Carlo algorithm using molecular dynamics forces' variances. *Computer Physics Communications*, 234(??):179–187, January 2019. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302625.

Bocquet:2019:TSD

[BMF+19] F. C. Bocquet, G. Mercurio, M. Franke, G. van Straaten, S. Weiß, S. Soubatch, C. Kumpf, and F. S. Tautz. Torricelli: a software to determine atomic spatial distributions from normal incidence X-ray standing wave data. *Computer Physics Communications*, 235(??):502–513, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302170.

Butykai:2015:COT

[BMG+15] A. Butykai, F. M. Mor, R. Gaál, P. Domínguez-García, L. Forró, and S. Jeney. Calibration of optical tweezers with non-spherical probes via high-resolution detection of Brownian motion. *Computer Physics Communications*, 196(??):599–610, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002702.

Bussone:2017:RTB

[BMHP17] Andrea Bussone, Michele Della Morte, Martin Hansen, and Claudio Pica. On reweighting for twisted boundary conditions. *Computer Physics Communications*, 219(??):91–98, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301534.

Bouazra:2014:NMI

[BMNS14] A. Bouazra, S. Mnasri, S. Abdi-Ben Nasrallah, and M. Said. Numerical modeling of the InAs quantum dot with application of coordinate transformation and the finite difference method. *Computer Physics Communications*, 185(4):1290–1298, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000046.

Bna:2016:VLI

[BMS+16] S. Bnà, S. Manservisi, R. Scardovelli, P. Yecko, and S. Zaleski. Vofi — a library to initialize the volume fraction scalar field. *Computer Physics Communications*, 200(??):291–299, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004087.

Baver:2011:LEC

[BMU11] D. A. Baver, J. R. Myra, and M. V. Umansky. Linear eigenvalue code for edge plasma in full tokamak X-point geometry. *Computer Physics Communications*, 182(8):1610–1620, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001251.

Boblest:2014:MES

[BMW14] S. Boblest, D. Meyer, and G. Wunner. Multi-electron systems in strong magnetic fields II: a fixed-phase diffusion quantum Monte Carlo application based on trial functions from a Hartree–Fock–Roothaan method. *Computer Physics Communications*, 185(11):2992–3000, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002446.

Broberg:2018:PPT

[BMZ+18] Danny Broberg, Bharat Medasani, Nils E. R. Zimmermann, Guodong Yu, Andrew Canning, Maciej Haranczyk, Mark Asta, and Geoffroy Hautier. PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators. *Computer Physics Communications*, 226(??):165–179, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300079.

Burrows:2011:PRS

[BNAB11] Adam Burrows, Jason Nordhaus, Ann Almgren, and John Bell. The potential role of spatial dimension in the neutrino-driving mechanism of core-collapse supernova explosions. *Computer Physics Communications*, 182(9):1764–1766, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004091.

Brower:2017:MDW

[BNO17] Richard C. Brower, Harmut Neff, and Kostas Orginos. The Möbius domain wall fermion algorithm. *Computer Physics Communications*, 220(??):1–19, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730036X.

Bartel:2019:TCF

[BNPPD19] J. Bartel, B. Nerlo-Pomorska, K. Pomorski, and A. Dobrowolski. Transport coefficients in the Fourier shape parametrization. *Computer Physics Communications*, 241 (??):139–145, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300888.

Baran:2018:JCC

[BNV18] Á. Baran, Cs. Noszály, and T. Vertse. JOZSO, a computer code for calculating broad neutron resonances in phenomenological nuclear potentials. *Computer Physics Communications*, 228(??):185–191, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300857.

Bresolin:2012:ABC

[BO12] C. S. Bresolin and A. A. M. Oliveira. An algorithm based on collision theory for the lattice Boltzmann simulation of isothermal mass diffusion with chemical reaction. *Computer Physics Communications*, 183(12):2542–2549, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002317.

Boer:2014:GBS

[Boe14] Attila Boer. GPU-based simulation of the long-range Potts model via parallel tempering. *Computer Physics Communications*, 185(7):1932–1937, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465514001027.

Boer:2018:IRE

[Boe18] A. Boer. Implementation of the replica-exchange Wang–Landau sampling on Graphics Processing Units (GPUs). *Computer Physics Communications*, 233(??):62–66, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302509.

Bogner:2016:MPC

[Bog16] Christian Bogner. MPL — a program for computations with iterated integrals on moduli spaces of curves of genus zero. *Computer Physics Communications*, 203(??):339–353, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300595.

Bigay:2017:WCC

[BOGL17] P. Bigay, G. Oger, P.-M. Guilcher, and D. Le Touzé. A weakly-compressible Cartesian grid approach for hydrodynamic flows. *Computer Physics Communications*, 220(??):31–43, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301923.

Bonhommeau:2015:MVM

[Bon15] David A. Bonhommeau. MCMC^2 (version 1.1.1): a Monte Carlo code for multiply charged clusters. *Computer Physics Communications*, 196(??):614–616, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002623.

Bonhommeau:2016:MVM

[Bon16] David A. Bonhommeau. MCMC^2 (version 1.1.2): a Monte Carlo code for multiply charged clusters. *Computer Physics Communications*, 207(??):533–535, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301710.

Bacchini:2017:NPC

[BOPL17] Fabio Bacchini, Vyacheslav Olshevsky, Stefaan Poedts, and Giovanni Lapenta. A new particle-in-cell method for modeling magnetized fluids. *Computer Physics Communications*, 210(??):79–91, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303071`.

Borinsky:2014:FGG

[Bor14] Michael Borinsky. Feynman graph generation and calculations in the Hopf algebra of Feynman graphs. *Computer Physics Communications*, 185(12):3317–3330, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002665`.

Botje:2011:QFQ

[Bot11] M. Botje. QCDNUM: Fast QCD evolution and convolution. *Computer Physics Communications*, 182(2):490–532, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004212`.

Botha:2012:GMA

[Bot12] A. E. Botha. General R-matrix approach for integrating the multiband $k \cdot p$ equation in layered semiconductor structures. *Computer Physics Communications*, 183(1):197–202, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003067`.

Botto:2013:GMP

[Bot13] Lorenzo Botto. A geometric multigrid Poisson solver for domains containing solid inclusions. *Computer Physics Communications*, 184(3):1033–1044, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003840`.

Boyd:2015:FWC

[Boy15] John P. Boyd. Four ways to compute the inverse of the complete elliptic integral of the first kind. *Computer Physics*

Communications, 196(??):13–18, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001733.

Babaev:2012:RCE

[BP12] A. Babaev and Yu. L. Pivovarov. Resonant coherent excitation of hydrogen-like ions planar channeled in a crystal: Transition into the first excited state. *Computer Physics Communications*, 183(3):705–710, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003717.

Bart:2017:MPM

[BPB+17] G. Bart, C. Peltz, N. Bigaouette, T. Fennel, T. Brabec, and C. Varin. Massively parallel microscopic particle-in-cell. *Computer Physics Communications*, 219(??):269–285, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301868.

Batic:2012:ICC

[BPC12] Matej Batic, Maria Grazia Pia, and Sam J. Cipolla. ISICSoo: a class for the calculation of ionization cross sections from ECPSSR and PWBA theory. *Computer Physics Communications*, 183(2):398–404, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003328.

Batic:2013:CIC

[BPC13] Matej Batic, Maria Grazia Pia, and Sam J. Cipolla. Corrected ISICSoo class version. *Computer Physics Communications*, 184(9):2232–2233, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000751.

Biarnes:2012:MVI

[BPML12] Xevi Biarnés, Fabio Pietrucci, Fabrizio Marinelli, and Alessandro Laio. METAGUI. A VMD interface for analyzing metadynamics and molecular dynamics simulations.

Computer Physics Communications, 183(1):203–211, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003079.

Bhattacharya:2014:EPT

[BPMM14] Kolahal Bhattacharya, Arnab K. Pal, Gobinda Majumder, and Naba K. Mondal. Error propagation of the track model and track fitting strategy for the Iron CALorimeter detector in India-based neutrino observatory. *Computer Physics Communications*, 185(12):3259–3268, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003087.

Brazzano:2016:BMA

[BPMS16] L. Ciocci Brazzano, L. J. Pellizza, C. L. Matteo, and P. A. Sorichetti. A Bayesian method for analysing relaxation spectra. *Computer Physics Communications*, 198(??):22–30, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500332X.

Bernaschi:2011:BGC

[BPP11] M. Bernaschi, G. Parisi, and L. Parisi. Benchmarking GPU and CPU codes for Heisenberg spin glass over-relaxation. *Computer Physics Communications*, 182(6):1265–1271, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000749.

Brock:2016:FBO

[BPS+16] Casey N. Brock, Brandon C. Paikoff, Muhammad I. Md Sallih, Alan R. Tackett, and D. Greg Walker. Force-based optimization of pseudopotentials for non-equilibrium configurations. *Computer Physics Communications*, 201(??):106–118, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000072.

Bhat:2018:OES

[BPSS18] Pushpalatha C. Bhat, Harrison B. Prosper, Sezen Sekmen, and Chip Stewart. Optimizing event selection with the random grid search. *Computer Physics Communications*, 228(??):245–257, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830047X.

Braga:2011:DLA

[BR11] F. L. Braga and M. S. Ribeiro. Diffusion Limited Aggregation: Algorithm optimization revisited. *Computer Physics Communications*, 182(8):1602–1605, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001238.

Bhar:2013:CPW

[BR13] Shyamal Bhar and Soumen Kumar Roy. A comparison of the performance of Wang–Landau-Transition-Matrix algorithm with Wang–Landau algorithm for the determination of the joint density of states for continuous spin models. *Computer Physics Communications*, 184(5):1387–1394, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300009X.

Bertsch:2014:CLD

[BR14] G. F. Bertsch and L. M. Robledo. Combinatorial level densities by the real-time method. *Computer Physics Communications*, 185(12):3406–3411, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002884.

Bradler:2015:HGD

[Brá15] Kamil Brádler. Hiking a generalized Dyck path: a tractable way of calculating multimode boson evolution operators. *Computer Physics Communications*, 196(??):80–91, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002003.

Barrio:2012:CAP

[BRB12] Roberto Barrio, Marcos Rodríguez, and Fernando Blesa. Computer-assisted proof of skeletons of periodic orbits. *Computer Physics Communications*, 183(1):80–85, January 2012.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003031.

Brewin:2010:BIC

[Bre10] Leo Brewin. A brief introduction to Cadabra: a tool for tensor computations in General Relativity. *Computer Physics Communications*, 181(3):489–498, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003415.

Bruneval:2016:MMB

[BRH+16] Fabien Bruneval, Tonatiuh Rangel, Samia M. Hamed, Meiyue Shao, Chao Yang, and Jeffrey B. Neaton. molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. *Computer Physics Communications*, 208(??):149–161, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301990.

Bespamyatnov:2012:ANB

[BRL12] I. O. Bespamyatnov, W. L. Rowan, and K. T. Liao. ALCBEAM — neutral beam formation and propagation code for beam-based plasma diagnostics. *Computer Physics Communications*, 183(3):669–676, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003511.

Brunetti:2013:FFG

[Bru13] Antonio Brunetti. A fast fine-grained genetic algorithm for spectrum fitting: an application to X-ray spectra. *Computer Physics Communications*, 184(3):573–578, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003438.

Barash:2011:RPL

[BS11] L. Yu. Barash and L. N. Shchur. RNGSSELIB: Program library for random number generation, SSE2 realization. *Computer Physics Communications*, 182(7):1518–1527, July

2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001159.

Buraczewski:2012:NMM

[BS12] A. Buraczewski and M. Stobińska. Numerical model for macroscopic quantum superpositions based on phase-covariant quantum cloning. *Computer Physics Communications*, 183(10):2245–2253, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200166X.

Barash:2013:RPL

[BS13a] L. Yu. Barash and L. N. Shchur. RNGSSELIB: Program library for random number generation. More generators, parallel streams of random numbers and Fortran compatibility. *Computer Physics Communications*, 184(10):2367–2369, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001422.

Bondarenko:2013:NEQ

[BS13b] Sergey G. Bondarenko and Andrey A. Sapronov. NLO EW and QCD proton-proton cross section calculations with mcsanc-v1.01. *Computer Physics Communications*, 184(10):2343–2350, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001707.

Barash:2014:PGA

[BS14a] L. Yu. Barash and L. N. Shchur. PRAND: GPU accelerated parallel random number generation library: Using most reliable algorithms and applying parallelism of modern GPUs and CPUs. *Computer Physics Communications*, 185(4):1343–1353, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000204.

Barettin:2014:ORD

[BS14b] Daniele Barettin and Paolo Sibani. Optimization by record dynamics. *Computer Physics Communications*, 185(3):

730–735, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003755.

Barker:2015:DDT

[BS15a] Andrew T. Barker and Martin Stoll. Domain decomposition in time for PDE-constrained optimization. *Computer Physics Communications*, 197(??):136–143, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003227.

Begau:2015:ADL

[BS15b] Christoph Begau and Godehard Sutmann. Adaptive dynamic load-balancing with irregular domain decomposition for particle simulations. *Computer Physics Communications*, 190(??):51–61, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000181.

Bernal:2013:AGM

[BSC+13] M. A. Bernal, D. Sikansi, F. Cavalcante, S. Incerti, C. Champion, V. Ivanchenko, and Z. Francis. An atomistic geometrical model of the B-DNA configuration for DNA-radiation interaction simulations. *Computer Physics Communications*, 184(12):2840–2847, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002439.

Borgoo:2010:MED

[BSGG10] A. Borgoo, O. Scharf, G. Gaigalas, and M. Godefroid. Multiconfiguration electron density function for the ATSP2K-package. *Computer Physics Communications*, 181(2):426–439, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003270.

Blinne:2018:SAN

[BSK+18] Alexander Blinne, David Schinkel, Stephan Kuschel, Nina Elkina, Sergey G. Rykovanov, and Matt Zepf. A systematic approach to numerical dispersion in Maxwell solvers.

Computer Physics Communications, 224(??):273–281, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303508.

Bae:2013:GCS

[BSM13] C. Bae, W. M. Stacey, and T. D. Morley. GTROTA: a code for the solution of the coupled nonlinear extended neoclassical rotation equations in tokamak plasmas using successive over-relaxation and simulated annealing. *Computer Physics Communications*, 184(11):2571–2587, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002002.

Buckley:2012:FSP

[BSW12] A. Buckley, A. Shilton, and M. J. White. Fast supersymmetry phenomenology at the Large Hadron Collider using machine learning techniques. *Computer Physics Communications*, 183(4):960–970, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000021.

Buckeridge:2014:APD

[BSWC14] J. Buckeridge, D. O. Scanlon, A. Walsh, and C. R. A. Catlow. Automated procedure to determine the thermodynamic stability of a material and the range of chemical potentials necessary for its formation relative to competing phases and compounds. *Computer Physics Communications*, 185(1):330–338, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002993.

Basko:2017:HML

[BT17a] Mikhail M. Basko and Ilia P. Tsygvintsev. A hybrid model of laser energy deposition for multi-dimensional simulations of plasmas and metals. *Computer Physics Communications*, 214(??):59–70, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730022X.

Bierwage:2017:BMP

[BT17b] A. Bierwage and Y. Todo. Benchmark of multi-phase method for the computation of fast ion distributions in a tokamak plasma in the presence of low-amplitude resonant MHD activity. *Computer Physics Communications*, 220(??):279–284, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302424.

Bonelli:2017:MCA

[BTC+17] Francesco Bonelli, Michele Tuttafesta, Gianpiero Colonna, Luigi Cutrone, and Giuseppe Pascazio. An MPI–CUDA approach for hypersonic flows with detailed state-to-state air kinetics using a GPU cluster. *Computer Physics Communications*, 219(??):178–195, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301613.

Blumers:2017:GAR

[BTL+17] Ansel L. Blumers, Yu-Hang Tang, Zhen Li, Xuejin Li, and George E. Karniadakis. GPU-accelerated red blood cells simulations with transport dissipative particle dynamics. *Computer Physics Communications*, 217(??):171–179, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301042.

Beland:2017:ACS

[BTM+17] Laurent Karim Béland, Artur Tamm, Sai Mu, German D. Samolyuk, Yuri N. Osetsky, Alvo Aabloo, Mattias Klintenberg, Alfredo Caro, and Roger E. Stoller. Accurate classical short-range forces for the study of collision cascades in Fe–Ni–Cr. *Computer Physics Communications*, 219(??):11–19, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301315.

Buckeridge:2019:EPD

[Buc19] J. Buckeridge. Equilibrium point defect and charge carrier concentrations in a material determined through calculation of the self-consistent Fermi energy. *Computer Physics*

Communications, 244(??):329–342, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302048.

Bessarab:2015:MFM

[BUJ15] Pavel F. Bessarab, Valery M. Uzdin, and Hannes Jónsson. Method for finding mechanism and activation energy of magnetic transitions, applied to skyrmion and antivortex annihilation. *Computer Physics Communications*, 196(??):335–347, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002696.

Broeckhove:2013:ACC

[BV13] J. Broeckhove and K. Vanmechelen. An adaptor for C++ callbacks with C and Fortran libraries. *Computer Physics Communications*, 184(3):824–832, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003591.

Blochliger:2013:SAO

[BVC13] Nicolas Blöchliger, Andreas Vitalis, and Amedeo Caflisch. A scalable algorithm to order and annotate continuous observations reveals the metastable states visited by dynamical systems. *Computer Physics Communications*, 184(11):2446–2453, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002038.

Bury:2015:NEM

[BvH15] M. Bury and A. van Hameren. Numerical evaluation of multi-gluon amplitudes for high energy factorization. *Computer Physics Communications*, 196(??):592–598, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002684.

Block:2010:MGA

[BVP10] Benjamin Block, Peter Virnau, and Tobias Preis. Multi-GPU accelerated multi-spin Monte Carlo simulations of the 2D Ising model. *Computer Physics Communications*, 181(9):1549–1556, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001463.

Brenes:2019:MPI

[BVSG19] Marlon Brenes, Vipin Kerala Varma, Antonello Scardicchio, and Ivan Girotto. Massively parallel implementation and approaches to simulate quantum dynamics using Krylov subspace techniques. *Computer Physics Communications*, 235(??):477–488, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303060.

Beyer:2011:SSV

[BW11] Frank Beyer and Martin Weigel. Spin stiffness of vector spin glasses. *Computer Physics Communications*, 182(9):1883–1887, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004935.

Berg:2012:FCL

[BW12a] Bernd A. Berg and Hao Wu. Fortran code for SU(3) lattice gauge theory with and without MPI checkerboard parallelization. *Computer Physics Communications*, 183(10):2145–2157, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001269.

Bergner:2012:AAM

[BW12b] Georg Bergner and Jaïr Wuilloud. Acceleration of the Arnoldi method and real eigenvalues of the non-Hermitian Wilson–Dirac operator. *Computer Physics Communications*, 183(2):299–304, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003353.

Brown:2015:ITI

[BW15] Aaron H. Brown and Tiffany R. Walsh. An improved TIGER2 implementation for NAMD suitable for the Blue Gene architecture. *Computer Physics Communications*, 192(??):278–281, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000831.

Barrett:2016:SFP

[BW16] Christopher Barrett and Lin-Wang Wang. A systematic fitting procedure for accurate force field models to reproduce ab initio phonon spectra of nanostructures. *Computer Physics Communications*, 200(??):27–36, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003999.

Barash:2017:GAP

[BWB+17] Lev Yu. Barash, Martin Weigel, Michal Borovský, Wolfhard Janke, and Lev N. Shchur. GPU accelerated population annealing algorithm. *Computer Physics Communications*, 220(??):341–350, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302023.

Brown:2011:IMD

[BWPT11] W. Michael Brown, Peng Wang, Steven J. Plimpton, and Arnold N. Tharrington. Implementing molecular dynamics on hybrid high performance computers — short range forces. *Computer Physics Communications*, 182(4):898–911, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005102.

Baral:2019:DLS

[BWWM19] Suman Baral, Travis Whyte, Walter Wilcox, and Ronald B. Morgan. Disconnected loop subtraction methods in lattice QCD. *Computer Physics Communications*, 241(??):64–79, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930089X.

Brown:2013:IMD

[BY13] W. Michael Brown and Masako Yamada. Implementing molecular dynamics on hybrid high performance computers — three-body potentials. *Computer Physics Communications*, 184(12):2785–2793, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002634.

Buaria:2017:HSP

[BY17] D. Buaria and P. K. Yeung. A highly scalable particle tracking algorithm using partitioned global address space (PGAS) programming for extreme-scale turbulence simulations. *Computer Physics Communications*, 221(??):246–258, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302680.

Comesana:2013:SSP

[CAGL13] E. Comesaña, M. Aldegunde, and A. J. Garcia-Loureiro. Simulation of the spin polarization and the charge transport in Zener tunnel junctions based on ferromagnetic GaAs and ZnO. *Computer Physics Communications*, 184(3):746–756, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003864.

Cai:2011:CSB

[Cai11] Liang-Wu Cai. On the computation of spherical Bessel functions of complex arguments. *Computer Physics Communications*, 182(3):663–668, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004650.

Chaabane:2011:ATD

[CAN11] Raoudha Chaabane, Faouzi Askri, and Sassi Ben Nasrallah. Analysis of two-dimensional transient conduction-radiation problems in an anisotropically scattering participating enclosure using the lattice Boltzmann method and the control volume finite element method. *Computer Physics Communications*, 182(7):1402–1413, July 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000841.

Caplan:2013:NNS

[Cap13] R. M. Caplan. NLSEmagic: Nonlinear Schrödinger equation multi-dimensional Matlab-based GPU-accelerated integrators using compact high-order schemes. *Computer Physics Communications*, 184(4):1250–1271, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004067.

Carasco:2010:MODa

[Car10a] C. Carasco. MCNP output data analysis with ROOT (MODAR). *Computer Physics Communications*, 181(6):1161–1166, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000055X.

Carasco:2010:MODb

[Car10b] C. Carasco. MCNP output data analysis with ROOT (MODAR). *Computer Physics Communications*, 181(12):2210–2211, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000322X.

Carasco:2016:CNM

[Car16] C. Carasco. COuntLOss in NEutron multiplicity assessment (COLONEMA). *Computer Physics Communications*, 200(??):285–290, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004051.

Casperson:2012:IIB

[Cas12] R. J. Casperson. IBAR: Interacting boson model calculations for large system sizes. *Computer Physics Communications*, 183(4):1029–1035, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004127.

Charsooghi:2011:MPC

[CATK11] Mohammad A. Charsooghi, Ehsan A. Akhlaghi, Sharareh Tavaddod, and H. R. Khalesifard. A Matlab program to calculate translational and rotational diffusion coefficients of a single particle. *Computer Physics Communications*, 182(2):400–408, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003620.

Cardoso:2013:GPG

[CB13a] Nuno Cardoso and Pedro Bicudo. Generating SU(N_c) pure gauge lattice QCD configurations on GPUs with CUDA. *Computer Physics Communications*, 184(3):509–518, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003347.

Caruntu:2013:APS

[CB13b] Bogdan Caruntu and Constantin Bota. Approximate polynomial solutions of the nonlinear Lane–Emden type equations arising in astrophysics using the squared remainder minimization method. *Computer Physics Communications*, 184(7):1643–1648, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000647.

Cardall:2015:GBO

[CB15a] Christian Y. Cardall and Reuben D. Budiardja. GenASiS basics: Object-oriented utilitarian functionality for large-scale physics simulations. *Computer Physics Communications*, 196(??):506–534, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002453.

Chen:2015:SKP

[CB15b] Ziguang Chen and Florin Bobaru. Selecting the kernel in a peridynamic formulation: a study for transient heat diffusion. *Computer Physics Communications*, 197(??):51–60, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002908.

Cheng:2015:JHN

[CB15c] Xiang Cheng and Stefan Boettcher. Jamming in hierarchical networks. *Computer Physics Communications*, 196(??):19–26, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001873.

Ciaramella:2015:SFS

[CB15d] G. Ciaramella and A. Borzì. SKRYN: a fast semismooth-Krylov–Newton method for controlling Ising spin systems. *Computer Physics Communications*, 190(??):213–223, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000156.

Ciaramella:2016:LCS

[CB16a] G. Ciaramella and A. Borzì. A LONE code for the sparse control of quantum systems. *Computer Physics Communications*, 200(??):312–323, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004105.

Cooper:2016:PBM

[CB16b] Christopher D. Cooper and Lorena A. Barba. Poisson–Boltzmann model for protein-surface electrostatic interactions and grid-convergence study using the PyGBe code. *Computer Physics Communications*, 202(??):23–32, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004579.

Cardall:2017:GNB

[CB17] Christian Y. Cardall and Reuben D. Budiardja. GenASiS Basics: Object-oriented utilitarian functionality for large-scale physics simulations (version 2). *Computer Physics Communications*, 214(??):247–248, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300097.

Cardall:2018:GNM

[CB18] Christian Y. Cardall and Reuben D. Budiardja. GenASiS mathematics: Object-oriented manifolds, operations, and solvers for large-scale physics simulations. *Computer Physics Communications*, 222(??):384–412, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303429.

Colagrossi:2012:PPA

[CBAM12] Andrea Colagrossi, B. Bouscasse, M. Antuono, and S. Marrone. Particle packing algorithm for SPH schemes. *Computer Physics Communications*, 183(8):1641–1653, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001051.

Clark:2010:SLQ

[CBB+10] M. A. Clark, R. Babich, K. Barros, R. C. Brower, and C. Rebbi. Solving lattice QCD systems of equations using mixed precision solvers on GPUs. *Computer Physics Communications*, 181(9):1517–1528, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001426.

Cooper:2014:BES

[CBB14] Christopher D. Cooper, Jaydeep P. Bardhan, and L. A. Barba. A biomolecular electrostatics solver using Python, GPUs and boundary elements that can handle solvent-filled cavities and Stern layers. *Computer Physics Communications*, 185(3):720–729, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003731.

Clay:2017:DCD

[CBGY17] M. P. Clay, D. Buaria, T. Gotoh, and P. K. Yeung. A dual communicator and dual grid-resolution algorithm for petascale simulations of turbulent mixing at high Schmidt number. *Computer Physics Communications*, 219(??):313–328, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301911.

Clay:2018:GAP

[CBYG18] M. P. Clay, D. Buaria, P. K. Yeung, and T. Gotoh. GPU acceleration of a petascale application for turbulent mixing at high Schmidt number using OpenMP 4.5. *Computer Physics Communications*, 228(??):100–114, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300596.

Carrettoni:2010:GNT

[CC10a] M. Carrettoni and O. Cremonesi. Generation of noise time series with arbitrary power spectrum. *Computer Physics Communications*, 181(12):1982–1985, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003486.

Cho:2010:WFM

[CC10b] Min Hyung Cho and Wei Cai. A Wideband Fast Multipole Method for the two-dimensional complex Helmholtz equation. *Computer Physics Communications*, 181(12):2086–2090, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003553.

Cho:2012:RWW

[CC12] Min Hyung Cho and Wei Cai. Revision of wFMM — a Wideband Fast Multipole Method for the two-dimensional complex Helmholtz equation. *Computer Physics Communications*, 183(2):446–447, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003420.

Chen:2014:ECC

[CC14] G. Chen and L. Chacón. An energy- and charge-conserving, nonlinearly implicit, electromagnetic 1D-3V Vlasov–Darwin particle-in-cell algorithm. *Computer Physics Communications*, 185(10):2391–2402, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465514001647.

Chen:2015:MDE

[CC15] G. Chen and L. Chacón. A multi-dimensional, energy- and charge-conserving, nonlinearly implicit, electromagnetic Vlasov–Darwin particle-in-cell algorithm. *Computer Physics Communications*, 197(??):73–87, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002921.

Chakraborty:2016:MUI

[CC16] Souvik Chakraborty and Rajib Chowdhury. Modelling uncertainty in incompressible flow simulation using Galerkin based generalized ANOVA. *Computer Physics Communications*, 208(??):73–91, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302326.

Coradeschi:2019:RTM

[CC19] F. Coradeschi and T. Cridge. reSolve — a transverse momentum resummation tool. *Computer Physics Communications*, 238(??):262–294, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304168.

Canelas:2016:SDM

[CCD+16] Ricardo B. Canelas, Alejandro J. C. Crespo, Jose M. Domínguez, Rui M. L. Ferreira, and Moncho Gómez-Gesteira. SPH-DCDEM model for arbitrary geometries in free surface solid-fluid flows. *Computer Physics Communications*, 202(??):131–140, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000254.

Cabellos:2011:SWO

[CCdC+11] Luis Cabellos, Isabel Campos, Enol Fernández del Castillo, Michal Owsiak, Bartek Palak, and Marcin Plóciennik. Scientific workflow orchestration interoperating HTC and HPC resources. *Computer Physics Communications*, 182(4):890–897, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005096.

Colo:2013:SCR

[CCGC13] Gianluca Colò, Ligang Cao, Nguyen Van Giai, and Luigi Capelli. Self-consistent RPA calculations with Skyrme-type interactions: the skyrme_rpa program. *Computer Physics Communications*, 184(1):142–161, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002627.

Chu:2011:ABC

[CCHL11] Yuchuan Chu, Yong Cao, Xiaoming He, and Min Luo. Asymptotic boundary conditions with immersed finite elements for interface magnetostatic/electrostatic field problems with open boundary. *Computer Physics Communications*, 182(11):2331–2338, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002372.

Chen:2023:CSI

[CCK23] Ruyun Chen, Juan Chen, and Xuesong Kuang. Comment on 'Symbolic integration of a product of two spherical Bessel functions with an additional exponential and polynomial factor' by B. Gebremariam, T. Duguet and S. K. Bogner. *Computer Physics Communications*, 282(??):Article 108498, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552200217X. See [GDB10].

Chen:2015:BOM

[CCL15] Rong-Bin Chen, Yu-Huang Chiu, and Ming-Fa Lin. Beating oscillations of magneto-optical spectra in simple hexagonal graphite. *Computer Physics Communications*, 189(??):60–65, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004147.

Chen:2018:GPF

[CCL18] Jen-Hao Chen, Ren-Chuen Chen, and Jinn-Liang Liu. A GPU Poisson–Fermi solver for ion channel simulations. *Computer Physics Communications*, 229(??):99–105, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301024.

Cai:2018:PFE

[CCLL18] Yong Cai, Xiangyang Cui, Guangyao Li, and Wenyang Liu. A parallel finite element procedure for contact-impact problems using edge-based smooth triangular element and GPU. *Computer Physics Communications*, 225(??):47–58, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304113.

Charbonnier:2012:CCR

[CCM12] Aldée Charbonnier, Céline Combet, and David Maurin. clumpy: a code for γ-ray signals from dark matter structures. *Computer Physics Communications*, 183(3):656–668, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003493.

Cowan:2017:RAF

[CCN17] G. A. Cowan, D. C. Craik, and M. D. Needham. RapidSim: an application for the fast simulation of heavy-quark hadron decays. *Computer Physics Communications*, 214(??):239–246, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300413.

Chien:2010:TSC

[CCW10] C.-S. Chien, S.-L. Chang, and Biao Wu. Two-stage continuation algorithms for Bloch waves of Bose–Einstein condensates in optical lattices. *Computer Physics Communications*, 181(10):1727–1737, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002079.

Chen:2011:USF

[CCWL11] Chien-Fu Chen, An-Chung Cheng, Yi-Duen Wang, and Chai-Yu Lin. Universal scaling functions of a dissipative Manna model. *Computer Physics Communications*, 182(1):226–228, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002663.

Chen:2015:CPP

[CCXC15] Xiang Chen, Aleksandr Chernatynskiy, Liming Xiong, and Youping Chen. A coherent phonon pulse model for transient phonon thermal transport. *Computer Physics Communications*, 195(??):112–116, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001861.

Choi:2018:PPB

[CCY18] Wonqook Choi, Kihyeon Cho, and Insung Yeo. Performance profiling for brachytherapy applications. *Computer Physics Communications*, 226(??):180–186, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300055.

Chen:2012:SEH

[CD12] Xi Chen and Z. J. Ding. Solving extra-high-order Rubik's Cube problem by a dynamic simulated annealing. *Computer Physics Communications*, 183(8):1658–1663, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001087.

Charpentier:2015:HOA

[CD15] Isabelle Charpentier and Claude Dal Cappello. Higher-order automatic differentiation of mathematical functions. *Computer Physics Communications*, 189(??):66–71, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004305.

Camporeale:2016:VSD

[CDBM16] E. Camporeale, G. L. Delzanno, B. K. Bergen, and J. D. Moulton. On the velocity space discretization for the Vlasov–Poisson system: Comparison between implicit Hermite spectral and Particle-in-Cell methods. *Computer Physics Communications*, 198(??):47–58, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003409.

Carli:2014:MPI

[CDdM14] H. Carli, L. G. S. Duarte, and L. A. C. P. da Mota. A Maple package for improved global mapping forecast. *Computer Physics Communications*, 185(3):1115–1129, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300413X.

Corno:2016:ISL

[CdFDS16] Jacopo Corno, Carlo de Falco, Herbert De Gersemo, and Sebastian Schöps. Isogeometric simulation of Lorentz detuning in superconducting accelerator cavities. *Computer Physics Communications*, 201(??):1–7, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004373.

Chen:2012:RTI

[CDL+12] Bokui Chen, Chuanfei Dong, Yike Liu, Wei Tong, Wenyao Zhang, Jie Liu, and Binghong Wang. Real-time information feedback based on a sharp decay weighted function. *Computer Physics Communications*, 183(10):2081–2088, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001786.

Chiron:2019:FAS

[CdLOL19] L. Chiron, M. de Leffe, G. Oger, and D. Le Touzé. Fast and accurate SPH modelling of 3D complex wall boundaries in viscous and non viscous flows. *Computer Physics Communications*, 234(??):93–111, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465518302832.

Castro:2011:UOO

[CDMCN11] María Eugenia Castro, Javier Díaz, Camelia Muñoz-Caro, and Alfonso Niño. A uniform object-oriented solution to the eigenvalue problem for real symmetric and Hermitian matrices. *Computer Physics Communications*, 182(9):2059–2064, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004686.

Crespo:2015:DOS

[CDR+15] A. J. C. Crespo, J. M. Domínguez, B. D. Rogers, M. Gómez-Gesteira, S. Longshaw, R. Canelas, R. Vacondio, A. Barreiro, and O. García-Feal. DualSPHysics: Open-source parallel CFD solver based on Smoothed Particle Hydrodynamics (SPH). *Computer Physics Communications*, 187(??):204–216, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003397.

Capuzzo-Dolcetta:2013:PCD

[CDS13a] R. Capuzzo-Dolcetta and M. Spera. A performance comparison of different graphics processing units running direct N-body simulations. *Computer Physics Communications*, 184(11):2528–2539, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002336.

Chowdhury:2013:EAT

[CDS+13b] Abhishek Chowdhury, Asit K. De, Sangita De Sarkar, A. Harindranath, Jyotirmoy Maiti, Santanu Mondal, and Anwesa Sarkar. Exploring autocorrelations in two-flavor Wilson Lattice QCD using DD-HMC algorithm. *Computer Physics Communications*, 184(5):1439–1445, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000295.

Carapelle:2011:HMC

[CDSG11] Alain Carapelle, Jean-Marc Defise, David Strivay, and Henri-Pierre Garnir. Handheld modern computer brings new features to portable X-ray fluorescence coating thickness measurement device. *Computer Physics Communications*, 182(6):1304–1306, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000865`.

Consiglio:2018:PR

[CdSM+18] R. Consiglio, P. F. de Salas, G. Mangano, G. Miele, S. Pastor, and O. Pisanti. PArthENoPE reloaded. *Computer Physics Communications*, 233(??):237–242, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302303`.

Carlsson:2010:SSC

[CDTV10] B. G. Carlsson, J. Dobaczewski, J. Toivanen, and P. Veselý. Solution of self-consistent equations for the N^3 LO nuclear energy density functional in spherical symmetry. The program hosphe (v1.02). *Computer Physics Communications*, 181(9):1641–1657, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001773`.

Cardoso:2016:ICL

[CECGS16] Nuno Cardoso, David Emmanuel-Costa, Nuno Gonçalves, and C. Simões. SOSpin, a C++ library for Yukawa decomposition in SO($2N$) models. *Computer Physics Communications*, 203(??):178–200, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516000308`.

Crouseilles:2016:APS

[CEF16] Nicolas Crouseilles, Lukas Einkemmer, and Erwan Faou. An asymptotic preserving scheme for the relativistic Vlasov–Maxwell equations in the classical limit. *Computer Physics Communications*, 209(??):13–26, December 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302302.

Crouseilles:2018:EID

[CEP18] Nicolas Crouseilles, Lukas Einkemmer, and Martina Prugger. An exponential integrator for the drift-kinetic model. *Computer Physics Communications*, 224(??):144–153, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303867.

Conte:2010:SNU

[CEPI10] D. Conte, E. Esposito, B. Paternoster, and L. Gr. Ixaru. Some new uses of the $\eta m(Z)$ functions. *Computer Physics Communications*, 181(1):128–137, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002574.

Carrazza:2016:QCF

[CEZ16] Stefano Carrazza, R. Keith Ellis, and Giulia Zanderighi. QCDLoop: a comprehensive framework for one-loop scalar integrals. *Computer Physics Communications*, 209(??):134–143, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302491.

Checinski:2016:MMF

[CF16] Jakub Checiński and Marek Frankowski. MAGE (M-file/Mif Automatic GEnerator): a graphical interface tool for automatic generation of Object Oriented Micromagnetic Framework configuration files and Matlab scripts for results analysis. *Computer Physics Communications*, 207(??):487–498, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302016.

Cota:2017:OGA

[CF17] Wesley Cota and Silvio C. Ferreira. Optimized Gillespie algorithms for the simulation of Markovian epidemic processes on large and heterogeneous networks. *Computer Physics*

Communications, 219(??):303–312, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301893.

Carles:2012:DIS

[CFCB12] Guillem Carles, Carme Ferran, Artur Carnicer, and Salvador Bosch. Design and implementation of a scene-dependent dynamically selfadaptable wavefront coding imaging system. *Computer Physics Communications*, 183(1):147–154, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002761.

Clauser:2019:FFO

[CFF19] C. F. Clauser, R. Farengo, and H. E. Ferrari. FOCUS: a full-orbit CUDA solver for particle simulations in magnetized plasmas. *Computer Physics Communications*, 234(??):126–136, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302753.

Cuoci:2015:OOO

[CFFR15] A. Cuoci, A. Frassoldati, T. Faravelli, and E. Ranzi. OpenSMOKE++: an object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms. *Computer Physics Communications*, 192(??):237–264, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000715.

Calvo:2010:SSE

[CFMR10] M. Calvo, J. M. Franco, J. I. Montijano, and L. Rández. Symmetric and symplectic exponentially fitted Runge–Kutta methods of high order. *Computer Physics Communications*, 181(12):2044–2056, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003103.

Conte:2013:MUF

[CFS13] Eric Conte, Benjamin Fuks, and Guillaume Serret. MadAnalysis 5, a user-friendly framework for collider phenomenology. *Computer Physics Communications*, 184(1):222–256, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002950`.

Chang:2014:CPP

[CFSK14] Yuan-Pin Chang, Frank Filsinger, Boris G. Sartakov, and Jochen Küpper. CMIstark: Python package for the stark-effect calculation and symmetry classification of linear, symmetric and asymmetric top wavefunctions in dc electric fields. *Computer Physics Communications*, 185(1):339–349, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003019`.

Chilenski:2017:EME

[CFW17] M. A. Chilenski, I. C. Faust, and J. R. Walk. eqtools: Modular, extensible, open-source, cross-machine Python tools for working with magnetic equilibria. *Computer Physics Communications*, 210(??):155–162, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551630282X`.

Contino:2014:EIH

[CGG+14] Roberto Contino, Margherita Ghezzi, Christophe Grojean, Margarete Mühlleitner, and Michael Spira. eHDECAY: an implementation of the Higgs effective Lagrangian into HDECAY. *Computer Physics Communications*, 185(12):3412–3423, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002896`.

Cullen:2011:GLO

[CGH+11] G. Cullen, J.-Ph. Guillet, G. Heinrich, T. Kleinschmidt, E. Pilon, T. Reiter, and M. Rodgers. Golem95C: a library for one-loop integrals with complex masses. *Computer Physics Communications*, 182(10):2276–2284, October 2011. CO-

DEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001810.

Cimrak:2014:EIE

[CGJ14] I. Cimrák, M. Gusenbauer, and I. Jancigová. An ESPResSo implementation of elastic objects immersed in a fluid. *Computer Physics Communications*, 185(3):900–907, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004256.

Castro:2017:JFA

[CGM17] Manuel J. Castro, José M. Gallardo, and Antonio Marquina. Jacobian-free approximate solvers for hyperbolic systems: Application to relativistic magnetohydrodynamics. *Computer Physics Communications*, 219(??):108–120, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301558.

Clark:2017:MMN

[CGO17] D. B. Clark, E. Godat, and F. I. Olness. ManeParse: a Mathematica reader for parton distribution functions. *Computer Physics Communications*, 216(??):126–137, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300802.

Chu:2014:AAF

[CGRB14] Yanbiao Chu, Pierre Gautreau, Tarek Ragab, and Cemal Basaran. An accelerated algorithm for full band electron-phonon scattering rate computation. *Computer Physics Communications*, 185(12):3392–3397, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002768.

Chaudhury:2018:ASM

[CGSB18] Bhaskar Chaudhury, Anurag Gupta, Henil Shah, and Saumya Bhadani. Accelerated simulation of microwave breakdown in gases on Xeon Phi based cluster-application to self-organized plasma pattern formation. *Computer Physics*

Communications, 229(??):20–35, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300961.

Chowdhury:2013:SPS

[CGV13] Debtosh Chowdhury, Raghuveer Garani, and Sudhir K. Vempati. SuSeFLAV 1.2: Program for supersymmetric mass spectra with seesaw mechanism and rare lepton flavor violating decays. *Computer Physics Communications*, 184(3):899–918, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003748.

Carter:2011:SGP

[CH11a] Jonathon Carter and Gudrun Heinrich. SecDec: a general program for sector decomposition. *Computer Physics Communications*, 182(7):1566–1581, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001196.

Colberg:2011:HAS

[CH11b] Peter H. Colberg and Felix Höfling. Highly accelerated simulations of glassy dynamics using GPUs: Caveats on limited floating-point precision. *Computer Physics Communications*, 182(5):1120–1129, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000294.

Cazeaux:2019:PMT

[CH19] P. Cazeaux and J. S. Hesthaven. Projective multiscale time-integration for electrostatic particle-in-cell methods. *Computer Physics Communications*, 236(??):34–50, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303606.

Chen:2011:MSP

[CHA11] Ke-Jung Chen, Alexander Heger, and Ann S. Almgren. Multidimensional simulations of pair-instability supernovae.

Computer Physics Communications, 182(1):254–256, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002092.

Charpentier:2016:OHO

[Cha16] Isabelle Charpentier. Optimized higher-order automatic differentiation for the Faddeeva function. *Computer Physics Communications*, 205(??):132–137, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300984.

Chandar:2019:OIS

[Cha19] Dominic D. J. Chandar. On overset interpolation strategies and conservation on unstructured grids in OpenFOAM. *Computer Physics Communications*, 239(??):72–83, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300153.

Cheng:2011:ODS

[CHC+11] K.-W. Cheng, C.-T. Hung, M.-H. Chiang, F.-N. Hwang, and J.-S. Wu. One-dimensional simulation of nitrogen dielectric barrier discharge driven by a quasi-pulsed power source and its comparison with experiments. *Computer Physics Communications*, 182(1):164–166, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002055.

Cecilia:2017:ECE

[CHDCJA17] José M. Cecilia, A. M. Hernández-Díaz, Pedro Castrillo, and J. F. Jiménez-Alonso. Enhanced calculation of eigen-stress field and elastic energy in atomistic interdiffusion of alloys. *Computer Physics Communications*, 211(??):23–30, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301941.

Cheng:2010:LAM

[CHDF10] Jie Cheng, Yanqing Hu, Zengru Di, and Ying Fan. Local adaptive mechanism and hierarchic social entropy in opinion formation on complex networks. *Computer Physics Communications*, 181(10):1697–1701, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000189X.

Chetty:2011:NMS

[Che11] N. Chetty. New modalities for scientific engagement in Africa — the case for computational physics. *Computer Physics Communications*, 182(9):2065–2070, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003772.

Cheviakov:2017:SCE

[Che17] Alexei F. Cheviakov. Symbolic computation of equivalence transformations and parameter reduction for nonlinear physical models. *Computer Physics Communications*, 220(??):56–73, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301959. See comment [Mel19].

Chiu:2011:EPC

[CHH+11] Y.-M. Chiu, C.-T. Hung, F.-N. Hwang, M.-H. Chiang, J.-S. Wu, and S.-H. Chen. Effect of plasma chemistry on the simulation of helium atmospheric-pressure plasmas. *Computer Physics Communications*, 182(1):167–169, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001979.

Carter:2018:GPS

[CHNS18] Francisco Carter, Nancy Hitschfeld, Cristóbal A. Navarro, and Rodrigo Soto. GPU parallel simulation algorithm of Brownian particles with excluded volume using Delaunay triangulations. *Computer Physics Communications*, 229(??):148–161, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301061.

Chou:2011:KBE

[Cho11] Chung-I Chou. A Knowledge-based Evolution Algorithm approach to political districting problem. *Computer Physics Communications*, 182(1):209–212, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002870.

Christensen:2018:DHT

[Chr18] Neil Christensen. Diagonalizing the Hamiltonian of $\lambda\phi^4$ theory in 2 space-time dimensions. *Computer Physics Communications*, 222(??):167–188, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303405.

Cheng:2015:PSM

[CHW+15] Hai-Xia Cheng, Yao-Wen Hu, Xiao-Xu Wang, Guo-Hua Zhang, Zhi-Wei An, Zhen-Feng Zhang, Biao Zhang, Tao Zhou, Ping Qian, Ying Liu, and Nan-Xian Chen. The phase stability, magnetic and vibrational properties of $A_2Ni_{21}B_6$ (A = Th, U) and $Ce_3Pd_{20}Si_6$. *Computer Physics Communications*, 193(??):72–77, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500123X.

Crouseilles:2018:MPC

[CHZ18] Nicolas Crouseilles, Sever A. Hirstoaga, and Xiaofei Zhao. Multiscale Particle-in-Cell methods and comparisons for the long-time two-dimensional Vlasov–Poisson equation with strong magnetic field. *Computer Physics Communications*, 222(??):136–151, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730334X.

Czyz:2011:EMC

[CI11] Henryk Czyz and Sergiy Ivashyn. EKHARA: a Monte Carlo generator for $e^+e^- \to e^+e^-\pi^0$ and $e^+e^- \to e^+e^-\pi^+\pi^-$ processes. *Computer Physics Communications*, 182(6):1338–1349, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000671.

Cipolla:2011:IUV

[Cip11] Sam J. Cipolla. ISICS2011, an updated version of ISICS: a program for calculation K-, L-, and M-shell cross sections from PWBA and ECPSSR theories using a personal computer. *Computer Physics Communications*, 182 (11):2439–2440, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002141.

Cipolla:2013:CIP

[Cip13] Sam J. Cipolla. Corrected ISICS program versions available due to a minor calculation error involving M3 X-ray production cross sections. *Computer Physics Communications*, 184(9):2230–2231, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300074X.

Catterall:2012:OOC

[CJ12] Simon Catterall and Anosh Joseph. An object oriented code for simulating supersymmetric Yang–Mills theories. *Computer Physics Communications*, 183(6):1336–1353, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000537.

Chang:2011:ESQ

[CJH11] Tay-Rong Chang, Horng-Tay Jeng, and Chen-Shiung Hsue. Electronic structures of quasi-one-dimensional ferrimagnetic insulator $Ca_3Co_2O_6$. *Computer Physics Communications*, 182(1):93–95, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003073.

Chen:2017:SFE

[CJJ+17] Zhanghui Chen, Weile Jia, Xiangwei Jiang, Shu-Shen Li, and Lin-Wang Wang. SGO: a fast engine for ab initio atomic structure global optimization by differential evolution. *Computer Physics Communications*, 219(??):35–44, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301352.

Ciappina:2012:SSC

[CK12] M. F. Ciappina and T. Kirchner. SymbMat: Symbolic computation of quantum transition matrix elements. *Computer Physics Communications*, 183(8):1832–1840, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001257.

Cunningham:2018:CSG

[CK18] William J. Cunningham and Dmitri Krioukov. Causal set generator and action computer. *Computer Physics Communications*, 233(??):123–133, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302169.

Czyz:2019:EUE

[CK19] Henryk Czyz and Patrycja Kisza. EKHARA 3.0: an update of the EKHARA Monte Carlo event generator. *Computer Physics Communications*, 234(??):245–255, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302789.

Cichy:2013:LHA

[CKCS13] Krzysztof Cichy, Agnieszka Kujawa-Cichy, and Marcin Szyniszewski. Lattice Hamiltonian approach to the massless Schwinger model: Precise extraction of the mass gap. *Computer Physics Communications*, 184(7):1666–1672, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000672.

Chojnacki:2012:TTH

[CKFB12] Mikolaj Chojnacki, Adam Kisiel, Wojciech Florkowski, and Wojciech Broniowski. THERMINATOR 2: THERMal heavy I o N gener ATOR 2. *Computer Physics Communications*, 183(3):746–773, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465511003808.

Cho:2011:CPB

[CKhN11] Kihyeon Cho, Junghyun Kim, and Soo hyeon Nam. Collider physics based on e-Science paradigm of experiment-computing-theory. *Computer Physics Communications*, 182(9):1756–1759, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005084.

Cullen:2011:SFL

[CKJR11] G. Cullen, M. Koch-Janusz, and T. Reiter. spinney: a Form library for helicity spinors. *Computer Physics Communications*, 182(11):2368–2387, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002177.

Chun:2013:GPP

[CKK+13] Kyungwon Chun, Huioon Kim, Hyounggyu Kim, Kil Su Jung, and Youngjoo Chung. GMES: a Python package for solving Maxwell's equations using the FDTD method. *Computer Physics Communications*, 184(4):1272–1279, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004079.

Cai:2010:CCN

[CKLM10] Weiwei Cai, Laura Kranendonk, Tonghun Lee, and Lin Ma. Characterization of composite nanoparticles using an improved light scattering program for coated spheres. *Computer Physics Communications*, 181(5):978–984, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000470.

Ciappina:2010:MCE

[CKS10] M. F. Ciappina, T. Kirchner, and M. Schulz. Monte Carlo event generators in atomic collisions: a new tool to tackle the few-body dynamics. *Computer Physics Communications*, 181(4):813–820, April 2010. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004068.

Cebrecos:2019:FET

[CKSM+19] Alejandro Cebrecos, Dimitri Krattiger, Victor J. Sánchez-Morcillo, Vicent Romero-García, and Mahmoud I. Hussein. The finite-element time-domain method for elastic band-structure calculations. *Computer Physics Communications*, 238(??):77–87, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304387.

Calderin:2017:KGE

[CKT17] L. Calderín, V. V. Karasiev, and S. B. Trickey. Kubo–Greenwood electrical conductivity formulation and implementation for projector augmented wave datasets. *Computer Physics Communications*, 221(??):118–142, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302539.

Chen:2010:NME

[CL10] Jen-Hao Chen and Jinn-Liang Liu. A numerical method for exact diagonalization of semiconductor quantum dot model. *Computer Physics Communications*, 181(5):937–946, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000196.

Cheng:2011:MCM

[CL11] Guoxin Cheng and Lie Liu. Monte Carlo modeling of secondary electron emission and its incorporation in particle simulations of electron-surface interaction. *Computer Physics Communications*, 182(6):1295–1303, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000798.

Cosden:2013:HAC

[CL13] Ian A. Cosden and Jennifer R. Lukes. A hybrid atomistic-continuum model for fluid flow using LAMMPS and Open-

FOAM. *Computer Physics Communications*, 184(8):1958–1965, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001069.

Chiodo:2014:MSO

[CL14] Sandro Giuseppe Chiodo and Monica Leopoldini. MolSOC: a spin-orbit coupling code. *Computer Physics Communications*, 185(2):676–683, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003421.

Cao:2015:CMF

[CL15a] Danping Cao and Wenyuan Liao. A computational method for full waveform inversion of crosswell seismic data using automatic differentiation. *Computer Physics Communications*, 188(??):47–58, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003725.

Chugunov:2015:PII

[CL15b] Svyatoslav Chugunov and Changying Li. Parallel implementation of inverse adding-doubling and Monte Carlo multilayered programs for high performance computing systems with shared and distributed memory. *Computer Physics Communications*, 194(??):64–75, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000892.

Cundy:2016:EIO

[CL16] Nigel Cundy and Weonjong Lee. The eigSUMR inverter for overlap fermions. *Computer Physics Communications*, 203(??):1–17, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003665.

Cruz:2011:HOE

[CLB11] Felipe A. Cruz, Simon K. Layton, and L. A. Barba. How to obtain efficient GPU kernels: An illustration using FMM & FGT algorithms. *Computer Physics Communications*, 182(10):2084–2098, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100155X.

Chan:2014:ECM

[CLC14] Tzu-Liang Chan, Alex J. Lee, and James R. Chelikowsky. An effective capacitance model for computing the electronic properties of charged defects in crystals. *Computer Physics Communications*, 185(6):1564–1569, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000642.

Cruz-Lopez:2018:AAL

[CLF18] Carlos-Antonio Cruz-López and Juan-Luis François. An alternative algorithm for the linearization process of transmutation and decay networks. *Computer Physics Communications*, 231(??):122–139, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301401.

Cao:2017:PAI

[CLH+17] Yang Cao, Chun Liu, Yuehui Huang, Tieqiang Wang, Chenjun Sun, Yue Yuan, Xinsong Zhang, and Shuyun Wu. Parallel algorithms for islanded microgrid with photovoltaic and energy storage systems planning optimization problem: Material selection and quantity demand optimization. *Computer Physics Communications*, 211(??):45–53, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301916.

Cao:2019:HAN

[CLHL19] Thanh-Xuan H. Cao, Duy-Nhat Ly, Ngoc-Tram D. Hoang, and Van-Hoang Le. High-accuracy numerical calculations of the bound states of a hydrogen atom in a constant magnetic field with arbitrary strength. *Computer Physics Communications*, 240(??):138–151, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL `http://www.sciencedirect.com/science/article/pii/S0010465519300657`.

Chen:2012:RFT

[CLJ12] Liang Chen, Cheng Lv, and Xunya Jiang. A re-formulation of the transfer matrix method for calculating wave-functions in higher dimensional disordered open systems. *Computer Physics Communications*, 183(12):2513–2518, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002275`.

Choi:2011:IGC

[CLKK11] Jaewon Choi, Gyuchang Lim, Soo Yong Kim, and Kyungsik Kim. Information of group-correlations in Korean financial market. *Computer Physics Communications*, 182(1):219–222, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003061`.

Chen:2016:PEC

[CLL16] Ren-Chuen Chen, Chun-Hsien Li, and Jinn-Liang Liu. A posteriori error control in numerical simulations of semiconductor nanodevices. *Computer Physics Communications*, 207(??):287–297, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302089`.

Cha:2011:WDW

[CLLK11] Moon-Yong Cha, Jae Woo Lee, Deok-Sun Lee, and Doo Hwan Kim. Wealth dynamics in world trade. *Computer Physics Communications*, 182(1):216–218, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003449`.

Chau:2011:MAS

[CLW11] S. W. Chau, S. Y. Lu, and P. J. Wang. Modeling of axis-symmetric steam plasma flow in a non-transferred torch. *Computer Physics Communications*, 182(1):152–154, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003024`.

Cheng:2011:IRE

[CLY11] Hui-Wen Cheng, Yiming Li, and Jung-Yen Yang. Investigation of Raman enhancement in hydrothermally roughened SERS-active substrates. *Computer Physics Communications*, 182(1):260–262, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002584.

Cai:2010:ACT

[CM10a] Weiwei Cai and Lin Ma. Applications of critical temperature in minimizing functions of continuous variables with simulated annealing algorithm. *Computer Physics Communications*, 181(1):11–16, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002392.

Cai:2010:CAB

[CM10b] Weiwei Cai and Lin Ma. Comparison of approaches based on optimization and algebraic iteration for binary tomography. *Computer Physics Communications*, 181(12):1974–1981, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003498.

Crouseilles:2014:APS

[CM14a] Nicolas Crouseilles and Giovanni Manfredi. Asymptotic preserving schemes for the Wigner–Poisson–BGK equations in the diffusion limit. *Computer Physics Communications*, 185(2):448–458, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001963.

Czakon:2014:TPC

[CM14b] Michal Czakon and Alexander Mitov. Top++: a program for the calculation of the top-pair cross-section at hadron colliders. *Computer Physics Communications*, 185(11):2930–2938, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002264.

Chang:2015:SOE

[CM15] Y. C. Chang and Waleed E. Mahmoud. Simulation of optical excitation spectra of semiconductor nanowires within effective bond orbital model. *Computer Physics Communications*, 196(??):92–112, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002039.

Cantwell:2015:NOS

[CMC+15] C. D. Cantwell, D. Moxey, A. Comerford, A. Bolis, G. Rocco, G. Mengaldo, D. De Grazia, S. Yakovlev, J.-E. Lombard, D. Ekelschot, B. Jordi, H. Xu, Y. Mohamied, C. Eskilsson, B. Nelson, P. Vos, C. Biotto, R. M. Kirby, and S. J. Sherwin. Nektar++: an open-source spectral/*hp* element framework. *Computer Physics Communications*, 192(??):205–219, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000533.

CostaRibeiro:2011:DTK

[CMdB11] Leonardo Costa Ribeiro, Ricardo Machado Ruiz, Eduardo da Motta e Albuquerque, and Américo T. Bernardes. The diffusion of technological knowledge through interlaced networks. *Computer Physics Communications*, 182(9):1875–1878, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004789.

Chen:2011:NSP

[CMJ+11] C.-C. Chen, B. Moritz, C. J. Jia, S. Johnston, A. P. Sorini, L.-Q. Lee, K. Ko, and T. P. Devereaux. Numerical studies of photon-based spectroscopies on high-T_c superconductors. *Computer Physics Communications*, 182(1):106–108, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003085.

Ceriotti:2014:PPI

[CMM14] Michele Ceriotti, Joshua More, and David E. Manolopoulos. i-PI: a Python interface for ab initio path integral molecular dynamics simulations. *Computer Physics*

Communications, 185(3):1019–1026, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300372X.

Casas:2012:ECZ

[CMN12] Fernando Casas, Ander Murua, and Mladen Nadinic. Efficient computation of the Zassenhaus formula. *Computer Physics Communications*, 183(11):2386–2391, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200207X.

Costa:2017:EPD

[CMR17] B. V. Costa, L. A. S. Mól, and J. C. S. Rocha. Energy probability distribution zeros: a route to study phase transitions. *Computer Physics Communications*, 216(??):77–83, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300796.

Cardenas-Montes:2014:PPH

[CMRVVR+14] Miguel Cárdenas-Montes, Juan José Rodríguez-Vázquez, Miguel A. Vega-Rodríguez, Ignacio Sevilla-Noarbe, and Eusebio Sánchez Alvaro. Performance and precision of histogram calculation on GPUs: Cosmological analysis as a case study. *Computer Physics Communications*, 185(10):2558–2565, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002069.

Cardenas-Montes:2016:RSI

[CMRVVR16] Miguel Cárdenas-Montes, Juan José Rodríguez-Vázquez, and Miguel A. Vega-Rodríguez. Bin recycling strategy for improving the histogram precision on GPU. *Computer Physics Communications*, 204(??):55–63, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300649.

Cyrol:2017:FMT

[CMS17] Anton K. Cyrol, Mario Mitter, and Nils Strodthoff. FormTracer: A Mathematica tracing package using FORM. *Computer Physics Communications*, 219(??):346–352, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301662.

Cardenas-Montes:2018:VTR

[CMSN18] Miguel Cárdenas-Montes and Ignacio Sevilla-Noarbe. Voronoi tessellation for reducing the processing time of correlation functions. *Computer Physics Communications*, 222(??):158–166, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303399.

Chekanov:2014:PIO

[CMSV14] S. V. Chekanov, E. May, K. Strand, and P. Van Gemmeren. ProMC: Input-output data format for HEP applications using varint encoding. *Computer Physics Communications*, 185(10):2629–2635, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002215.

Cardenas-Montes:2014:GBS

[CMVRB+14] Miguel Cárdenas-Montes, Miguel A. Vega-Rodríguez, Christopher Bonnett, Ignacio Sevilla-Noarbe, Rafael Ponce, Eusebio Sánchez Alvaro, and Juan José Rodríguez-Vázquez. GPU-based shear-shear correlation calculation. *Computer Physics Communications*, 185(1):11–18, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300266X.

Cunha-Netto:2011:CBH

[CND11] A. G. Cunha-Netto and R. Dickman. Critical behavior of hard-core lattice gases: Wang–Landau sampling with adaptive windows. *Computer Physics Communications*, 182(3):719–725, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465510004923.

Castro:2010:HCR

[CNMC10a] M. E. Castro, A. Niño, and C. Muñoz-Caro. Heuristic computation of the rovibrational G matrix in optimized molecule-fixed axes. Gmat 2.1. *Computer Physics Communications*, 181(8):1471–1475, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001396.

Castro:2010:MAO

[CNMC10b] M. E. Castro, A. Niño, and C. Muñoz-Caro. A metaheuristic approach to the optimal definition of molecule-fixed axes in rovibrational Hamiltonians. *Computer Physics Communications*, 181(5):967–977, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000469.

Cunha:2014:UQT

[CNS+14] Americo Cunha, Jr., Rafael Nasser, Rubens Sampaio, Hélio Lopes, and Karin Breitman. Uncertainty quantification through the Monte Carlo method in a cloud computing setting. *Computer Physics Communications*, 185(5):1355–1363, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000198.

Cerda:2018:HST

[CNS+18] Mauricio Cerda, Cristóbal A. Navarro, Juan Silva, Scott R. Waitukaitis, Nicolás Mujica, and Nancy Hitschfeld. A high-speed tracking algorithm for dense granular media. *Computer Physics Communications*, 227(??):8–16, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300389.

Czerwinski:2011:TVL

[CO11] Fabian Czerwinski and Lene B. Oddershede. TimeSeriesStreaming.vi: LabVIEW program for reliable data streaming of large analog time series. *Computer Physics*

Communications, 182(2):485–489, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004200.

Campoli:2019:KKA

[COK19] L. Campoli, G. P. Oblapenko, and E. V. Kustova. KAPPA: Kinetic approach to physical processes in atmospheres library in C++. *Computer Physics Communications*, 236(??):244–267, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303643.

Colavecchia:2014:ASA

[Col14] F. D. Colavecchia. Accelerating spectral atomic and molecular collisions methods with graphics processing units. *Computer Physics Communications*, 185(7):1955–1964, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001064.

Corsetti:2014:OMM

[Cor14] Fabiano Corsetti. The orbital minimization method for electronic structure calculations with finite-range atomic basis sets. *Computer Physics Communications*, 185(3):873–883, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004207.

Cobanoglu:2011:OLE

[ÇÖSÜ11] Özgür Çobanoğlu, Erkcan Özcan, Saleh Sultansoy, and Gökhan Ünel. OPUCEM: a library with error checking mechanism for computing oblique parameters. *Computer Physics Communications*, 182(8):1732–1743, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001494.

Coufal:2013:MASa

[Cou13a] O. Coufal. A method for the accurate and smooth approximation of standard thermodynamic functions. *Computer Physics Communications*, 184(1):194–200, January 2013.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002810.

Coufal:2013:MASb

[Cou13b] O. Coufal. A method for the accurate and smooth approximation of standard thermodynamic functions. *Computer Physics Communications*, 184(7):1810–1811, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000799.

Cercos-Pita:2015:ANF

[CP15a] J. L. Cercos-Pita. AQUAgpusph, a new free 3D SPH solver accelerated with OpenCL. *Computer Physics Communications*, 192(??):295–312, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000909.

Chernatynskiy:2015:PTS

[CP15b] Aleksandr Chernatynskiy and Simon R. Phillpot. Phonon transport simulator (PhonTS). *Computer Physics Communications*, 192(??):196–204, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500017X.

Cercos-Pita:2018:NGF

[CPCDdM18] J. L. Cercos-Pita, I. R. Cal, D. Duque, and G. Sanjuán de Moreta. NASAL-Geom, a free upper respiratory tract 3D model reconstruction software. *Computer Physics Communications*, 223(??):55–68, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730348X.

Ciappina:2014:CCS

[CPHL14] M. F. Ciappina, J. A. Pérez-Hernández, and M. Lewenstein. ClassSTRONG: Classical simulations of strong field processes. *Computer Physics Communications*, 185(1):398–406, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300310X.

Cherfils:2012:JPS

[CPR12] J. M. Cherfils, G. Pinon, and E. Rivoalen. JOSEPHINE: a parallel SPH code for free-surface flows. *Computer Physics Communications*, 183(7):1468–1480, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000604.

Certik:2013:DRG

[CPV13] Ondrej Certík, John E. Pask, and Jirí Vackár. `dftatom`: a robust and general Schrödinger and Dirac solver for atomic structure calculations. *Computer Physics Communications*, 184(7):1777–1791, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000714.

Chekanov:2017:CPV

[CPW17] S. V. Chekanov, I. Pogrebnyak, and D. Wilbern. Cross-platform validation and analysis environment for particle physics. *Computer Physics Communications*, 220(??):91–96, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301996.

Chrzaszcz:2018:TLD

[CPWZ18] M. Chrzaszcz, T. Przedzinski, Z. Was, and J. Zaremba. TAUOLA of τ lepton decays — framework for hadronic currents, matrix elements and anomalous decays. *Computer Physics Communications*, 232(??):220–236, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301802.

Cieslinski:2012:DGA

[CR12] Jan L. Cieśliński and Boguslaw Ratkiewicz. Discrete gradient algorithms of high order for one-dimensional systems. *Computer Physics Communications*, 183(3):617–627, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003961.

Caliari:2013:GMC

[CR13] Marco Caliari and Stefan Rainer. GSGPEs: a MATLAB code for computing the ground state of systems of Gross–Pitaevskii equations. *Computer Physics Communications*, 184(3):812–823, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003402.

Clausen:2010:PPL

[CRA10] Jonathan R. Clausen, Daniel A. Reasor, Jr., and Cyrus K. Aidun. Parallel performance of a lattice-Boltzmann/finite element cellular blood flow solver on the IBM Blue Gene/P architecture. *Computer Physics Communications*, 181(6):1013–1020, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000391.

Cossio:2017:BGA

[CRB+17] Pilar Cossio, David Rohr, Fabio Baruffa, Markus Rampp, Volker Lindenstruth, and Gerhard Hummer. BioEM: GPU-accelerated computing of Bayesian inference of electron microscopy images. *Computer Physics Communications*, 210(??):163–171, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302855.

Crivellin:2013:SVC

[CRC+13] A. Crivellin, J. Rosiek, P. H. Chankowski, A. Dedes, S. Jäger, and P. Tanedo. SUSY_FLAVOR v2: a computational tool for FCNC and CP-violating processes in the MSSM. *Computer Physics Communications*, 184(3):1004–1032, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003839.

Criado:2018:MPL

[Cri18] Juan C. Criado. MatchingTools: A Python library for symbolic effective field theory calculations. *Computer Physics Communications*, 227(??):42–50, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300456.

Chow:2018:ISI

[CRLS18] Alex D. Chow, Benedict D. Rogers, Steven J. Lind, and Peter K. Stansby. Incompressible SPH (ISPH) with fast Poisson solver on a GPU. *Computer Physics Communications*, 226(??):81–103, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300092.

Curtis:2012:SPS

[CRNK12] Joseph E. Curtis, Sindhu Raghunandan, Hirsh Nanda, and Susan Krueger. SASSIE: a program to study intrinsically disordered biological molecules and macromolecular ensembles using experimental scattering restraints. *Computer Physics Communications*, 183(2):382–389, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003286.

Croker:2016:NDG

[Cro16] K. A. S. Croker. ngravs: Distinct gravitational interactions in GADGET-2. *Computer Physics Communications*, 207(??):478–486, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301989.

Chun:2010:HPT

[CS10] Changbum Chun and Rathinasamy Sakthivel. Homotopy perturbation technique for solving two-point boundary value problems — comparison with other methods. *Computer Physics Communications*, 181(6):1021–1024, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000445.

Chandrasekar:2016:EEC

[CS16] K. Silpaja Chandrasekar and M. V. Sangaranarayanan. Exact enumeration of conformations for two and three dimensional lattice proteins. *Computer Physics Communications*, 199(??):8–11, February 2016. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003653.

Chen:2017:RLO

[CS17] Parry Y. Chen and Yonatan Sivan. Robust location of optical fiber modes via the argument principle method. *Computer Physics Communications*, 214(??):105–116, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303630.

Cardoso:2013:LGF

[CSBO13] Nuno Cardoso, Paulo J. Silva, Pedro Bicudo, and Orlando Oliveira. Landau gauge fixing on GPUs. *Computer Physics Communications*, 184(1):124–129, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002937.

Campolongo:2011:SQS

[CSC11] Francesca Campolongo, Andrea Saltelli, and Jessica Cariboni. From screening to quantitative sensitivity analysis. A unified approach. *Computer Physics Communications*, 182(4):978–988, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005321.

Chen:2017:UHS

[CSJ+17] Yongpin P. Chen, Wei E. I. Sha, Lijun Jiang, Min Meng, Yu Mao Wu, and Weng Cho Chew. A unified Hamiltonian solution to Maxwell–Schrödinger equations for modeling electromagnetic field-particle interaction. *Computer Physics Communications*, 215(??):63–70, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300486.

Choi:2019:CMP

[CSK+19] Sangkook Choi, Patrick Semon, Byungkyun Kang, Andrey Kutepov, and Gabriel Kotliar. ComDMFT: a massively parallel computer package for the electronic structure of correlated-electron systems. *Computer Physics*

Communications, 244(??):277–294, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302140.

Cho:2013:EOP

[CSL+13] T. H. Cho, W. S. Su, T. C. Leung, Wei Ren, and C. T. Chan. Electronic and optical properties of bundled single-walled carbon nanotubes investigated by the first-principles method. *Computer Physics Communications*, 184(4):1077–1085, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003876.

Chmiela:2019:SCA

[CSP+19] Stefan Chmiela, Huziel E. Sauceda, Igor Poltavsky, Klaus-Robert Müller, and Alexandre Tkatchenko. sGDML: Constructing accurate and data efficient molecular force fields using machine learning. *Computer Physics Communications*, 240(??):38–45, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300591.

Chakraborty:2010:AIC

[CSPAD10] Monodeep Chakraborty, Jürgen Spitaler, Peter Puschnig, and Claudia Ambrosch-Draxl. ATAT@WIEN2k: An interface for cluster expansion based on the linearized augmented planewave method. *Computer Physics Communications*, 181(5):913–920, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000160.

Chudoba:2013:UPS

[CSRV13] R. Chudoba, V. Sadílek, R. Rypl, and M. Vorechovský. Using Python for scientific computing: Efficient and flexible evaluation of the statistical characteristics of functions with multivariate random inputs. *Computer Physics Communications*, 184(2):414–427, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003086.

Cheng:2015:AGP

[CSSB15] Way Lee Cheng, Ali Sheharyar, Reza Sadr, and Othmane Bouhali. Application of GPU processing for Brownian particle simulation. *Computer Physics Communications*, 186(??):39–47, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400318X.

Clark:2018:PMB

[CSV+18] M. A. Clark, Alexei Strelchenko, Alejandro Vaquero, Mathias Wagner, and Evan Weinberg. Pushing memory bandwidth limitations through efficient implementations of block-Krylov space solvers on GPUs. *Computer Physics Communications*, 233(??):29–40, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302273.

Chen:2015:KNF

[CTL15] Y. L. Chen, C. Z. Tian, and L. X. Li. A key-node finite element method and its application to porous materials. *Computer Physics Communications*, 195(??):102–111, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001721.

Carreras:2017:DCE

[CTT17] Abel Carreras, Atsushi Togo, and Isao Tanaka. DynaPhoPy: a code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, 221(??):221–234, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302631.

Childers:2017:ASA

[CUL+17] J. T. Childers, T. D. Uram, T. J. LeCompte, M. E. Papka, and D. P. Benjamin. Adapting the serial alpgen parton-interaction generator to simulate LHC collisions on millions of parallel threads. *Computer Physics Communications*, 210(??):54–59, January 2017. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302843.

Carrete:2017:ASS

[CVK+17] Jesús Carrete, Bjorn Vermeersch, Ankita Katre, Ambroise van Roekeghem, Tao Wang, Georg K. H. Madsen, and Natalio Mingo. almaBTE: a solver of the space-time dependent Boltzmann transport equation for phonons in structured materials. *Computer Physics Communications*, 220(??):351–362, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302059.

Clason:2012:GSMa

[CvW12a] Christian Clason and Gregory von Winckel. A general spectral method for the numerical simulation of one-dimensional interacting fermions. *Computer Physics Communications*, 183(2):405–417, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100333X.

Clason:2012:GSMb

[CvW12b] Christian Clason and Gregory von Winckel. A general spectral method for the numerical simulation of one-dimensional interacting fermions. *Computer Physics Communications*, 183(8):1843–1844, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001208.

Chen:2013:QQC

[CW13] Y. G. Chen and J. B. Wang. Qcompiler: Quantum compilation with the CSD method. *Computer Physics Communications*, 184(3):853–865, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003621.

Chen:2016:TDD

[CW16] Juan Chen and Jianguo Wang. Three-dimensional dispersive hybrid implicit-explicit finite-difference time-domain method for simulations of graphene. *Computer Physics Communications*, 207(??):211–216, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301692.

Cai:2019:LSP

[CWJ19] Jiaxiang Cai, Yushun Wang, and Chaolong Jiang. Local structure-preserving algorithms for general multi-symplectic Hamiltonian PDEs. *Computer Physics Communications*, 235(??):210–220, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303114.

Cai:2014:DMC

[CWS14] Wenjun Cai, Yushun Wang, and Yongzhong Song. Derivation of the multisymplectic Crank–Nicolson scheme for the nonlinear Schrödinger equation. *Computer Physics Communications*, 185(10):2403–2411, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001659.

Chang:2010:GUV

[CWW10] Chao-Hsi Chang, Jian-Xiong Wang, and Xing-Gang Wu. GENXICC2.0: An upgraded version of the generator for hadronic production of double heavy baryons Ξcc, Ξbc, and Ξbb. *Computer Physics Communications*, 181(6):1144–1149, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000457.

Chang:2015:BNU

[CWW15] Chao-Hsi Chang, Xian-You Wang, and Xing-Gang Wu. BCVEGPY2.2: a newly upgraded version for hadronic production of the meson B_c and its excited states. *Computer Physics Communications*, 197(??):335–338, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002842.

Chen:2017:PSP

[CWY+17] R. J. Chen, M. Wang, X. L. Yan, Q. Yang, Y. H. Lam, L. Yang, and Y. H. Zhang. A parallelization scheme of the periodic signals tracking algorithm for isochronous mass spectrometry on GPUs. *Computer Physics Communications*, 221(??):216–220, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730262X.

Chen:2019:POO

[CXG+19] Zhenping Chen, Jinsen Xie, Qian Guo, Qin Xie, Zijing Liu, Wenjie Zeng, Chao Xie, Pengcheng Zhao, and Tao Yu. Physics-oriented optimization strategy for the energy lookup algorithm in continuous energy Monte Carlo neutron transport simulation. *Computer Physics Communications*, 234(??):146–158, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830273X.

Chen:2015:IPA

[CXH+15] Mohan Chen, Junchao Xia, Chen Huang, Johannes M. Dieterich, Linda Hung, Ilgyou Shin, and Emily A. Carter. Introducing PROFESS 3.0: an advanced program for orbital-free density functional theory molecular dynamics simulations. *Computer Physics Communications*, 190(??):228–230, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000077.

Chen:2019:ELF

[CXL19] J. G. Chen, X. Q. Xu, and Y. A. Lei. Extension of Landau-fluid closure to weakly collisional plasma regime. *Computer Physics Communications*, 236(??):128–134, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303722.

Chane-Yook:2011:UUC

[CYD11] M. Chane-Yook and J. Dubau. Update of UCL computer codes for the calculation of fine-structure electron-atom collision cross-section. *Computer Physics Communications*, 182(1):134–135, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001955`.

Cartalade:2019:MRT

[CYN19] Alain Cartalade, Amina Younsi, and Marie-Christine Néel. Multiple-Relaxation-Time Lattice Boltzmann scheme for fractional advection–diffusion equation. *Computer Physics Communications*, 234(??):40–54, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551830300X`.

Chikano:2019:IOS

[CYOS19] Naoya Chikano, Kazuyoshi Yoshimi, Junya Otsuki, and Hiroshi Shinaoka. `irbasis`: Open-source database and software for intermediate-representation basis functions of imaginary-time Green's function. *Computer Physics Communications*, 240(??):181–188, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930058X`.

Chen:2012:SSE

[CYSL12] Zhaoxia Chen, Xiong You, Wei Shi, and Zhongli Liu. Symmetric and symplectic ERKN methods for oscillatory Hamiltonian systems. *Computer Physics Communications*, 183(1):86–98, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003043`.

Caliari:2017:IFE

[CZ17] Marco Caliari and Simone Zuccher. INFFTM: Fast evaluation of 3D Fourier series in MATLAB with an application to quantum vortex reconnections. *Computer Physics Communications*, 213(??):197–207, April 2017. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303691.

Caliari:2018:RTS

[CZ18a] M. Caliari and S. Zuccher. Reliability of the time splitting Fourier method for singular solutions in quantum fluids. *Computer Physics Communications*, 222(??):46–58, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303004.

Chakraborty:2018:EDD

[CZ18b] Souvik Chakraborty and Nicholas Zabaras. Efficient data-driven reduced-order models for high-dimensional multi-scale dynamical systems. *Computer Physics Communications*, 230(??):70–88, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301176.

Cichy:2019:WCP

[CZ19] Krzysztof Cichy and Savvas Zafeiropoulos. Wilson chiral perturbation theory for dynamical twisted mass fermions vs lattice data — a case study. *Computer Physics Communications*, 237(??):143–153, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304120.

Cai:2015:ALO

[CZD15] Dan Cai, Lijun Zhang, and Yong Du. Application of locally one-dimensional semi-implicit scheme in phase-field equations. *Computer Physics Communications*, 192(??):148–155, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500106X.

Chen:2018:MFE

[CZF18] Kaifeng Chen, Bo Zhao, and Shanhui Fan. MESH: A free electromagnetic solver for far-field and near-field radiative heat transfer for layered periodic structures. *Computer Physics Communications*, 231(??):163–172, October 2018.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301486.

Chrobak:2019:DBC

[CZGC19] Artur Chrobak, Grzegorz Ziólkowski, Krzysztof Granek, and Dariusz Chrobak. Disorder-based cluster Monte Carlo algorithm and its application in simulations of magnetization processes. *Computer Physics Communications*, 238(??):157–164, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304211.

Cho:2011:IRC

[CZL+11] Min Hyung Cho, Haiyu Zheng, Yuehui Lu, YoungPak Lee, and Wei Cai. Improved rigorous coupled-wave analysis for polar magnetic gratings. *Computer Physics Communications*, 182(2):360–365, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004078.

Curtis:2014:STS

[CZN14] Joseph E. Curtis, Hailiang Zhang, and Hirsh Nanda. SLDMOL: a tool for the structural characterization of thermally disordered membrane proteins. *Computer Physics Communications*, 185(11):3010–3015, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002483.

Chen:2010:MSS

[CZS10] Yaming Chen, Huajun Zhu, and Songhe Song. Multi-symplectic splitting method for the coupled nonlinear Schrödinger equation. *Computer Physics Communications*, 181(7):1231–1241, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000895.

Chen:2019:AEA

[CZZ+19] Lizhen Chen, Jun Zhang, Jia Zhao, Waixiang Cao, Hong Wang, and Jiwei Zhang. An accurate and efficient algorithm for the time-fractional molecular beam epitaxy model with slope selection. *Computer Physics Communications*, 245(??):Article 106842, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930219X.

Dixit:2016:ICX

[DA16] Anant Dixit and M. Alouani. Ab initio calculations of X-ray magnetic circular dichroism spectra within the projector augmented wave method: an implementation into the VASP code. *Computer Physics Communications*, 207(??):136–144, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301461.

Dupuy:2011:PSD

[DADS11] P. M. Dupuy, P. Austin, G. W. Delaney, and M. P. Schwarz. Pore scale definition and computation from tomography data. *Computer Physics Communications*, 182(10):2249–2258, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001664.

Filho:2012:TDE

[dAFdSVM12] Luciano M. de Andrade Filho, José Manoel de Seixas, Roberto Agostino Vitillo, and Brian Thomas Martin. Three-dimensional event visualization for the ATLAS calorimeter. *Computer Physics Communications*, 183(2):245–250, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003092.

deAquino:2012:AAL

[dALM+12] Priscila de Aquino, William Link, Fabio Maltoni, Olivier Mattelaer, and Tim Stelzer. ALOHA: Automatic libraries of helicity amplitudes for Feynman diagram computations. *Computer Physics Communications*, 183(10):2254–2263, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001725.

Daniluk:2010:MDDa

[Dan10a] Andrzej Daniluk. Model-driven development for scientific computing. computations of RHEED intensities for a disordered surface. Part I. *Computer Physics Communications*, 181(3):707–708, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003841.

Daniluk:2010:MDDb

[Dan10b] Andrzej Daniluk. Model-driven development for scientific computing. computations of RHEED intensities for a disordered surface. Part II. *Computer Physics Communications*, 181(3):709–710, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003865.

Daniluk:2011:CCC

[Dan11] Andrzej Daniluk. Cooperative and competitive concurrency in scientific computing. A full open-source upgrade of the program for dynamical calculations of RHEED intensity oscillations. *Computer Physics Communications*, 182(6):1389–1390, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000804.

Daniluk:2012:VMS

[Dan12] Andrzej Daniluk. Visual modeling for scientific software architecture design. A practical approach. *Computer Physics Communications*, 183(2):213–230, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002700.

Daniluk:2014:RIT

[Dan14] Andrzej Daniluk. RHEED intensities from two-dimensional heteroepitaxial nanoscale systems. *Computer Physics Communications*, 185(11):3001–3009, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002458.

Daniluk:2016:RIT

[Dan16] Andrzej Daniluk. RHEED intensities from two-dimensional heteroepitaxial nanoscale systems of GaN on a Si surface. *Computer Physics Communications*, 207(??):536–538, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301722.

Daniluk:2017:RIT

[Dan17] Andrzej Daniluk. RHEED intensities from two-dimensional heteroepitaxial nanoscale systems of GaN on a 3C–SiC(111) surface. *Computer Physics Communications*, 221(??):419–420, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302655.

Daniluk:2019:RIT

[Dan19] Andrzej Daniluk. RHEED intensities from two-dimensional heteroepitaxial nanoscale systems of GaN on AlN(0 0 0 1) and AlN(0 0 0 $\bar{1}$) surfaces. *Computer Physics Communications*, 244(??):487–489, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301717.

deAnda-Suarez:2019:POS

[dASJC+19] Juan de Anda-Suárez, Solai Jeyakumar, Martín Carpio, Héctor J. Puga, Alfonso Rojas-Domínguez, Laura Cruz-Reyes, and Juan F. Mosiño. Parameter optimization for the smoothed-particle hydrodynamics method by means of evolutionary metaheuristics. *Computer Physics Communications*, 243(??):30–40, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301572.

Dattani:2013:FMP

[Dat13] Nikesh S. Dattani. FeynDyn: a MATLAB program for fast numerical Feynman integral calculations for open quantum system dynamics on GPUs. *Computer Physics Communications*, 184(12):2828–2833, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465513002294.

Dalitz:2019:ATR

[DAW+19] Christoph Dalitz, Yassid Ayyad, Jens Wilberg, Lukas Aymans, Daniel Bazin, and Wolfgang Mittig. Automatic trajectory recognition in Active Target Time Projection Chambers data by means of hierarchical clustering. *Computer Physics Communications*, 235(??):159–168, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303242.

DiNapoli:2013:BIE

[DB13] Edoardo Di Napoli and Mario Berljafa. Block iterative eigensolvers for sequences of correlated eigenvalue problems. *Computer Physics Communications*, 184(11):2478–2488, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002117.

deBuyl:2014:VPN

[dB14] Pierre de Buyl. The vmf90 program for the numerical resolution of the Vlasov equation for mean-field systems. *Computer Physics Communications*, 185(6):1822–1827, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000848.

DiNapoli:2012:CSG

[DBB12] Edoardo Di Napoli, Stefan Blügel, and Paolo Bientinesi. Correlations in sequences of generalized eigenproblems arising in Density Functional Theory. *Computer Physics Communications*, 183(8):1674–1682, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001117.

deBuyl:2014:HSE

[dBCH14] Pierre de Buyl, Peter H. Colberg, and Felix Höfling. H5MD: a structured, efficient, and portable file format for molecular data. *Computer Physics Communications*, 185(6):1546–1553, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000447.

Deconinck:2017:ALN

[DBD+17] Willem Deconinck, Peter Bauer, Michail Diamantakis, Mats Hamrud, Christian Kühnlein, Pedro Maciel, Gianmarco Mengaldo, Tiago Quintino, Baudouin Raoult, Piotr K. Smolarkiewicz, and Nils P. Wedi. Atlas: a library for numerical weather prediction and climate modelling. *Computer Physics Communications*, 220(??):188–204, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302138.

Daly:2012:MPC

[DBDP12] Kevin B. Daly, Jay B. Benziger, Pablo G. Debenedetti, and Athanassios Z. Panagiotopoulos. Massively parallel chemical potential calculation on graphics processing units. *Computer Physics Communications*, 183(10):2054–2062, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001749.

Davis:2011:SSO

[DBJ11] Sergio M. Davis, Anatoly B. Belonoshko, and Börje Johansson. SearchFill: a stochastic optimization code for detecting atomic vacancies in crystalline and non-crystalline systems. *Computer Physics Communications*, 182(5):1105–1110, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000487X.

Dolfi:2014:MPS

[DBK+14] Michele Dolfi, Bela Bauer, Sebastian Keller, Alexandr Kosenkov, Timothée Ewart, Adrian Kantian, Thierry Giamarchi, and Matthias Troyer. Matrix product state applications for the ALPS project. *Computer Physics Communications*, 185(12):3430–3440, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003002.

Ducrozet:2016:HOO

[DBLF16] Guillaume Ducrozet, Félicien Bonnefoy, David Le Touzé, and Pierre Ferrant. HOS-ocean: Open-source solver for nonlinear waves in open ocean based on High-Order Spectral method. *Computer Physics Communications*, 203(??):245–254, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300327.

DAlessandro:2018:DOS

[DBMR18] Valerio D'Alessandro, Lorenzo Binci, Sergio Montelpare, and Renato Ricci. On the development of OpenFOAM solvers based on explicit and implicit high-order Runge–Kutta schemes for incompressible flows with heat transfer. *Computer Physics Communications*, 222(??):14–30, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302965.

Derouillat:2018:SCO

[DBP+18] J. Derouillat, A. Beck, F. Pérez, T. Vinci, M. Chiaramello, A. Grassi, M. Flé, G. Bouchard, I. Plotnikov, N. Aunai, J. Dargent, C. Riconda, and M. Grech. Smilei: a collaborative, open-source, multi-purpose particle-in-cell code for plasma simulation. *Computer Physics Communications*, 222(??):351–373, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303314.

Dobrowolski:2019:NMP

[DBP19] A. Dobrowolski, J. Bartel, and K. Pomorski. Nuclear mass parameters and moments of inertia in a folded-Yukawa mean-field approach. *Computer Physics Communications*, 237(??):253–262, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304090.

DAngola:2010:EEC

[DCC+10] A. D'Angola, G. Coppa, M. Capitelli, C. Gorse, and G. Colonna. An efficient energy-conserving numerical model for the electron energy distribution function in the presence of electron-electron collisions. *Computer Physics Communications*, 181(7):1204–1211, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000858.

deCastro:2019:IIA

[dCD19] Pablo de Castro and Tommaso Dorigo. INFERNO: Inference-Aware Neural Optimisation. *Computer Physics Communications*, 244(??):170–179, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301948.

Dominguez:2013:OSC

[DCGG13] Jose M. Domínguez, Alejandro J. C. Crespo, and Moncho Gómez-Gesteira. Optimization strategies for CPU and GPU implementations of a smoothed particle hydrodynamics method. *Computer Physics Communications*, 184(3):617–627, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200358X.

Dalena:2012:SGC

[DCM+12] S. Dalena, P. Chuychai, R. L. Mace, A. Greco, G. Qin, and W. H. Matthaeus. Streamline generation code for particle dynamics description in numerical models of turbulence. *Computer Physics Communications*, 183(9):1974–1985, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001610.

DiIlio:2019:MGA

[DCU+19] G. Di Ilio, D. Chiappini, S. Ubertini, G. Bella, and S. Succi. A moving-grid approach for fluid-structure interaction problems with hybrid lattice Boltzmann method. *Computer Physics Communications*, 234(??):137–145, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302741.

Dominguez:2013:NMG

[DCVB+13] J. M. Domínguez, A. J. C. Crespo, D. Valdez-Balderas, B. D. Rogers, and M. Gómez-Gesteira. New multi-GPU implementation for smoothed particle hydrodynamics on heterogeneous clusters. *Computer Physics Communications*, 184(8):1848–1860, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001057`.

Degrande:2012:UUF

[DDF+12] Céline Degrande, Claude Duhr, Benjamin Fuks, David Grellscheid, Olivier Mattelaer, and Thomas Reiter. UFO — the Universal FeynRules Output. *Computer Physics Communications*, 183(6):1201–1214, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000379`.

Denner:2017:CFB

[DDH17] Ansgar Denner, Stefan Dittmaier, and Lars Hofer. Collier: a Fortran-based complex one-loop library in extended regularizations. *Computer Physics Communications*, 212(??):220–238, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303320`.

Ben:2019:LSG

[DdJC+19] Mauro Del Ben, Felipe H. da Jornada, Andrew Canning, Nathan Wichmann, Karthik Raman, Ruchira Sasanka, Chao Yang, Steven G. Louie, and Jack Deslippe. Large-scale GW calculations on pre-exascale HPC systems. *Computer Physics Communications*, 235(??):187–195, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303175`.

Drees:2015:CCY

[DDK+15] Manuel Drees, Herbert K. Dreiner, Jong Soo Kim, Daniel Schmeier, and Jamie Tattersall. CheckMATE: Confronting your favourite new physics model with LHC data. *Computer Physics Communications*, 187(??):227–265, February

2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003646.

Dercks:2017:CML

[DDK+17] Daniel Dercks, Nishita Desai, Jong Soo Kim, Krzysztof Rolbiecki, Jamie Tattersall, and Torsten Weber. CheckMATE 2: From the model to the limit. *Computer Physics Communications*, 221(??):383–418, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302679.

Denner:2015:HMC

[DDKM15] Ansgar Denner, Stefan Dittmaier, Stefan Kallweit, and Alexander Mück. HAWK 2.0: a Monte Carlo program for Higgs production in vector-boson fusion and Higgs strahlung at hadron colliders. *Computer Physics Communications*, 195(??):161–171, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001630.

Donker:2014:EES

[DDM14] Hylke C. Donker, Hans De Raedt, and Kristel Michielsen. Event-by-event simulation of a quantum delayed-choice experiment. *Computer Physics Communications*, 185 (12):3109–3118, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002689.

Duarte:2016:FFO

[DdMN16] L. G. S. Duarte, L. A. C. P. da Mota, and E. Nunez. Finding first order differential invariants through the S-function. *Computer Physics Communications*, 207(??):542–544, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301746.

deDoncker:2018:RNE

[dDYK+18] E. de Doncker, F. Yuasa, K. Kato, T. Ishikawa, J. Kapenga, and O. Olagbemi. Regularization with numerical extrapolation for finite and UV-divergent multi-loop integrals. *Computer Physics Communications*, 224(??):164–185, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303703.

DeMichele:2011:OED

[De 11] C. De Michele. Optimizing event-driven simulations. *Computer Physics Communications*, 182(9):1846–1850, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004583.

Doi:2013:UCA

[DE13] Takumi Doi and Michael G. Endres. Unified contraction algorithm for multi-baryon correlators on the lattice. *Computer Physics Communications*, 184(1):117–123, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002901.

Degrande:2015:AEU

[Deg15] Celine Degrande. Automatic evaluation of UV and R_2 terms for beyond the standard model Lagrangians: a proof-of-principle. *Computer Physics Communications*, 197(??):239–262, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500301X.

Demchik:2011:PRN

[Dem11] Vadim Demchik. Pseudo-random number generators for Monte Carlo simulations on ATI Graphics Processing Units. *Computer Physics Communications*, 182(3):692–705, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004868.

Demeter:2013:SMB

[Dem13] G. Demeter. Solving the Maxwell–Bloch equations for resonant nonlinear optics using GPUs. *Computer Physics Communications*, 184(4):1203–1210, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465512004250.

DePalma:2019:PPI

[DEMM19] Barbara De Palma, Marco Erba, Luca Mantovani, and Nicola Mosco. A Python program for the implementation of the Γ-method for Monte Carlo simulations. *Computer Physics Communications*, 234(??):294–301, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302534.

Deng:2010:RNM

[Den10] Shaozhong Deng. A robust numerical method for self-polarization energy of spherical quantum dots with finite confinement barriers. *Computer Physics Communications*, 181(4):787–799, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004032.

Deppisch:2017:EMP

[Dep17] Thomas Deppisch. E6Tensors: a Mathematica package for E_6 tensors. *Computer Physics Communications*, 213(??):130–135, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302818.

Deublein:2011:MMS

[DES$^+$11] Stephan Deublein, Bernhard Eckl, Jürgen Stoll, Sergey V. Lishchuk, Gabriela Guevara-Carrion, Colin W. Glass, Thorsten Merker, Martin Bernreuther, Hans Hasse, and Jadran Vrabec. ms 2: a molecular simulation tool for thermodynamic properties. *Computer Physics Communications*, 182(11):2350–2367, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002025.

Descouvemont:2016:MPC

[Des16] P. Descouvemont. An R-matrix package for coupled-channel problems in nuclear physics. *Computer Physics*

Communications, 200(??):199–219, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003951.

Das:2012:NFC

[DET12] Debottam Das, Ulrich Ellwanger, and Ana M. Teixeira. NMSDECAY: a Fortran code for supersymmetric particle decays in the Next-to-Minimal Supersymmetric Standard Model. *Computer Physics Communications*, 183(3):774–779, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003833.

Deuar:2016:TPL

[Deu16] P. Deuar. A tractable prescription for large-scale free flight expansion of wavefunctions. *Computer Physics Communications*, 208(??):92–102, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630234X.

Deveikis:2012:CPT

[Dev12] A. Deveikis. A computer program for two-particle intrinsic coefficients of fractional parentage. *Computer Physics Communications*, 183(6):1397–1401, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000574.

Degiacomi:2016:ECP

[DEW16] Matteo T. Degiacomi, Valentina Erastova, and Mark R. Wilson. Easy creation of polymeric systems for molecular dynamics with Assemble! *Computer Physics Communications*, 202(??):304–309, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000187.

Delzanno:2011:FDA

[DF11a] Gian Luca Delzanno and John M. Finn. The fluid dynamic approach to equidistribution methods for grid adaptation.

Computer Physics Communications, 182(2):330–346, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004054.

Duhr:2011:SMF

[DF11b] Claude Duhr and Benjamin Fuks. A superspace module for the FeynRules package. *Computer Physics Communications*, 182(11):2404–2426, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002190.

Delaney:2013:PFT

[DF13] Kris T. Delaney and Glenn H. Fredrickson. Polymer field-theory simulations on graphics processing units. *Computer Physics Communications*, 184(9):2102–2110, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001379.

Deng:2014:OMR

[DF14] Wenjun Deng and Guo-Yong Fu. Optimization by marker removal for δf particle simulations. *Computer Physics Communications*, 185(1):96–105, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002828.

Duff:2015:MRF

[DFM+15] Andrew Ian Duff, M. W. Finnis, Philippe Maugis, Barend J. Thijsse, and Marcel H. F. Sluiter. MEAMfit: a reference-free modified embedded atom method (RF-MEAM) energy and force-fitting code. *Computer Physics Communications*, 196(??):439–445, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001964.

Dehghan:2010:ADR

[DG10a] Mehdi Dehghan and Arezou Ghesmati. Application of the dual reciprocity boundary integral equation technique to solve the nonlinear Klein–Gordon equation. *Computer*

Physics Communications, 181(8):1410–1418, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001190.

Dehghan:2010:NST

[DG10b] Mehdi Dehghan and Arezou Ghesmati. Numerical simulation of two-dimensional sine–Gordon solitons via a local weak meshless technique based on the radial point interpolation method (RPIM). *Computer Physics Communications*, 181(4):772–786, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004020.

Duchemin:2010:SAA

[DG10c] Ivan Duchemin and François Gygi. A scalable and accurate algorithm for the computation of Hartree–Fock exchange. *Computer Physics Communications*, 181(5):855–860, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004135.

Durand:2016:ECP

[DG16] Marc Durand and Etienne Guesnet. An efficient Cellular Potts Model algorithm that forbids cell fragmentation. *Computer Physics Communications*, 208(??):54–63, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302284.

Dugan:2013:CGP

[DGG13] Nazim Dugan, Luigi Genovese, and Stefan Goedecker. A customized 3D GPU Poisson solver for free boundary conditions. *Computer Physics Communications*, 184(8):1815–1820, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000817.

Dasgupta:2019:FSO

[DGJH19] Adhiraj Dasgupta, Esteban Gonzalez-Juez, and Daniel C. Haworth. Flame simulations with an open-source code. *Computer Physics Communications*, 237(??):219–229, April 2019.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830403X.

Dhote:2015:SMA

[DGMZ15] R. P. Dhote, H. Gomez, R. N. V. Melnik, and J. Zu. Shape memory alloy nanostructures with coupled dynamic thermo-mechanical effects. *Computer Physics Communications*, 192(??):48–53, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000764.

Dominguez-Garcia:2018:JIA

[DGPOR18] P. Domínguez-García, M. Pancorbo, F. Ortega, and M. A. Rubio. JColloids: Image analysis for video-microscopy studies of colloidal suspensions. *Computer Physics Communications*, 231(??):243–244, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301516.

Davidson:2011:MTV

[DGPW11] N. Davidson, P. Golonka, T. Przedziński, and Z. Was. MC-TESTER v. 1.23: a universal tool for comparisons of Monte Carlo predictions for particle decays in high energy physics. *Computer Physics Communications*, 182(3):779–789, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004698.

Donnel:2019:MSC

[DGS+19] P. Donnel, X. Garbet, Y. Sarazin, V. Grandgirard, Y. Asahi, N. Bouzat, E. Caschera, G. Dif-Pradalier, C. Ehrlacher, P. Ghendrih, C. Gillot, G. Latu, and C. Passeron. A multi-species collisional operator for full-F global gyrokinetics codes: Numerical aspects and verification with the GYSELA code. *Computer Physics Communications*, 234(??):1–13, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303035.

Dunster:2017:CEM

[DGST17] T. M. Dunster, A. Gil, J. Segura, and N. M. Temme. Conical: an extended module for computing a numerically satisfactory pair of solutions of the differential equation for conical functions. *Computer Physics Communications*, 217(??):193–197, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301212`.

deHaan:2011:IIW

[dHGCS11] Hendrick W. de Haan, Michel G. Gauthier, Mykyta V. Chubynsky, and Gary W. Slater. The importance of introducing a waiting time for lattice Monte Carlo simulations of a polymer translocation process. *Computer Physics Communications*, 182(1):29–32, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510002924`.

Dennis:2013:XFS

[DHJ13] Graham R. Dennis, Joseph J. Hope, and Mattias T. Johnsson. XMDS2: Fast, scalable simulation of coupled stochastic partial differential equations. *Computer Physics Communications*, 184(1):201–208, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002822`.

Dion:2014:PQW

[DHR14] C. M. Dion, A. Hashemloo, and G. Rahali. Program for quantum wave-packet dynamics with time-dependent potentials. *Computer Physics Communications*, 185(1):407–414, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003135`.

DelDebbio:2014:MPC

[DHS14] Luigi Del Debbio, Nathan Hartland, and Steffen Schumann. MCgrid: Projecting cross section calculations on grids. *Computer Physics Communications*, 185(7):2115–2126, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001039`.

Dima:2014:FVA

[Dim14] M. Dima. Flash vertexing algorithms for trigger applications. *Computer Physics Communications*, 185(1):177–180, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003056.

DAmbrosio:2011:CEB

[DIP11] R. D'Ambrosio, L. Gr. Ixaru, and B. Paternoster. Construction of the ef-based Runge–Kutta methods revisited. *Computer Physics Communications*, 182(2):322–329, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004042.

Dai:2019:MBB

[DIR+19] De-Chang Dai, Cigdem Issever, Eram Rizvi, Glenn Starkman, Dejan Stojkovic, and Jeff Tseng. Manual of BlackMax. A black-hole event generator with rotation, recoil, split branes, and brane tension. Version 2.02. *Computer Physics Communications*, 236(??):285–301, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303692.

Dehghan:2011:HON

[DJ11] Mehdi Dehghan and Rooholah Jazlanian. A high-order non-oscillatory central scheme with non-staggered grids for hyperbolic conservation laws. *Computer Physics Communications*, 182(6):1284–1294, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000786.

Deinega:2012:FDD

[DJ12] Alexei Deinega and Sajeev John. Finite difference discretization of semiconductor drift-diffusion equations for nanowire solar cells. *Computer Physics Communications*, 183(10):2128–2135, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001853.

Doerk:2014:TOE

[DJ14] H. Doerk and F. Jenko. Towards optimal explicit time-stepping schemes for the gyrokinetic equations. *Computer Physics Communications*, 185(7):1938–1946, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001040`.

deJong:2016:MSB

[dJBIM16] Djurre H. de Jong, Svetlana Baoukina, Helgi I. Ingólfsson, and Siewert J. Marrink. Martini straight: Boosting performance using a shorter cutoff and GPUs. *Computer Physics Communications*, 199(??):1–7, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003628`. See comment [BL18a].

DeRaedt:2019:MPQ

[DJW+19] Hans De Raedt, Fengping Jin, Dennis Willsch, Madita Willsch, Naoki Yoshioka, Nobuyasu Ito, Shengjun Yuan, and Kristel Michielsen. Massively parallel quantum computer simulator, eleven years later. *Computer Physics Communications*, 237(??):47–61, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303977`.

Dieterich:2014:SMP

[DKG+14] Johannes M. Dieterich, David B. Krisiloff, Alexander Gaenko, Florian Libisch, Theresa L. Windus, Mark S. Gordon, and Emily A. Carter. Shared-memory parallelization of a local correlation multi-reference CI program. *Computer Physics Communications*, 185(12):3175–3188, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551400294X`.

Djouadi:2019:HTY

[DKMS19] Abdelhak Djouadi, Jan Kalinowski, Margarete Mühlleitner, and Michael Spira. HDECAY: Twenty++ years after. *Computer Physics Communications*, 238(??):214–231, May 2019.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304260.

Dolgov:2014:CEE

[DKOS14] S. V. Dolgov, B. N. Khoromskij, I. V. Oseledets, and D. V. Savostyanov. Computation of extreme eigenvalues in higher dimensions using block tensor train format. *Computer Physics Communications*, 185(4):1207–1216, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004293.

Dewhurst:2016:EAT

[DKSG16] J. K. Dewhurst, K. Krieger, S. Sharma, and E. K. U. Gross. An efficient algorithm for time propagation as applied to linearized augmented plane wave method. *Computer Physics Communications*, 209(??):92–95, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302715.

Druzhinin:2014:GMC

[DKT14] V. P. Druzhinin, L. V. Kardapoltsev, and V. A. Tayursky. GGRESRC: a Monte Carlo generator for the two-photon process $e^+e^- \to e^+e^-R(J^{PC} = 0^{-+})$ in the single-tag mode. *Computer Physics Communications*, 185(1):236–243, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002452.

Davis:2010:PMD

[DLGP10] Sergio Davis, Claudia Loyola, Felipe González, and Joaquín Peralta. Las Palmeras Molecular Dynamics: a flexible and modular molecular dynamics code. *Computer Physics Communications*, 181(12):2126–2139, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000336X.

delaHoz:2010:IFN

[dlHV10] Francisco de la Hoz and Fernando Vadillo. An integrating factor for nonlinear Dirac equations. *Computer Physics*

Communications, 181(7):1195–1203, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000846.

delaHoz:2012:NSD

[dlHV12] Francisco de la Hoz and Fernando Vadillo. Numerical simulation of the N-dimensional sine–Gordon equation via operational matrices. *Computer Physics Communications*, 183(4):864–879, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004000.

Dulat:2018:INI

[DLM18] Falko Dulat, Achilleas Lazopoulos, and Bernhard Mistlberger. iHixs 2-inclusive Higgs cross sections. *Computer Physics Communications*, 233(??):243–260, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302479.

Otero-de-la-Roza:2011:GNVb

[dlRAPL11] A. Otero de-la Roza, David Abbasi-Pérez, and Víctor Luaña. Gibbs 2: a new version of the quasiharmonic model code. II. Models for solid-state thermodynamics, features and implementation. *Computer Physics Communications*, 182(10):2232–2248, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001652.

Otero-de-la-Roza:2014:CPR

[dlRJL14] A. Otero de-la Roza, Erin R. Johnson, and Víctor Luaña. Critic 2: a program for real-space analysis of quantum chemical interactions in solids. *Computer Physics Communications*, 185(3):1007–1018, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003718.

Otero-de-la-Roza:2011:GNVa

[dlRL11] A. Otero de-la Roza and Víctor Luaña. Gibbs 2: a new version of the quasi-harmonic model code. I. Robust treatment of the static data. *Computer Physics Communications*, 182(8):1708–1720, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001470.

laRosa:2018:HDF

[dlRM18] Jonatan Núñez de la Rosa and Claus-Dieter Munz. Hybrid DG/FV schemes for magnetohydrodynamics and relativistic hydrodynamics. *Computer Physics Communications*, 222(??):113–135, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303338.

Denner:2018:RRC

[DLU18] Ansgar Denner, Jean-Nicolas Lang, and Sandro Uccirati. RECOLA2: REcursive Computation of One-Loop Amplitudes 2. *Computer Physics Communications*, 224(??):346–361, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S001046551730396X.

Dong:2018:TFL

[DLW+18] Shao-Jun Dong, Wen-Yuan Liu, Chao Wang, Yongjian Han, G.-C. Guo, and Lixin He. TNSPackage: A Fortran2003 library designed for tensor network state methods. *Computer Physics Communications*, 228(??):163–177, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830078X.

Dziubak:2012:OOI

[DM12] Tomasz Dziubak and Jacek Matulewski. An object-oriented implementation of a solver of the time-dependent Schrödinger equation using the CUDA technology. *Computer Physics Communications*, 183(3):800–812, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003948.

Dehghan:2017:NSB

[DM17] Mehdi Dehghan and Vahid Mohammadi. A numerical scheme based on radial basis function finite difference (RBF–FD) technique for solving the high-dimensional nonlinear Schrödinger equations using an explicit time discretization: Runge–Kutta method. *Computer Physics Communications*, 217(??):23–34, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300991.

Doctors:2010:CEM

[DMC10] G. M. Doctors, M. D. Mazzeo, and P. V. Coveney. A computationally efficient method for simulating fluid flow in elastic pipes in three dimensions. *Computer Physics Communications*, 181(9):1584–1592, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001669.

Ding:2015:PPF

[DMC+15] Hong Ding, Bharat Medasani, Wei Chen, Kristin A. Persson, Maciej Haranczyk, and Mark Asta. PyDII: a Python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds. *Computer Physics Communications*, 193(??):118–123, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001149.

Raedt:2016:DCM

[DMH16] Hans De Raedt, Kristel Michielsen, and Karl Hess. The digital computer as a metaphor for the perfect laboratory experiment: Loophole-free Bell experiments. *Computer Physics Communications*, 209(??):42–47, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302405.

Dytrych:2016:ESS

[DML+16] T. Dytrych, P. Maris, K. D. Launey, J. P. Draayer, J. P. Vary, D. Langr, E. Saule, M. A. Caprio, U. Catalyurek, and

M. Sosonkina. Efficacy of the SU(3) scheme for ab initio large-scale calculations beyond the lightest nuclei. *Computer Physics Communications*, 207(??):202–210, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301680.

DAmbrosio:2018:PEI

[DMP18] Raffaele D'Ambrosio, Martina Moccaldi, and Beatrice Paternoster. Parameter estimation in IMEX-trigonometrically fitted methods for the numerical solution of reaction–diffusion problems. *Computer Physics Communications*, 226(??):55–66, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300110.

Dehghan:2013:SWS

[DN13] Mehdi Dehghan and Ahmad Nikpour. The solitary wave solution of coupled Klein–Gordon–Zakharov equations via two different numerical methods. *Computer Physics Communications*, 184(9):2145–2158, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001458.

Dawson:2018:MPS

[DN18] William Dawson and Takahito Nakajima. Massively parallel sparse matrix function calculations with NTPoly. *Computer Physics Communications*, 225(??):154–165, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304150.

Davidson:2012:UIT

[DNP+12] N. Davidson, G. Nanava, T. Przedziński, E. Richter-Was, and Z. Was. Universal interface of TAUOLA: Technical and physics documentation. *Computer Physics Communications*, 183(3):821–843, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003973.

Dreiner:2013:FLC

[DNPS13] H. Dreiner, K. Nickel, W. Porod, and F. Staub. Full 1-loop calculation of $BR(B^0_{s,d} \to \ell\bar{\ell})$ in models beyond the MSSM with SARAH and SPheno. *Computer Physics Communications*, 184(11):2604–2617, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002282.

Duy:2014:DMM

[DO14a] Truong Vinh Truong Duy and Taisuke Ozaki. A decomposition method with minimum communication amount for parallelization of multi-dimensional FFTs. *Computer Physics Communications*, 185(1):153–164, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003020.

Duy:2014:TDD

[DO14b] Truong Vinh Truong Duy and Taisuke Ozaki. A three-dimensional domain decomposition method for large-scale DFT electronic structure calculations. *Computer Physics Communications*, 185(3):777–789, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004013.

Deluzet:2017:DAS

[DOP17] Fabrice Deluzet, Maurizio Ottaviani, and Stefan Possanner. A drift-asymptotic scheme for a fluid description of plasmas in strong magnetic fields. *Computer Physics Communications*, 219(??):164–177, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301601.

Dobrowolski:2016:SEP

[DPB16] A. Dobrowolski, K. Pomorski, and J. Bartel. Solving the eigenvalue problem of the nuclear Yukawa-folded mean-field Hamiltonian. *Computer Physics Communications*, 199(??):118–132, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465515003720.

Napoli:2017:HPG

[DPHB17] Edoardo Di Napoli, Elmar Peise, Markus Hrywniak, and Paolo Bientinesi. High-performance generation of the Hamiltonian and overlap matrices in FLAPW methods. *Computer Physics Communications*, 211(??):61–72, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303095.

Delage:2015:PID

[DPK+15] E. Delage, Q. T. Pham, M. Karamitros, H. Payno, V. Stepan, S. Incerti, L. Maigne, and Y. Perrot. PDB4DNA: Implementation of DNA geometry from the Protein Data Bank (PDB) description for Geant4-DNA Monte-Carlo simulations. *Computer Physics Communications*, 192(??):282–288, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000843.

Davidson:2016:PIC

[DPW16] N. Davidson, T. Przedzinski, and Z. Was. PHOTOS interface in C++: Technical and physics documentation. *Computer Physics Communications*, 199(??):86–101, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003513.

Dubray:2012:NSD

[DR12] N. Dubray and D. Regnier. Numerical search of discontinuities in self-consistent potential energy surfaces. *Computer Physics Communications*, 183(10):2035–2041, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001671.

Gallo:2016:CBM

[DRI+16] L. Di Gallo, C. Reux, F. Imbeaux, J.-F. Artaud, M. Owsiak, B. Saoutic, G. Aiello, P. Bernardi, G. Ciraolo, J. Bucalossi, J.-L. Duchateau, C. Fausser, D. Galassi, P. Hertout, J.-C. Jaboulay, A. Li-Puma, and L. Zani. Coupling between a multi-physics workflow engine and an optimization framework. *Computer Physics Communications*, 200(??):76–86, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004130.

Dimitroulis:2015:PTC

[DRR15] Christos Dimitroulis, Theophanes Raptis, and Vasilios Raptis. POLYANA — a tool for the calculation of molecular radial distribution functions based on molecular dynamics trajectories. *Computer Physics Communications*, 197(??):220–226, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002970.

Davina:2016:OAI

[DRR16] A. Lamas Daviña, E. Ramos, and J. E. Roman. Optimized analysis of isotropic high-nuclearity spin clusters with GPU acceleration. *Computer Physics Communications*, 209(??):70–78, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302442.

Deuzeman:2012:LMP

[DRUE12] Albert Deuzeman, Siebren Reker, Carsten Urbach, and ETM Collaboration. Lemon: An MPI parallel I/O library for data encapsulation using LIME. *Computer Physics Communications*, 183(6):1321–1335, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000318.

Dehghan:2010:SNT

[DS10] Mehdi Dehghan and Rezvan Salehi. Solution of a nonlinear time-delay model in biology via semi-analytical approaches. *Computer Physics Communications*, 181(7):1255–1265, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000949.

Decyk:2011:APC

[DS11a] Viktor K. Decyk and Tajendra V. Singh. Adaptable particle-in-cell algorithms for graphical processing units. *Computer Physics Communications*, 182(3):641–648, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004558.

Dehghan:2011:SWS

[DS11b] Mehdi Dehghan and Rezvan Salehi. The solitary wave solution of the two-dimensional regularized long-wave equation in fluids and plasmas. *Computer Physics Communications*, 182(12):2540–2549, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002670.

DeVuyst:2013:GAN

[DS13a] Florian De Vuyst and Francesco Salvarani. GPU-accelerated numerical simulations of the Knudsen gas on time-dependent domains. *Computer Physics Communications*, 184(3):532–536, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003372.

Dlamini:2013:QDC

[DS13b] Nkosinathi Dlamini and Alessandro Sergi. Quantum dynamics in classical thermal baths. *Computer Physics Communications*, 184(11):2474–2477, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002099.

Dlotko:2013:PIA

[DS13c] Pawel Dlotko and Ruben Specogna. Physics inspired algorithms for (co)homology computations of three-dimensional combinatorial manifolds with boundary. *Computer Physics Communications*, 184(10):2257–2266, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001665.

Decyk:2014:PCA

[DS14] Viktor K. Decyk and Tajendra V. Singh. Particle-in-Cell algorithms for emerging computer architectures. *Computer Physics Communications*, 185(3):708–719, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300341X.

Dybiec:2015:ESE

[DS15] Bartlomiej Dybiec and Igor M. Sokolov. Estimation of the smallest eigenvalue in fractional escape problems: Semi-analytics and fits. *Computer Physics Communications*, 187(??):29–37, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003427.

daSilva:2012:TVT

[dSdO12] Evandro F. da Silva and Mário J. de Oliveira. Two versions of the threshold contact model in two dimensions. *Computer Physics Communications*, 183(9):2001–2005, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001701.

daSilva:2018:HDC

[dSF18] Roberto da Silva and Henrique A. Fernandes. Highly detailed computational study of a surface reaction model with diffusion: Four algorithms analyzed via time-dependent and steady-state Monte Carlo simulations. *Computer Physics Communications*, 230(??):1–9, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301206.

daSilva:2013:NCA

[dSFdFF13] Roberto da Silva, Henrique A. Fernandes, J. R. Drugowich de Felício, and Wagner Figueiredo. Novel considerations about the non-equilibrium regime of the tricritical point in a metamagnetic model: Localization and tricritical exponents. *Computer Physics Communications*, 184(11):2371–2377, November 2013. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001653.

Danielson:2017:SDR

[DSHS17] Thomas Danielson, Jonathan E. Sutton, Céline Hin, and Aditya Savara. SQERTSS: Dynamic rank based throttling of transition probabilities in kinetic Monte Carlo simulations. *Computer Physics Communications*, 219(??):149–163, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301583.

Damian:2019:OST

[DSK19] Santiago Márquez Damián, Federico Schaumburg, and Pablo A. Kler. Open-source toolbox for electromigrative separations. *Computer Physics Communications*, 237(??):244–252, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304077.

daSilva:2013:PMI

[dSLF13] P. R. O. da Silva, F. W. S. Lima, and R. N. Costa Filho. Potts model with $q = 3$ and 4 states on directed small-world network. *Computer Physics Communications*, 184(12):2746–2750, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300249X.

Dixit:2011:APD

[DSLP11] H. Dixit, R. Saniz, D. Lamoen, and B. Partoens. Accurate pseudopotential description of the GW bandstructure of ZnO. *Computer Physics Communications*, 182(9):2029–2031, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000488.

Dhaka:2011:EMD

[DSM+11] M. S. Dhaka, G. Sharma, M. C. Mishra, K. B. Joshi, R. K. Kothari, and B. K. Sharma. Electron momentum density distribution in Cd_3P_2. *Computer Physics Communications*, 182(9):2017–2020, September 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005175.

Dunzlaff:2015:SPT

[DSP15] P. Dunzlaff, R. D. Strauss, and M. S. Potgieter. Solving Parker's transport equation with stochastic differential equations on GPUs. *Computer Physics Communications*, 192(??):156–165, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001071.

Dupuy:2010:FDS

[DSPJ10] Pablo M. Dupuy, H. F. Svendsen, Luciano E. Patruno, and Hugo A. Jakobsen. Finite-difference stable stencils based on least-square quadric fitting. *Computer Physics Communications*, 181(10):1671–1681, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001815.

Deslippe:2012:BMP

[DSS+12] Jack Deslippe, Georgy Samsonidze, David A. Strubbe, Manish Jain, Marvin L. Cohen, and Steven G. Louie. BerkeleyGW: a massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures. *Computer Physics Communications*, 183(6):1269–1289, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003912.

Dunsch:2019:RIL

[DSS+19] Mario Dunsch, Jan Soedingrekso, Alexander Sandrock, Maximilian Meier, Thorben Menne, and Wolfgang Rhode. Recent improvements for the lepton propagator PROPOSAL. *Computer Physics Communications*, 242(??):132–144, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301201.

daSilva:2013:SNM

[dSVLP13] Roberto da Silva, Mendeli H. Vainstein, Luis C. Lamb, and Sandra D. Prado. A simple non-Markovian computational model of the statistics of soccer leagues: Emergence and scaling effects. *Computer Physics Communications*, 184(3):661–670, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003736.

DelBen:2015:ESF

[DSW+15a] Mauro Del Ben, Ole Schütt, Tim Wentz, Peter Messmer, Jürg Hutter, and Joost VandeVondele. Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. *Computer Physics Communications*, 187(??):120–129, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003671.

Delgado:2015:SQI

[DSW15b] Carlos A. Argüelles Delgado, Jordi Salvado, and Christopher N. Weaver. A simple quantum integro-differential solver (SQuIDS). *Computer Physics Communications*, 196(??):569–591, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002672.

Dehghan:2010:CSS

[DT10] Mehdi Dehghan and Ameneh Taleei. A compact split-step finite difference method for solving the nonlinear Schrödinger equations with constant and variable coefficients. *Computer Physics Communications*, 181(1):43–51, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002768.

Dehghan:2011:CPM

[DT11a] Mehdi Dehghan and Ameneh Taleei. A Chebyshev pseudospectral multidomain method for the soliton solution of coupled nonlinear Schrödinger equations. *Computer Physics*

Communications, 182(12):2519–2529, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002475.

Diaz-Torres:2011:PCR

[DT11b] Alexis Diaz-Torres. PLATYPUS: a code for reaction dynamics of weakly-bound nuclei at near-barrier energies within a classical dynamical model. *Computer Physics Communications*, 182(4):1100–1104, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000129.

Diaz-Torres:2018:OCT

[DT18] Alexis Diaz-Torres. OWL: a code for the two-center shell model with spherical Woods–Saxon potentials. *Computer Physics Communications*, 224(??):381–386, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303715.

duToit:2018:PPS

[dTOV18] E. J. du Toit, M. R. O'Brien, and R. G. L. Vann. Positivity-preserving scheme for two-dimensional advection-diffusion equations including mixed derivatives. *Computer Physics Communications*, 228(??):61–68, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300766.

Duarte:2010:CII

[Dua10] C. A. Duarte. Convergence and instability of iterative procedures on the one-dimensional Schrödinger–Poisson problem. *Computer Physics Communications*, 181(9):1501–1509, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001402.

Duarte:2012:CEM

[Dua12] C. A. Duarte. Compact expressions for the magnetoresistance and the electron/hole density of states under the application of magnetic fields. *Computer Physics*

Communications, 183(4):993–997, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000100.

Duff:2016:MRF

[Duf16] Andrew Ian Duff. MEAMfit: a reference-free modified embedded atom method (RF-MEAM) energy and force-fitting code. *Computer Physics Communications*, 203(??):354–355, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300303.

Deinega:2011:LTB

[DV11] Alexei Deinega and Ilya Valuev. Long-time behavior of PML absorbing boundaries for layered periodic structures. *Computer Physics Communications*, 182(1):149–151, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001839.

Degroote:2011:FRP

[DVB11] Matthias Degroote, Dimitri Van Neck, and Carlo Barbieri. Faddeev Random Phase Approximation for molecules. *Computer Physics Communications*, 182(9):1995–1998, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000425X.

Dai:2019:GSI

[DXY+19] Zongliang Dai, Yingfeng Xu, Lei Ye, Xiaotao Xiao, and Shaojie Wang. Gyrokinetic simulation of ITG turbulence with toroidal geometry including the magnetic axis by using field-aligned coordinates. *Computer Physics Communications*, 242(??):72–82, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930116X.

Deng:2013:FNF

[DZ13] Dingwen Deng and Chengjian Zhang. A family of new fourth-order solvers for a nonlinear damped wave equation. *Computer Physics Communications*, 184(1):86–101, January

2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002858.

Dai:2015:ASM

[DZ15] Fu-Zhi Dai and Wen-Zheng Zhang. An automatic and simple method for specifying dislocation features in atomistic simulations. *Computer Physics Communications*, 188(??):103–109, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400397X.

Ebadi:2013:BSC

[Eba13] Hossein Ebadi. Bound state calculation of two-component Klein–Gordon equation with damped-relaxation technique. *Computer Physics Communications*, 184(3):550–556, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003396.

Eder:2014:AMA

[EBCB+14] S. J. Eder, D. Bianchi, U. Cihak-Bayr, A. Vernes, and G. Betz. An analysis method for atomistic abrasion simulations featuring rough surfaces and multiple abrasive particles. *Computer Physics Communications*, 185(10):2456–2466, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001830.

Eder:2017:MAA

[EBCBG17] S. J. Eder, D. Bianchi, U. Cihak-Bayr, and K. Gkagkas. Methods for atomistic abrasion simulations of laterally periodic polycrystalline substrates with fractal surfaces. *Computer Physics Communications*, 212(??):100–112, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303368.

Eilert:2017:FNM

[EBDM17] Tobias Eilert, Maximilian Beckers, Florian Drechsler, and Jens Michaelis. Fast-NPS — a Markov chain Monte Carlo-based analysis tool to obtain structural information from single-molecule FRET measurements. *Computer Physics Communications*, 219(??):377–389, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301807.

Edgar:2010:EHT

[ECD+10] R. G. Edgar, M. A. Clark, K. Dale, D. A. Mitchell, S. M. Ord, R. B. Wayth, H. Pfister, and L. J. Greenhill. Enabling a high throughput real time data pipeline for a large radio telescope array with GPUs. *Computer Physics Communications*, 181(10):1707–1714, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001967.

Eriksson:2016:CFN

[ECSH16] J. Eriksson, S. Conroy, E. Andersson Sundén, and C. Hellesen. Calculating fusion neutron energy spectra from arbitrary reactant distributions. *Computer Physics Communications*, 199(??):40–46, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003902.

Egorova:2019:PSM

[EDPZ19] M. S. Egorova, S. A. Dyachkov, A. N. Parshikov, and V. V. Zhakhovsky. Parallel SPH modeling using dynamic domain decomposition and load balancing displacement of Voronoi subdomains. *Computer Physics Communications*, 234(??):112–125, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302765.

Eremina:2012:NSD

[EEGW12] Elena Eremina, Yuri Eremin, Natalia Grishina, and Thomas Wriedt. New scheme of the Discrete Sources Method for investigation of a near field enhancement by coupled particles. *Computer Physics Communications*, 183(8):1753–1759, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001245.

Engelhard:2010:SSP

[EFG+10] Guy Engelhard, Jonathan L. Feng, Iftah Galon, David Sanford, and Felix Yu. SPICE: Simulation package for including flavor in collider events. *Computer Physics Communications*, 181(1):213–226, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003038`.

Exl:2019:PNC

[EFK+19] Lukas Exl, Johann Fischbacher, Alexander Kovacs, Harald Oezelt, Markus Gusenbauer, and Thomas Schrefl. Preconditioned nonlinear conjugate gradient method for micromagnetic energy minimization. *Computer Physics Communications*, 235(??):179–186, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303187`.

ElKacimi:2010:OUE

[EGPS10] M. ElKacimi, D. Goujdami, H. Przysiezniak, and P. Skands. One universal extra dimension in Pythia. *Computer Physics Communications*, 181(1):122–127, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509002586`.

Eichstadt:2018:AHO

[EGT+18] Jan Eichstädt, Mashy Green, Michael Turner, Joaquim Peiró, and David Moxey. Accelerating high-order mesh optimisation with an architecture-independent programming model. *Computer Physics Communications*, 229(??):36–53, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300973`.

Einkemmer:2016:HPC

[Ein16a] Lukas Einkemmer. High performance computing aspects of a dimension independent semi-Lagrangian discontinuous Galerkin code. *Computer Physics Communications*, 202(??):326–336, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465516300017.

Einkemmer:2016:RMS

[Ein16b] Lukas Einkemmer. A resistive magnetohydrodynamics solver using modern C++ and the Boost library. *Computer Physics Communications*, 206(??):69–77, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301047.

Ekman:2019:RPR

[EJG+19] J. Ekman, P. Jönsson, M. Godefroid, C. Nazé, G. Gaigalas, and J. Bieroń. ris 4: a program for relativistic isotope shift calculations. *Computer Physics Communications*, 235(??):433–446, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303138.

El-Kurdi:2015:PFE

[EKDGG15] Yousef El-Kurdi, Maryam Mehri Dehnavi, Warren J. Gross, and Dennis Giannacopoulos. Parallel finite element technique using Gaussian belief propagation. *Computer Physics Communications*, 193(??):38–48, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001186.

Eitzlmayr:2014:NMM

[EKK14] Andreas Eitzlmayr, Gerold Koscher, and Johannes Khinast. A novel method for modeling of complex wall geometries in smoothed particle hydrodynamics. *Computer Physics Communications*, 185(10):2436–2448, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001684.

Edvardsson:2016:CPA

[EKO16] S. Edvardsson, K. Karlsson, and H. Olin. corr3p_tr: a particle approach for the general three-body problem. *Computer Physics Communications*, 200(??):259–273, March

2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004038.

Ekstrand:2011:LMP

[Eks11] Joel Ekstrand. Lambda: a Mathematica package for operator product expansions in vertex algebras. *Computer Physics Communications*, 182(2):409–418, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003760.

Efremenko:2014:MCC

[ELDS14] Dmitry S. Efremenko, Diego G. Loyola, Adrian Doicu, and Robert J. D. Spurr. Multi-core-CPU and GPU-accelerated radiative transfer models based on the discrete ordinate method. *Computer Physics Communications*, 185(12):3079–3089, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002616.

Eisenbach:2017:GAL

[ELL$^+$17a] Markus Eisenbach, Jeff Larkin, Justin Lutjens, Steven Rennich, and James H. Rogers. GPU acceleration of the Locally Selfconsistent Multiple Scattering code for first principles calculation of the ground state and statistical physics of materials. *Computer Physics Communications*, 211(??):2–7, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301953.

Ellis:2017:TZF

[Ell17b] Joshua P. Ellis. Ti*k*Z-Feynman: Feynman diagrams with Ti*k*Z. *Computer Physics Communications*, 210(??):103–123, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302521.

Emeliyanov:2011:NAF

[Eme11] D. Emeliyanov. A new algorithm for fitting tracks with energy losses due to Bremsstrahlung. *Computer Physics Communications*, 182(7):1491–1501, July 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001202.

Engeln:2019:NHB

[EMW19] Isabell Engeln, Margarete Mühlleitner, and Jonas Wittbrodt. N2HDECAY: Higgs boson decays in the different phases of the N2HDM. *Computer Physics Communications*, 234(??):256–262, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302777.

Endrodi:2011:MSI

[End11] Gergely Endrődi. Multidimensional spline integration of scattered data. *Computer Physics Communications*, 182 (6):1307–1314, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000877.

Edvardsson:2015:SET

[ENEO15] S. Edvardsson, M. Neuman, P. Edström, and H. Olin. Solving equations through particle dynamics. *Computer Physics Communications*, 197(??):169–181, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003276.

Erdelyi:2016:SKM

[EPB+16] Zoltán Erdélyi, Mykola Pasichnyy, Volodymyr Bezpalchuk, János J. Tomán, Bence Gajdics, and Andriy M. Gusak. Stochastic kinetic mean field model. *Computer Physics Communications*, 204(??):31–37, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300613.

Elking:2012:HHP

[EPP12] Dennis M. Elking, Lalith Perera, and Lee G. Pedersen. HPAM: Hirshfeld partitioned atomic multipoles. *Computer Physics Communications*, 183(2):390–397, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003316.

Endress:2015:VRP

[EPS15] E. Endress, C. Pena, and K. Sivalingam. Variance reduction with practical all-to-all lattice propagators. *Computer Physics Communications*, 195(??):35–48, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001496.

Er:2014:PSS

[Er14] Guo-Kang Er. Probabilistic solutions of some multi-degree-of-freedom nonlinear stochastic dynamical systems excited by filtered Gaussian white noise. *Computer Physics Communications*, 185(4):1217–1222, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004311.

Eibl:2019:SCR

[ER19] Sebastian Eibl and Ulrich Rüde. A systematic comparison of runtime load balancing algorithms for massively parallel rigid particle dynamics. *Computer Physics Communications*, 244(??):76–85, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302073.

Ermler:2018:JCB

[Erm18] Walter C. Ermler. jj-Coupling-based atomic self-consistent-field calculations with relativistic effective core potentials and two-component spinors. *Computer Physics Communications*, 229(??):182–198, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300894.

Espejo:2012:WFA

[ERP$^+$12] C. Espejo, T. Rangel, Y. Pouillon, A. H. Romero, and X. Gonze. Wannier functions approach to van der Waals interactions in ABINIT. *Computer Physics Communications*, 183(3):480–485, March 2012. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003651.

Estevez-Rams:2015:VLV

[ERPDFLS15] E. Estevez-Rams, C. Perez-Demydenko, B. Aragón Fernández, and R. Lora-Serrano. Visualizing long vectors of measurements by use of the Hilbert curve. *Computer Physics Communications*, 197(??):118–127, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003057.

Eriksson:2010:THDa

[ERS10a] David Eriksson, Johan Rathsman, and Oscar Stål. 2HDMC — two-Higgs-doublet model calculator. *Computer Physics Communications*, 181(1):189–205, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003014. See erratum [ERS10c].

Eriksson:2010:THDb

[ERS10b] David Eriksson, Johan Rathsman, and Oscar Stål. 2HDMC — two-Higgs-doublet model calculator. *Computer Physics Communications*, 181(4):833–834, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004081.

Eriksson:2010:ETH

[ERS10c] David Eriksson, Johan Rathsman, and Oscar Stål. Erratum for “2HDMC — two-Higgs-doublet model calculator” [Comput. Phys. Commun. **181** (2010) 189]. *Computer Physics Communications*, 181(5):985, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004184. See [ERS10a].

Erturk:2015:ETO

[Ert15] M. Erturk. Exponential type orbitals with generalized hyperbolic cosine functions for atomic systems. *Computer Physics Communications*, 194(??):59–63, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465515001484.

Engel:2011:TTM

[ES11] Georg P. Engel and Stefan Schaefer. Testing trivializing maps in the hybrid Monte Carlo algorithm. *Computer Physics Communications*, 182(10):2107–2114, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001573.

Eberl:2016:GDS

[ES16] Helmut Eberl and Vassilis C. Spanos. GravitinoPack and decays of supersymmetric metastable particles. *Computer Physics Communications*, 202(??):310–325, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000291.

Ervik:2017:RFE

[ESM17] Åsmund Ervik, Guadalupe Jiménez Serratos, and Erich A. Müller. raaSAFT: a framework enabling coarse-grained molecular dynamics simulations based on the SAFT-γ Mie force field. *Computer Physics Communications*, 212(??):161–179, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630251X.

Eremenko:2015:CWF

[EUT+15] V. Eremenko, N. J. Upadhyay, I. J. Thompson, Ch. Elster, F. M. Nunes, G. Arbanas, J. E. Escher, L. Hlophe, and on behalf of the TORUS Collaboration. Coulomb wave functions in momentum space. *Computer Physics Communications*, 187(??):195–203, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003373.

Eder:2014:MNA

[EVB14] S. Eder, A. Vernes, and G. Betz. Methods and numerical aspects of nanoscopic contact area estimation in atomistic tribological simulations. *Computer Physics Communications*, 185(1):217–228, January 2014. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003226.

Evstatiev:2014:APS

[Evs14] E. G. Evstatiev. Application of the phase space action principle to finite-size particle plasma simulations in the drift-kinetic approximation. *Computer Physics Communications*, 185(11):2851–2858, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400246X.

Einkemmer:2014:CDG

[EW14a] L. Einkemmer and M. Wiesenberger. A conservative discontinuous Galerkin scheme for the 2D incompressible Navier–Stokes equations. *Computer Physics Communications*, 185(11):2865–2873, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002495.

Eremin:2014:NSD

[EW14b] Yuri Eremin and Thomas Wriedt. New scheme of the Discrete Sources Method for light scattering analysis of a particle breaking interface. *Computer Physics Communications*, 185(12):3141–3150, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400277X.

Eremin:2016:DSM

[EW16] Yuri Eremin and Thomas Wriedt. Discrete sources method for light scattering analysis of non-axisymmetric features of a substrate. *Computer Physics Communications*, 198(??):12–21, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002933.

Exl:2017:GAE

[Exl17] Lukas Exl. A GPU accelerated and error-controlled solver for the unbounded Poisson equation in three dimensions. *Computer Physics Communications*, 221(??):352–357, December

2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302606.

Egami:2011:FPS

[EY11] Yoshiyuki Egami and Keita Yamada. First-principles study on quantum-transport properties of single molecule depending on adsorption conditions. *Computer Physics Communications*, 182(1):103–105, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002651.

Eckert:2016:HAL

[EZBA16] C. H. J. Eckert, E. Zenker, M. Bussmann, and D. Albach. HASEonGPU — an adaptive, load-balanced MPI/GPU-code for calculating the amplified spontaneous emission in high power laser media. *Computer Physics Communications*, 207(??):362–374, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301436.

Eaves:2016:CRV

[EZL+16] Nick A. Eaves, Qingan Zhang, Fengshan Liu, Hongsheng Guo, Seth B. Dworkin, and Murray J. Thomson. CoFlame: a refined and validated numerical algorithm for modeling sooting laminar coflow diffusion flames. *Computer Physics Communications*, 207(??):464–477, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301813.

Fang:2019:FSD

[Fan19] Yao-Lung L. Fang. FDTD: Solving $1+1$D delay PDE in parallel. *Computer Physics Communications*, 235(??):422–432, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830314X.

Fawzy:2010:CAF

[Faw10] Wafaa M. Fawzy. A code for analysis of the fine structure in near-rigid weakly-bonded open-shell complexes that consist of a diatomic radical in a $^3\Sigma$ state and a closed-shell molecule. *Computer Physics Communications*, 181(10):1789–1801, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510002432`.

Furuseth:2019:PHP

[FB19] Sondre Vik Furuseth and Xavier Buffat. Parallel high-performance multi-beam multi-bunch simulations. *Computer Physics Communications*, 244(??):180–186, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465519301936`.

Foucar:2012:CCA

[FBC+12] Lutz Foucar, Anton Barty, Nicola Coppola, Robert Hartmann, Peter Holl, Uwe Hoppe, Stephan Kassemeyer, Nils Kimmel, Jochen Küpper, Mirko Scholz, Simone Techert, Thomas A. White, Lothar Strüder, and Joachim Ullrich. CASS–CFEL–ASG software suite. *Computer Physics Communications*, 183(10):2207–2213, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001622`.

Freire:2010:CSI

[FBG10] Joana G. Freire, Owen J. Brison, and Jason A. C. Gallas. Complete sets of initial vectors for pattern growth with elementary cellular automata. *Computer Physics Communications*, 181(4):750–755, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003993`.

Faugeras:2017:OCC

[FBHB17] Blaise Faugeras, Jacques Blum, Holger Heumann, and Cédric Boulbe. Optimal control of a coupled partial and ordinary differential equations system for the assimilation of polarimetry Stokes vector measurements in tokamak free-boundary equilibrium reconstruction with application to ITER. *Computer Physics Communications*, 217(??):43–57, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301066.

Frances:2013:PAF

[FBN+13] J. Francés, S. Bleda, C. Neipp, A. Márquez, I. Pascual, and A. Beléndez. Performance analysis of the FDTD method applied to holographic volume gratings: Multi-core CPU versus GPU computing. *Computer Physics Communications*, 184(3):469–479, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003128.

Fischermeier:2014:SHS

[FBP+14] Ellen Fischermeier, Dominik Bartuschat, Tobias Preclik, Matthieu Marechal, and Klaus Mecke. Simulation of a hard-spherocylinder liquid crystal with the *pe*. *Computer Physics Communications*, 185(12):3156–3161, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002926.

Frankowski:2015:SSA

[FCC15] Marek Frankowski, Jakub Checiński, and Maciej Czapkiewicz. Spatial Spectrum Analyzer (SSA): a tool for calculations of spatial distribution of Fast Fourier Transform spectrum from Object Oriented Micromagnetic Framework output data. *Computer Physics Communications*, 189(??):207–212, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004159.

Ferro-Costas:2018:QPT

[FCCTFR18] David Ferro-Costas, M. Natália D. S. Cordeiro, Donald G. Truhlar, and Antonio Fernández-Ramos. Q2DTor: a program to treat torsional anharmonicity through coupled pair torsions in flexible molecules. *Computer Physics Communications*, 232(??):190–205, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302108.

Fan:2017:EMD

[FCVH17] Zheyong Fan, Wei Chen, Ville Vierimaa, and Ari Harju. Efficient molecular dynamics simulations with many-body potentials on graphics processing units. *Computer Physics Communications*, 218(??):10–16, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301339.

Fiore:2013:EBM

[FD13] Carlos E. Fiore and Cláudio J. DaSilva. Equivalence between microcanonical ensembles for lattice models. *Computer Physics Communications*, 184(5):1426–1431, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000271.

Ferrero:2012:SPM

[FDWC12] Ezequiel E. Ferrero, Juan Pablo De Francesco, Nicolás Wolovick, and Sergio A. Cannas. q-state Potts model metastability study using optimized GPU-based Monte Carlo algorithms. *Computer Physics Communications*, 183(8):1578–1587, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000884.

Fambri:2017:STA

[FDZ17] Francesco Fambri, Michael Dumbser, and Olindo Zanotti. Space-time adaptive ADER–DG schemes for dissipative flows: Compressible Navier–Stokes and resistive MHD equations. *Computer Physics Communications*, 220(??):297–318, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302448.

Fleischhaker:2011:MSS

[FE11] Robert Fleischhaker and Jörg Evers. A Maxwell–Schrödinger solver for quantum optical few-level systems. *Computer Physics Communications*, 182(3):739–747, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004194.

Frisch:2011:HPP

[FEH11] W. Frisch, H. Eberl, and H. Hluchá. HFOLD — a program package for calculating two-body MSSM Higgs decays at full one-loop level. *Computer Physics Communications*, 182(10):2219–2226, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001639`.

Feng:2012:AGM

[Fen12a] Feng Feng. $apart: a generalized Mathematica `Apart` function. *Computer Physics Communications*, 183(10):2158–2164, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001300`.

Feng:2012:RMC

[Fen12b] Feng Feng. A recursive method to calculate UV-divergent parts at one-loop level in dimensional regularization. *Computer Physics Communications*, 183(7):1519–1524, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000677`.

Feng:2016:AGM

[Fen16] Feng Feng. APart 2: a generalized Mathematica Apart function. *Computer Physics Communications*, 198(??):260–261, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003501`.

Ferrand:2015:GVG

[Fer15] Patrick Ferrand. GPScan.VI: a general-purpose LabVIEW program for scanning imaging or any application requiring synchronous analog voltage generation and data acquisition. *Computer Physics Communications*, 192(??):342–347, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001095`.

Filho:2011:SMP

[FF11] Tarcísio M. Rocha Filho and Annibal Figueiredo. [SADE]: a Maple package for the symmetry analysis of differential equations. *Computer Physics Communications*, 182(2):467–476, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003814.

Fujiwara:2011:MDS

[FFIH11] Susumu Fujiwara, Daiki Funaoka, Takashi Itoh, and Masato Hashimoto. Molecular dynamics simulation for phase behavior of amphiphilic solution. *Computer Physics Communications*, 182(1):192–194, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002456.

Fang:2014:PTS

[FFT+14] Ye Fang, Sheng Feng, Ka-Ming Tam, Zhifeng Yun, Juana Moreno, J. Ramanujam, and Mark Jarrell. Parallel tempering simulation of the three-dimensional Edwards–Anderson model with compact asynchronous multispin coding on GPU. *Computer Physics Communications*, 185(10):2467–2478, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001854.

Franco:2013:SPC

[FG13] J. M. Franco and I. Gómez. Some procedures for the construction of high-order exponentially fitted Runge–Kutta–Nyström methods of explicit type. *Computer Physics Communications*, 184(4):1310–1321, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004249.

Ferrando:2011:OBG

[FGC+11] N. Ferrando, M. A. Gosálvez, J. Cerdá, R. Gadea, and K. Sato. Octree-based, GPU implementation of a continuous cellular automaton for the simulation of complex, evolving surfaces. *Computer Physics Communications*, 182(3):628–640, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004509.

Frezzotti:2011:SBE

[FGG11] A. Frezzotti, G. P. Ghiroldi, and L. Gibelli. Solving the Boltzmann equation on GPUs. *Computer Physics Communications*, 182(12):2445–2453, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002402.

Farhi:2011:QMC

[FGGM11] Edward Farhi, Jeffrey Goldstone, David Gosset, and Harvey B. Meyer. A quantum Monte Carlo method at fixed energy. *Computer Physics Communications*, 182(8):1663–1673, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001524.

FroeseFischer:2019:GFV

[FGJB19] C. Froese Fischer, G. Gaigalas, P. Jönsson, and J. Bieroń. GRASP2018 — a Fortran 95 version of the General Relativistic Atomic Structure Package. *Computer Physics Communications*, 237(??):184–187, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303928.

Fillion-Gourdeau:2012:NST

[FGLB12] François Fillion-Gourdeau, Emmanuel Lorin, and André D. Bandrauk. Numerical solution of the time-dependent Dirac equation in coordinate space without fermion-doubling. *Computer Physics Communications*, 183(7):1403–1415, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000653.

Franco:2014:OET

[FGR14] J. M. Franco, I. Gómez, and L. Rández. Optimization of explicit two-step hybrid methods for solving orbital and oscillatory problems. *Computer Physics Communications*, 185(10):2527–2537, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002045.

Fu:2017:SSR

[FHA17] Lin Fu, Xiangyu Y. Hu, and Nikolaus A. Adams. Single-step reinitialization and extending algorithms for level-set based multi-phase flow simulations. *Computer Physics Communications*, 221(??):63–80, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730245X.

Fritzsche:2014:IRC

[FHH+14] T. Fritzsche, T. Hahn, S. Heinemeyer, F. von der Pahlen, H. Rzehak, and C. Schappacher. The implementation of the renormalized complex MSSM in FeynArts and FormCalc. *Computer Physics Communications*, 185(6):1529–1545, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400037X.

Fourey:2017:EFC

[FHTO17] G. Fourey, C. Hermange, D. Le Touzé, and G. Oger. An efficient FSI coupling strategy between smoothed particle hydrodynamics and finite element methods. *Computer Physics Communications*, 217(??):66–81, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301194.

Filho:2013:SVE

[Fil13] Tarcísio M. Rocha Filho. Solving the Vlasov equation for one-dimensional models with long range interactions on a GPU. *Computer Physics Communications*, 184(1):34–39, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002585.

Filho:2014:MDL

[Fil14] Tarcísio M. Rocha Filho. Molecular dynamics for long-range interacting systems on graphic processing units. *Computer Physics Communications*, 185(5):1364–1369, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000216.

Fischbacher:2012:NTV

[Fis12] Thomas Fischbacher. Numerical tools to validate stationary points of SO(8)-gauged $N = 8$, $D = 4$ supergravity. *Computer Physics Communications*, 183(3):780–784, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003845.

Fu:2019:OPS

[FJ19] Lin Fu and Zhe Ji. An optimal particle setup method with Centroidal Voronoi Particle dynamics. *Computer Physics Communications*, 234(??):72–92, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302972.

Ferrand:2017:UOB

[FJK+17] Martin Ferrand, Antoine Joly, Christophe Kassiotis, Damien Violeau, Agnès Leroy, François-Xavier Morel, and Benedict D. Rogers. Unsteady open boundaries for SPH using semi-analytical conditions and Riemann solver in 2D. *Computer Physics Communications*, 210(??):29–44, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302806.

Fitzgerald:2012:DPM

[FK12] M. Fitzgerald and J. Khachan. A 2-D PIC/MC/Vlasov method for electrostatic fusion discharges. *Computer Physics Communications*, 183(4):971–979, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000033.

Feger:2015:LMA

[FK15] Robert Feger and Thomas W. Kephart. LieART — a Mathematica application for Lie algebras and representation theory. *Computer Physics Communications*, 192(??):166–195, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000119.

Frijters:2015:PHK

[FKH15] S. Frijters, T. Krüger, and J. Harting. Parallelised Hoshen–Kopelman algorithm for lattice-Boltzmann simulations. *Computer Physics Communications*, 189(??):92–98, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004342.

Finkenrath:2013:FGC

[FKL13] Jacob Finkenrath, Francesco Knechtli, and Björn Leder. Fermions as global correction: the QCD case. *Computer Physics Communications*, 184(6):1522–1534, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000374.

Fucik:2019:MMH

[FKS+19] Radek Fucík, Jakub Klinkovský, Jakub Solovský, Tomás Oberhuber, and Jirí Mikyska. Multidimensional mixed-hybrid finite element method for compositional two-phase flow in heterogeneous porous media and its parallel implementation on GPU. *Computer Physics Communications*, 238(??):165–180, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830420X.

Falls:2016:XVR

[FLA+16] Zackary Falls, David C. Lonie, Patrick Avery, Andrew Shamp, and Eva Zurek. XtalOpt version r9: an open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 199(??):178–179, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003690.

Farris:2019:HFM

[FLE19] Alfred C. K. Farris, Ying Wai Li, and Markus Eisenbach. Histogram-free multicanonical Monte Carlo sampling to calculate the density of states. *Computer Physics Communications*, 235(??):297–304, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465518303485.

Fernandes:2010:BCM

[FLP10] F. P. Fernandes, F. W. S. Lima, and J. A. Plascak. Blume–Capel model on directed and undirected small-world Voronoi–Delaunay random lattices. *Computer Physics Communications*, 181(7):1218–1223, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000871.

Feng:2013:ICI

[FLSZ13] Y. Feng, T. Lunt, F. Sardei, and X. Zha. Implicit coupling of impurity transport at the SOL-core interface. *Computer Physics Communications*, 184(6):1555–1561, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000477.

Fang:2010:ERM

[FLW10] Yonglei Fang, Qinghong Li, and Xinyuan Wu. Extended RKN methods with FSAL property for oscillatory systems. *Computer Physics Communications*, 181(9):1538–1548, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001451.

Foerster:2017:CAC

[FLW17] A. Foerster, H. A. M. Leymann, and J. Wiersig. Computer-aided cluster expansion: an efficient algebraic approach for open quantum many-particle systems. *Computer Physics Communications*, 212(??):210–219, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303162.

Fan:2018:VCJ

[FLZ+18] Linyu Fan, Jianwei Liao, Junsen Zuo, Kebo Zhang, Chao Li, and Hailing Xiong. Version 4.0 of code Java for 3D simulation of the CCA model. *Computer Physics Communications*, 228(??):290–292, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465518300869.

Fiori:2012:NAA

[FM12] Marcelo Fiori and J. E. Miraglia. New approach for approximating the continuum wave function by Gaussian basis set. *Computer Physics Communications*, 183(12):2528–2534, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002299.

Furuichi:2015:ISM

[FM15] Mikito Furuichi and Dave A. May. Implicit solution of the material transport in Stokes flow simulation: Toward thermal convection simulation surrounded by free surface. *Computer Physics Communications*, 192(??):1–11, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000569.

Favata:2016:ABM

[FMRP16] Antonino Favata, Andrea Micheletti, Seunghwa Ryu, and Nicola M. Pugno. An analytical benchmark and a Mathematica program for MD codes: Testing LAMMPS on the 2nd generation Brenner potential. *Computer Physics Communications*, 207(??):426–431, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301679.

Fang:2010:ERT

[FMW10] Yonglei Fang, Qinghe Ming, and Xinyuan Wu. Extended RKN-type methods with minimal dispersion error for perturbed oscillators. *Computer Physics Communications*, 181(3):639–650, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003889.

Furuichi:2017:ILB

[FN17] Mikito Furuichi and Daisuke Nishiura. Iterative load-balancing method with multigrid level relaxation for particle simulation with short-range interactions. *Computer Physics*

Communications, 219(??):135–148, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301571`.

Frances:2010:RID

[FNPMB10] J. Francés, C. Neipp, M. Pérez-Molina, and A. Beléndez. Rigorous interference and diffraction analysis of diffractive optic elements using the finite-difference time-domain method. *Computer Physics Communications*, 181(12):1963–1973, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003504`.

Frances:2015:MGM

[FOB+15] J. Francés, B. Otero, S. Bleda, S. Gallego, C. Neipp, A. Márquez, and A. Beléndez. Multi-GPU and multi-CPU accelerated FDTD scheme for vibroacoustic applications. *Computer Physics Communications*, 191(??):43–51, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000375`.

Fonseca:2012:CRG

[Fon12] Renato M. Fonseca. Calculating the renormalisation group equations of a SUSY model with Susyno. *Computer Physics Communications*, 183(10):2298–2306, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001865`.

Fowlie:2018:FCI

[Fow18] Andrew Fowlie. A fast C++ implementation of thermal functions. *Computer Physics Communications*, 228(??):264–272, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300444`.

Francisco:2014:END

[FP14] E. Francisco and A. Martín Pendás. Electron number distribution functions from molecular wavefunctions. Version 2. *Computer Physics Communications*, 185(10):2663–2682, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001635.

Fu:2017:LJT

[FPY+17] S.-P. Fu, Z. Peng, H. Yuan, R. Kfoury, and Y. N. Young. Lennard-Jones type pair-potential method for coarse-grained lipid bilayer membrane simulations in LAMMPS. *Computer Physics Communications*, 210(??):193–203, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302892.

Frerichs:2015:SCI

[FR15] H. Frerichs and D. Reiter. Stability and control of iterated non-linear transport solvers for fusion edge plasmas. *Computer Physics Communications*, 188(??):82–87, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003798.

Frerichs:2010:BSG

[FRFH10] H. Frerichs, D. Reiter, Y. Feng, and D. Harting. Block-structured grids in Lagrangian 3D edge plasma transport simulations. *Computer Physics Communications*, 181(1):61–70, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002793.

Fattebert:2012:DLB

[FRG12] J.-L. Fattebert, D. F. Richards, and J. N. Glosli. Dynamic load balancing algorithm for molecular dynamics based on Voronoi cells domain decompositions. *Computer Physics Communications*, 183(12):2608–2615, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002524.

Frigori:2010:UST

[Fri10] Rafael B. Frigori. Universality in short-time critical gluodynamics with heat-bath-inspired algorithms. *Computer Physics Communications*, 181(8):1388–1391, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001165.

Fritzsche:2012:RPR

[Fri12] S. Fritzsche. The Ratip program for relativistic calculations of atomic transition, ionization and recombination properties. *Computer Physics Communications*, 183(7):1525–1559, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000690.

Frigori:2014:NLG

[Fri14a] Rafael B. Frigori. Nonextensive lattice gauge theories: Algorithms and methods. *Computer Physics Communications*, 185(8):2232–2239, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001398.

Fritzsche:2014:FTQ

[Fri14b] S. Fritzsche. The Feynman tools for quantum information processing: Design and implementation. *Computer Physics Communications*, 185(6):1697–1718, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000356.

Frigori:2017:PPL

[Fri17] Rafael B. Frigori. PHAST: Protein-like heteropolymer analysis by statistical thermodynamics. *Computer Physics Communications*, 215(??):165–172, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300334.

Fritzsche:2019:FCA

[Fri19] Stephan Fritzsche. A fresh computational approach to atomic structures, processes and cascades. *Computer Physics Communications*, 240(??):1–14, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300189.

FroeseFischer:2011:BSH

[Fro11] Charlotte Froese Fischer. A B-spline Hartree–Fock program. *Computer Physics Communications*, 182(6):1315–1326, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000324.

Falloon:2017:QMP

[FRW17] Peter E. Falloon, Jeremy Rodriguez, and Jingbo B. Wang. QSWalk: a Mathematica package for quantum stochastic walks on arbitrary graphs. *Computer Physics Communications*, 217(??):162–170, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301029.

Farhi:2017:NMC

[FS17] Asaf Farhi and Bipin Singh. A novel method for calculating relative free energy of similar molecules in two environments. *Computer Physics Communications*, 212(??):132–145, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303411.

Fischbacher:2013:FNS

[FSC13] Thomas Fischbacher and Franziska Synatschke-Czerwonka. FlowPy — a numerical solver for functional renormalization group equations. *Computer Physics Communications*, 184(8):1931–1945, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000994.

Florens:2011:OBA

[FSF11] M. Florens, B. Sapoval, and M. Filoche. The optimal branching asymmetry of a bidirectional distribution tree. *Computer Physics Communications*, 182(9):1932–1936, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004546.

Fan:2013:AMD

[FSH13] Zheyong Fan, Topi Siro, and Ari Harju. Accelerated molecular dynamics force evaluation on graphics processing units for thermal conductivity calculations. *Computer Physics Communications*, 184(5):1414–1425, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000258.

Fan:2016:MPM

[FSJ+16] Tian-E Fan, Gui-Fang Shao, Qing-Shuang Ji, Ji-Wen Zheng, Tun dong Liu, and Yu-Hua Wen. A multi-populations multi-strategies differential evolution algorithm for structural optimization of metal nanoclusters. *Computer Physics Communications*, 208(??):64–72, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302314.

Faik:2018:ESP

[FTI18] Steffen Faik, Anna Tauschwitz, and Igor Iosilevskiy. The equation of state package FEOS for high energy density matter. *Computer Physics Communications*, 227(??):117–125, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300122.

Fu:2019:LDF

[Fu19a] Lin Fu. A low-dissipation finite-volume method based on a new TENO shock-capturing scheme. *Computer Physics Communications*, 235(??):25–39, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303576.

Fu:2019:VHO

[Fu19b] Lin Fu. A very-high-order TENO scheme for all-speed gas dynamics and turbulence. *Computer Physics Communications*, 244(??):117–131, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302000.

Fuhrmann:2015:CNT

[Fuh15] Jürgen Fuhrmann. Comparison and numerical treatment of generalised Nernst–Planck models. *Computer Physics Communications*, 196(??):166–178, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002490`.

Fukushima:2017:NCE

[Fuk17] Toshio Fukushima. Numerical computation of electromagnetic field for general static and axisymmetric current distribution. *Computer Physics Communications*, 221(??):109–117, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302503`.

Fan:2014:ELS

[FUSH14] Zheyong Fan, Andreas Uppstu, Topi Siro, and Ari Harju. Efficient linear-scaling quantum transport calculations on graphics processing units and applications on electron transport in graphene. *Computer Physics Communications*, 185(1):28–39, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002701`.

Fan:2018:GEL

[FVH18] Zheyong Fan, Ville Vierimaa, and Ari Harju. GPUQT: An efficient linear-scaling quantum transport code fully implemented on graphics processing units. *Computer Physics Communications*, 230(??):113–120, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301280`.

Fernandes:2011:NRM

[FW11] Heitor C. M. Fernandes and Martin Weigel. Non-reversible Monte Carlo simulations of spin models. *Computer Physics Communications*, 182(9):1856–1859, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004637`.

Frust:2017:RDP

[FWS+17] Tobias Frust, Michael Wagner, Jan Stephan, Guido Juckeland, and André Bieberle. Rapid data processing for ultrafast X-ray computed tomography using scalable and modular CUDA based pipelines. *Computer Physics Communications*, 219(??):353–360, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301674.

Feng:2012:FPC

[FWZ+12] Wanxiang Feng, Jun Wen, Jinjian Zhou, Di Xiao, and Yugui Yao. First-principles calculation of Z_2 topological invariants within the FP–LAPW formalism. *Computer Physics Communications*, 183(9):1849–1859, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001312.

Feng:2014:SCM

[FXZ+14] Xueshang Feng, Changqing Xiang, Dingkun Zhong, Yufen Zhou, Liping Yang, and Xiaopeng Ma. SIP–CESE MHD model of solar wind with adaptive mesh refinement of hexahedral meshes. *Computer Physics Communications*, 185(7):1965–1980, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001076.

Fallahi:2018:MFW

[FYK18] Arya Fallahi, Alireza Yahaghi, and Franz X. Kärtner. MITHRA 1.0: A full-wave simulation tool for free electron lasers. *Computer Physics Communications*, 228(??):192–208, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300833.

Feldman:2016:PSI

[FZ16] Baruch Feldman and Yunkai Zhou. A partitioned shift-without-invert algorithm to improve parallel eigensolution efficiency in real-space electronic transport. *Computer Physics Communications*, 207(??):105–113, October 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301394.

Francisquez:2019:MTI

[FZR19] M. Francisquez, B. Zhu, and B. N. Rogers. Multigrid treatment of implicit continuum diffusion. *Computer Physics Communications*, 236(??):104–117, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303709.

Fu:2013:AMS

[FZY13] Hong Fu, Limin Zheng, and Minghui Yang. Accelerating modified Shepard interpolated potential energy calculations using graphics processing units. *Computer Physics Communications*, 184(4):1150–1154, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004018.

Fu:2017:PPC

[FZY17] Yongsheng Fu, Jiaolong Zeng, and Jianmin Yuan. PCTDSE: a parallel Cartesian-grid-based TDSE solver for modeling laser-atom interactions. *Computer Physics Communications*, 210(??):181–192, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302879.

Golbabai:2010:NMD

[GA10] A. Golbabai and M. M. Arabshahi. A numerical method for diffusion-convection equation using high-order difference schemes. *Computer Physics Communications*, 181(7):1224–1230, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000883.

Greppi:2013:ECP

[GA13] Paolo Greppi and Elisabetta Arato. Efficient computation paths for the systematic analysis of sensitivities. *Computer Physics Communications*, 184(1):79–85, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002846.

Gilbreth:2015:SCE

[GA15] C. N. Gilbreth and Y. Alhassid. Stabilizing canonical-ensemble calculations in the auxiliary-field Monte Carlo method. *Computer Physics Communications*, 188(??):1–6, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003075.

Grandgirard:2016:GFG

[GAB+16] V. Grandgirard, J. Abiteboul, J. Bigot, T. Cartier-Michaud, N. Crouseilles, G. Dif-Pradalier, Ch. Ehrlacher, D. Esteve, X. Garbet, Ph. Ghendrih, G. Latu, M. Mehrenberger, C. Norscini, Ch. Passeron, F. Rozar, Y. Sarazin, E. Sonnendrücker, A. Strugarek, and D. Zarzoso. A 5D gyrokinetic full-f global semi-Lagrangian code for flux-driven ion turbulence simulations. *Computer Physics Communications*, 207(??):35–68, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301230.

Gaenko:2017:UCL

[GAC+17] A. Gaenko, A. E. Antipov, G. Carcassi, T. Chen, X. Chen, Q. Dong, L. Gamper, J. Gukelberger, R. Igarashi, S. Iskakov, M. Könz, J. P. F. LeBlanc, R. Levy, P. N. Ma, J. E. Paki, H. Shinaoka, S. Todo, M. Troyer, and E. Gull. Updated core libraries of the ALPS project. *Computer Physics Communications*, 213(??):235–251, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303885.

Gagunashvili:2012:CCT

[Gag12a] N. D. Gagunashvili. CHICOM: a code of tests for comparing unweighted and weighted histograms and two weighted histograms. *Computer Physics Communications*, 183(1):193–196, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002864.

Gagunashvili:2012:CCG

[Gag12b] N. D. Gagunashvili. CHIWEI: a code of goodness of fit tests for weighted and unweighted histograms. *Computer Physics Communications*, 183(2):418–421, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003377.

Gao:2016:RMG

[GAGW16] Connie W. Gao, Joshua W. Allen, William H. Green, and Richard H. West. Reaction mechanism generator: Automatic construction of chemical kinetic mechanisms. *Computer Physics Communications*, 203(??):212–225, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300285.

Goicochea:2015:RDR

[GAHP15] A. Gama Goicochea, M. A. Balderas Altamirano, J. D. Hernández, and E. Pérez. The role of the dissipative and random forces in the calculation of the pressure of simple fluids with dissipative particle dynamics. *Computer Physics Communications*, 188(??):76–81, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003762.

Gainullin:2017:HPG

[Gai17] I. K. Gainullin. High-performance GPU parallel solver for 3D modeling of electron transfer during ion-surface interaction. *Computer Physics Communications*, 210(??):72–78, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303058.

Gao:2013:CPC

[Gao13a] Jun Gao. CIJET: a program for computation of jet cross sections induced by quark contact interactions at hadron colliders. *Computer Physics Communications*, 184(10):2362–2366, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001793.

Guo:2013:LSN

[GAO13b] Hua Guo, Peter Arbenz, and Benedikt Oswald. A large-scale nonlinear eigensolver for the analysis of dispersive nanostructures. *Computer Physics Communications*, 184(8):1898–1906, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001112.

Garnier:2019:DVC

[Gar19] Romain Garnier. Dual vibration configuration interaction (DVCI). An efficient factorization of molecular Hamiltonian for high performance infrared spectrum computation. *Computer Physics Communications*, 234(??):263–277, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302571.

Gramada:2011:CGE

[GB11] Apostol Gramada and Philip E. Bourne. Coarse-graining the electrostatic potential via distributed multipole expansions. *Computer Physics Communications*, 182(7):1455–1462, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000920.

Green:2014:IAP

[GB14] D. L. Green and L. A. Berry. Iterative addition of parallel temperature effects to finite-difference simulation of radio-frequency wave propagation in plasmas. *Computer Physics Communications*, 185(3):736–743, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003779.

Guo:2017:GIR

[GB17] Yachong Guo and Vladimir A. Baulin. GPU implementation of the Rosenbluth generation method for static Monte Carlo simulations. *Computer Physics Communications*, 216(??):95–101, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300929.

Gomes:2018:ERL

[GBC+18] Jorge Gomes, Emanuele Bagnaschi, Isabel Campos, Mario David, Luís Alves, João Martins, João Pina, Alvaro López-García, and Pablo Orviz. Enabling rootless Linux Containers in multi-user environments: the `udocker` tool. *Computer Physics Communications*, 232(??):84–97, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302042.

Gebremariam:2010:SCH

[GBD10] B. Gebremariam, S. K. Bogner, and T. Duguet. Symbolic computation of the Hartree–Fock energy from a chiral EFT three-nucleon interaction at N^2 LO. *Computer Physics Communications*, 181(6):1167–1177, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000603.

Grossu:2014:HPF

[GBFJ14] I. V. Grossu, C. Besliu, D. Felea, and Al. Jipa. High precision framework for chaos many-body engine. *Computer Physics Communications*, 185(4):1339–1342, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004360.

Grossu:2010:CCC

[GBJ+10] I. V. Grossu, C. Besliu, Al. Jipa, C. C. Bordeianu, D. Felea, E. Stan, and T. Esanu. Code C# for chaos analysis of relativistic many-body systems. *Computer Physics Communications*, 181(8):1464–1470, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001384.

Grossu:2012:CCC

[GBJ+12] I. V. Grossu, C. Besliu, Al. Jipa, E. Stan, T. Esanu, D. Felea, and C. C. Bordeianu. Code C# for chaos analysis of relativistic many-body systems with reactions. *Computer Physics Communications*, 183(4):1055–1059, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465512000124.

Grossu:2013:CMB

[GBJ+13] I. V. Grossu, C. Besliu, Al. Jipa, D. Felea, T. Esanu, E. Stan, and C. C. Bordeianu. Chaos Many-Body Engine v03: a new version of code C# for chaos analysis of relativistic many-body systems with reactions. *Computer Physics Communications*, 184(4):1346–1347, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004080.

Grossu:2015:SMP

[GBJ+15] I. V. Grossu, C. Besliu, Al. Jipa, D. Felea, E. Stan, and T. Esanu. Support for massless particles in Chaos Many-Body Engine simulations of nuclear collisions at relativistic energies. *Computer Physics Communications*, 195(??):218–220, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001915.

Grossu:2019:IQC

[GBJ+19] I. V. Grossu, C. Beşliu, Al. Jipa, D. Felea, E. Stan, and T. Eşanu. Implementation of quark confinement and retarded interactions algorithms for Chaos Many-Body Engine. *Computer Physics Communications*, 239(??):157–160, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300426.

Gray:2012:MAP

[GBK+12] A. Gray, I. Bethune, R. Kenway, L. Smith, M. Guest, C. Kitchen, P. Calleja, A. Korzynski, S. Rankin, M. Ashworth, A. Porter, I. Todorov, M. Plummer, E. Jones, L. Steenman-Clark, B. Ralston, and C. Laughton. Mapping application performance to HPC architecture. *Computer Physics Communications*, 183(3):520–529, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003754.

Gabay:2017:OKM

[GBN17] D. Gabay, A. Boag, and A. Natan. Optimizing kernel methods for Poisson integrals on a uniform grid. *Computer Physics Communications*, 215(??):1–6, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300280.

Garnier:2013:EPB

[GBP13] Romain Garnier, André Barka, and Olivier Pascal. Efficient periodic band diagram computation using a finite element method, Arnoldi eigensolver and sparse linear system solver. *Computer Physics Communications*, 184(7):1673–1682, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000684.

Ge:2014:THF

[GBR+14] Xiaochuan Ge, Simon J. Binnie, Dario Rocca, Ralph Gebauer, and Stefano Baroni. turboTDDFT 2.0-Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. *Computer Physics Communications*, 185(7):2080–2089, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400085X.

Gonzalez-Ballestero:2011:NSE

[GBRB11] C. González-Ballestero, L. M. Robledo, and G. F. Bertsch. Numeric and symbolic evaluation of the Pfaffian of general skew-symmetric matrices. *Computer Physics Communications*, 182(10):2213–2218, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001627.

Groen:2016:FFC

[GBS+16a] Derek Groen, Agastya P. Bhati, James Suter, James Hetherington, Stefan J. Zasada, and Peter V. Coveney. FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures. *Computer Physics Communications*, 207(??):375–385, October

2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301448.

Guskova:2016:RPL

[GBS16b] M. S. Guskova, L. Yu. Barash, and L. N. Shchur. RNGAVXLIB: Program library for random number generation, AVX realization. *Computer Physics Communications*, 200(??):402–405, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004117.

Green:2018:KJC

[GBSY18] David L. Green, Lee A. Berry, Adam B. Simpson, and Timothy R. Younkin. Kinetic-j: A computational kernel for solving the linearized Vlasov equation applied to calculations of the kinetic, configuration space plasma current for time harmonic wave electric fields. *Computer Physics Communications*, 225(??):122–127, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300043.

Gontchar:2010:CCD

[GC10] I. I. Gontchar and M. V. Chushnyakova. A C-code for the double folding interaction potential of two spherical nuclei. *Computer Physics Communications*, 181(1):168–182, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002860.

Gan:2012:HMI

[GC12] Yong Gan and J. K. Chen. A hybrid method for integrated atomistic-continuum simulation of ultrashort-pulsed laser interaction with semiconductors. *Computer Physics Communications*, 183(2):278–284, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003304.

Gontchar:2013:CCD

[GC13] I. I. Gontchar and M. V. Chushnyakova. A C-code for the double folding interaction potential for reactions involving deformed target nuclei. *Computer Physics Communications*, 184(1):172–182, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002792.

Gontchar:2016:DCC

[GC16] I. I. Gontchar and M. V. Chushnyakova. DFMSPH14: a C-code for the double folding interaction potential of two spherical nuclei. *Computer Physics Communications*, 206(??):97–102, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301011.

Gontchar:2018:DCC

[GC18] I. I. Gontchar and M. V. Chushnyakova. DFMDEF18: a C-code for the double folding interaction potential of a spherical nucleus with deformed nucleus. *Computer Physics Communications*, 222(??):414–417, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302953.

Guo:2018:GAL

[GCC+18] Xiangyu Guo, Qi Chu, Shin Kee Chung, Zhihui Du, Linqing Wen, and Yanqi Gu. GPU-acceleration on a low-latency binary-coalescence gravitational wave search pipeline. *Computer Physics Communications*, 231(??):62–71, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301504.

Ge:2017:IPS

[GCF+17] Xinmin Ge, Hua Chen, Yiren Fan, Juntao Liu, Jianchao Cai, and Jianyu Liu. An improved pulse sequence and inversion algorithm of T_2 spectrum. *Computer Physics Communications*, 212(??):82–89, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303186.

Guan:2018:RPA

[GCH+18] W. Guan, X. Cheng, J. Huang, G. Huber, W. Li, J. A. McCammon, and B. Zhang. RPYFMM: Parallel adaptive fast multipole method for Rotne–Prager–Yamakawa tensor in biomolecular hydrodynamics simulations. *Computer Physics Communications*, 227(??):99–108, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830033X.

Gu:2015:SCA

[GCHL15] Xian-Ming Gu, Markus Clemens, Ting-Zhu Huang, and Liang Li. The SCBiCG class of algorithms for complex symmetric linear systems with applications in several electromagnetic model problems. *Computer Physics Communications*, 191(??):52–64, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000387.

Gontchar:2019:DCC

[GCK19] I. I. Gontchar, M. V. Chushnyakova, and N. A. Khmyrova. DFMSPH19: a C-code for the double folding interaction potential of two spherical nuclei. *Computer Physics Communications*, 242(??):153–155, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301365.

Grosso:2015:VED

[GCP+15] Bastien Grosso, Valentino R. Cooper, Polina Pine, Adham Hashibon, Yuval Yaish, and Joan Adler. Visualization of electronic density. *Computer Physics Communications*, 195(??):1–13, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001332.

Gusev:2014:KNV

[GCVA14a] A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky, and A. G. Abrashkevich. KANTBP 3.0: New version of a program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel adiabatic approach. *Computer Physics Communications*, 185(12):3341–3343, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002690.

Gusev:2014:PPC

[GCVA14b] A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky, and A. G. Abrashkevich. POTHEA: a program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined 2D elliptic partial differential equation. *Computer Physics Communications*, 185(10):2636–2654, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001374.

Gonzalez:2014:FIP

[GD14] Diego González and Sergio Davis. Fitting of interatomic potentials without forces: a parallel particle swarm optimization algorithm. *Computer Physics Communications*, 185(12):3090–3093, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002628.

Gebremariam:2010:SIP

[GDB10] B. Gebremariam, T. Duguet, and S. K. Bogner. Symbolic integration of a product of two spherical Bessel functions with an additional exponential and polynomial factor. *Computer Physics Communications*, 181(6):1136–1143, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000408. See comment [CCK23].

Gins:2018:ACD

[GdGB+18] W. Gins, R. P. de Groote, M. L. Bissell, C. Granados Buitrago, R. Ferrer, K. M. Lynch, G. Neyens, and S. Sels. Analysis of counting data: Development of the SATLAS Python package. *Computer Physics Communications*, 222(??):286–294, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465517302990.

Geneste:2010:FEF

[Gen10] Grégory Geneste. Free energies of ferroelectric crystals from a microscopic approach. *Computer Physics Communications*, 181(4):732–745, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003968.

Grossu:2013:HFAb

[GES13] I. V. Grossu and S. A. El-Shamali. Hyper-Fractal Analysis v04: Implementation of a fuzzy box-counting algorithm for image analysis of artistic works. *Computer Physics Communications*, 184(7):1812–1813, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000970.

Grossu:2010:NVV

[GFB+10] I. V. Grossu, D. Felea, C. Besliu, Al. Jipa, C. C. Bordeianu, E. Stan, and T. Esanu. A new version of Visual [Basic] tool for estimating the fractal dimension of images. *Computer Physics Communications*, 181(4):831–832, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900397X.

Grossu:2014:CVI

[GFJ+14] I. V. Grossu, D. Felea, Al. Jipa, C. Besliu, E. Stan, O. Ristea, C. Ristea, M. Calin, T. Esanu, C. Bordeianu, and N. Tuturas. CMBE v05-implementation of a toy-model for chaos analysis of relativistic nuclear collisions at the present BNL energies. *Computer Physics Communications*, 185(11):3059–3061, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002197.

Graen:2016:NNS

[GG16] Timo Graen and Helmut Grubmüller. NuSol — numerical solver for the 3D stationary nuclear Schrödinger equation.

Computer Physics Communications, 198(??):169–178, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003203.

Grossu:2013:HFAa

[GGF+13] I. V. Grossu, I. Grossu, D. Felea, C. Besliu, Al. Jipa, T. Esanu, C. C. Bordeianu, and E. Stan. Hyper-Fractal Analysis: a visual tool for estimating the fractal dimension of 4D objects. *Computer Physics Communications*, 184(4):1344–1345, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003943.

Gillet:2016:EFI

[GGG16] Yannick Gillet, Matteo Giantomassi, and Xavier Gonze. Efficient on-the-fly interpolation technique for Bethe–Salpeter calculations of optical spectra. *Computer Physics Communications*, 203(??):83–93, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300236.

Goulko:2019:IHM

[GGG+19] Olga Goulko, Alexander Gaenko, Emanuel Gull, Nikolay Prokof'ev, and Boris Svistunov. Implementation of the bin hierarchy method for restoring a smooth function from a sampled histogram. *Computer Physics Communications*, 236(??):205–213, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303424.

Gehrmann-DeRidder:2014:EES

[GGGH14] A. Gehrmann-De Ridder, T. Gehrmann, E. W. N. Glover, and G. Heinrich. EERAD3: Event shapes and jet rates in electron-positron annihilation at order α_s^3. *Computer Physics Communications*, 185(12):3331–3340, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002677.

Galonska:2013:PUA

[GGI+13] A. Galonska, P. Gibbon, F. Imbeaux, Y. Frauel, B. Guillerminet, G. Manduchi, F. Wolf, and ITM-TF contributors. Parallel universal access layer: a scalable I/O library for integrated tokamak modeling. *Computer Physics Communications*, 184(3):638–646, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003670`.

Ghoshal:2011:DER

[GH11] Arijit Ghoshal and Y. K. Ho. Doubly excited resonance states of two-electron systems in exponential cosine-screened Coulomb potentials. *Computer Physics Communications*, 182(1):122–124, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001645`.

Green:2015:SSP

[GH15] D. G. Green and C. N. Harvey. SIMLA: Simulating particle dynamics in intense laser and other electromagnetic fields via classical and quantum electrodynamics. *Computer Physics Communications*, 192(??):313–321, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000910`.

Gagunashvili:2018:CCG

[GH18] Nikolay D. Gagunashvili and Helgi Halldorsson. CHIWEI: A code of goodness of fit tests for weighted and unweighted histograms in Fortran-77, C++, R and Python. *Computer Physics Communications*, 231(??):245, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301449`.

Gonzalez-Herrero:2018:PAI

[GHBL18] Diego Gonzalez-Herrero, Elisabetta Boella, and Giovanni Lapenta. Performance analysis and implementation details of the Energy Conserving Semi-Implicit Method code (ECsim). *Computer Physics Communications*, 229(??):162–169, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300924.

Giorgino:2010:DCV

[GHdF10] Toni Giorgino, M. J. Harvey, and Gianni de Fabritiis. Distributed computing as a virtual supercomputer: Tools to run and manage large-scale BOINC simulations. *Computer Physics Communications*, 181(8):1402–1409, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001189.

Garcia-Hernandez:2019:NVM

[GHK19] Rubén Jesús García-Hernández and Dieter Kranzlmüller. NOMAD VR: Multiplatform virtual reality viewer for chemistry simulations. *Computer Physics Communications*, 237(??):230–237, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304053.

Gonzalez-Herrero:2019:ECE

[GHMB+19] Diego Gonzalez-Herrero, Alfredo Micera, Elisabetta Boella, Jaeyoung Park, and Giovanni Lapenta. ECsim-CYL: Energy conserving semi-implicit particle in cell simulation in axially symmetric cylindrical coordinates. *Computer Physics Communications*, 236(??):153–163, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303746.

Gagunashvili:2019:CCC

[GHN19] Nikolay D. Gagunashvili, Helgi Halldorsson, and Helmut Neukirchen. CHICOM: Code for comparing weighted or unweighted histograms in Fortran-77, C++, R and Python. *Computer Physics Communications*, 245(??):Article 106872, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302590.

Gremse:2016:GAA

[GHR+16] Felix Gremse, Andreas Höfter, Lukas Razik, Fabian Kiessling, and Uwe Naumann. GPU-accelerated adjoint algorithmic differentiation. *Computer Physics Communications*, 200(??):300–311, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004099.

Gamillscheg:2011:NPT

[GHvdL11] Ralf Gamillscheg, Gundolf Haase, and Wolfgang von der Linden. A numerical projection technique for large-scale eigenvalue problems. *Computer Physics Communications*, 182(10):2168–2173, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002062.

Guillet:2014:TNA

[GHvSF14] J. Ph. Guillet, G. Heinrich, and J. F. von Soden-Fraunhofen. Tools for NLO automation: Extension of the golem95C integral library. *Computer Physics Communications*, 185(6):1828–1834, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000897.

Gingrich:2010:MCE

[Gin10] Douglas M. Gingrich. Monte Carlo event generator for black hole production and decay in proton-proton collisions — QBH version 1.02. *Computer Physics Communications*, 181(11):1917–1924, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002602.

Giorgino:2014:CDA

[Gio14a] Toni Giorgino. Computing 1-D atomic densities in macromolecular simulations: the density profile tool for VMD. *Computer Physics Communications*, 185(1):317–322, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002956.

Giorgino:2014:PGE

[Gio14b] Toni Giorgino. PLUMED-GUI: an environment for the interactive development of molecular dynamics analysis and biasing scripts. *Computer Physics Communications*, 185(3):1109–1114, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004128.

Giorgino:2018:HDC

[Gio18] Toni Giorgino. How to differentiate collective variables in free energy codes: Computer-algebra code generation and automatic differentiation. *Computer Physics Communications*, 228(??):258–263, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300468.

Giuliani:2019:BMC

[Giu19] Nicola Giuliani. BlackNUFFT: Modular customizable black box hybrid parallelization of type 3 NUFFT in 3D. *Computer Physics Communications*, 235(??):324–335, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303539.

Geng:2013:GAD

[GJ13] Weihua Geng and Ferosh Jacob. A GPU-accelerated direct-sum boundary integral Poisson–Boltzmann solver. *Computer Physics Communications*, 184(6):1490–1496, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000349.

Gelmi:2014:IGP

[GJ14] Claudio A. Gelmi and Héctor Jorquera. IDSOLVER: a general purpose solver for n th-order integro-differential equations. *Computer Physics Communications*, 185(1):392–397, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003093.

Ghale:2018:SMV

[GJ18a] Purnima Ghale and Harley T. Johnson. A sparse matrix–vector multiplication based algorithm for accurate density matrix computations on systems of millions of atoms. *Computer Physics Communications*, 227(??):17–26, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300365`.

Guterding:2018:EGA

[GJ18b] Daniel Guterding and Harald O. Jeschke. An efficient GPU algorithm for tetrahedron-based Brillouin-zone integration. *Computer Physics Communications*, 231(??):114–121, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301383`.

Gonze:2016:RDA

[GJA+16] X. Gonze, F. Jollet, F. Abreu Araujo, D. Adams, B. Amadon, T. Applencourt, C. Audouze, J.-M. Beuken, J. Bieder, A. Bokhanchuk, E. Bousquet, F. Bruneval, D. Caliste, M. Côté, F. Dahm, F. Da Pieve, M. Delaveau, M. Di Gennaro, B. Dorado, C. Espejo, G. Geneste, L. Genovese, A. Gerossier, M. Giantomassi, Y. Gillet, D. R. Hamann, L. He, G. Jomard, J. Laflamme Janssen, S. Le Roux, A. Levitt, A. Lherbier, F. Liu, I. Lukačević, A. Martin, C. Martins, M. J. T. Oliveira, S. Poncé, Y. Pouillon, T. Rangel, G.-M. Rignanese, A. H. Romero, B. Rousseau, O. Rubel, A. A. Shukri, M. Stankovski, M. Torrent, M. J. Van Setten, B. Van Troeye, and M. J. Verstraete. Recent developments in the ABINIT software package. *Computer Physics Communications*, 205(??):106–131, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300923`.

Gross:2011:MPR

[GJB11] Jonathan Gross, Wolfhard Janke, and Michael Bachmann. Massively parallelized replica-exchange simulations of polymers on GPUs. *Computer Physics Communications*, 182(8):1638–1644, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465511001433.

Gronbech-Jensen:2014:AGJ

[GJHF14] Niels Grønbech-Jensen, Natha Robert Hayre, and Oded Farago. Application of the G-JF discrete-time thermostat for fast and accurate molecular simulations. *Computer Physics Communications*, 185(2):524–527, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003342.

Gherardi:2012:HDS

[GJLB12] M. Gherardi, T. Jourdan, S. Le Bourdiec, and G. Bencteux. Hybrid deterministic/stochastic algorithm for large sets of rate equations. *Computer Physics Communications*, 183(9):1966–1973, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001592.

Gawronski:2011:CDB

[GK11] Przemyslaw Gawroński and Krzysztof Kulakowski. Crowd dynamics — being stuck. *Computer Physics Communications*, 182(9):1924–1927, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100083X.

Germanas:2010:CFP

[GKM10] D. Germanas, R. K. Kalinauskas, and S. Mickevicius. Calculation of four-particle harmonic-oscillator transformation brackets. *Computer Physics Communications*, 181(2):420–425, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003257.

Garcia:2013:SEP

[GLAC13] Eliseo García, Lorena Lozano, Maria-Jesús Algar, and Felipe Cátedra. A study of the efficiency of the parallelization of a high frequency electromagnetic approach for the computation of radiation and scattering considering multiple bounces. *Computer Physics Communications*, 184(1):45–50, January

2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002603`.

Gerhard:2013:RHG

[GLB13] Jochen Gerhard, Volker Lindenstruth, and Marcus Bleicher. Relativistic hydrodynamics on graphic cards. *Computer Physics Communications*, 184(2):311–319, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002998`.

Gong:2012:PTU

[GLHG12] Chunye Gong, Jie Liu, Haowei Huang, and Zhenghu Gong. Particle transport with unstructured grid on GPU. *Computer Physics Communications*, 183(3):588–593, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003870`.

Gerdt:2019:MPT

[GLHR19] Vladimir P. Gerdt, Markus Lange-Hegermann, and Daniel Robertz. The MAPLE package TDDS for computing Thomas decompositions of systems of nonlinear PDEs. *Computer Physics Communications*, 234(??):202–215, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302820`.

Gomez-Lobo:2012:SMP

[GLMG12] Alfonso García-Parrado Gómez-Lobo and José M. Martín-García. Spinors: a Mathematica package for doing spinor calculus in General Relativity. *Computer Physics Communications*, 183(10):2214–2225, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001634`.

Gavin:2011:FCH

[GLPQ11] Ryan Gavin, Ye Li, Frank Petriello, and Seth Quackenbush. FEWZ 2.0: a code for hadronic Z production at next-to-next-to-leading order. *Computer Physics Communications*, 182(11):2388–2403, November 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002189.

Giorgino:2017:MGU

[GLR17] Toni Giorgino, Alessandro Laio, and Alex Rodriguez. METAGUI 3: a graphical user interface for choosing the collective variables in molecular dynamics simulations. *Computer Physics Communications*, 217(??):204–209, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301236.

Gao:2013:MPC

[GLS+13] Jun Gao, Zhihua Liang, Davison E. Soper, Hung-Liang Lai, Pavel M. Nadolsky, and C.-P. Yuan. MEKS: a program for computation of inclusive jet cross sections at hadron colliders. *Computer Physics Communications*, 184(6):1626–1642, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000611.

Guo:2014:CFE

[GLW14] Zhenlin Guo, Ping Lin, and Yangfan Wang. Continuous finite element schemes for a phase field model in two-layer fluid Bénard–Marangoni convection computations. *Computer Physics Communications*, 185(1):63–78, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002798.

Guan:2014:NAS

[GLX+14] Xin Guan, Kristina D. Launey, Mingxia Xie, Lina Bao, Feng Pan, and Jerry P. Draayer. Numerical algorithm for the standard pairing problem based on the Heine–Stieltjes correspondence and the polynomial approach. *Computer Physics Communications*, 185(10):2714–2723, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001970.

Georgoudis:2017:AAG

[GLZ17] Alessandro Georgoudis, Kasper J. Larsen, and Yang Zhang. Azurite: an algebraic geometry based package for finding bases of loop integrals. *Computer Physics Communications*, 221(??):203–215, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551730259X`.

Ghodrat:2011:MDS

[GM11] Malihe Ghodrat and Afshin Montakhab. Molecular dynamics simulation of a relativistic gas: Thermostatistical properties. *Computer Physics Communications*, 182(9):1909–1913, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000385`.

Grisins:2014:MHT

[GM14] Pjotrs Grisins and Igor E. Mazets. Metropolis–Hastings thermal state sampling for numerical simulations of Bose–Einstein condensates. *Computer Physics Communications*, 185(7):1926–1931, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001015`.

Gonoskov:2016:SSP

[GM16] Ivan Gonoskov and Mattias Marklund. Single-step propagators for calculation of time evolution in quantum systems with arbitrary interactions. *Computer Physics Communications*, 202(??):211–215, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300212`.

Gituliar:2017:FTR

[GM17] Oleksandr Gituliar and Vitaly Magerya. Fuchsia: a tool for reducing differential equations for Feynman master integrals to epsilon form. *Computer Physics Communications*, 219(??):329–338, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301340`.

Gupta:2018:ALQ

[GM18] Sourendu Gupta and Pushan Majumdar. Accelerating lattice QCD simulations with 2 flavors of staggered fermions on multiple GPUs using OpenACC — a first attempt. *Computer Physics Communications*, 228(??):44–53, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300808`.

Garcia:2018:SCM

[GMC18] Eliseo García, Javier Moreno, and Felipe Cátedra. Speeding-up the CBFM–MLFMA approach for scattering analysis of very large electromagnetic problems. *Computer Physics Communications*, 232(??):177–189, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301565`.

Gao:2017:PDF

[GMF+17] Xingyu Gao, Zeyao Mo, Jun Fang, Haifeng Song, and Han Wang. Parallel 3-dim fast Fourier transforms with load balancing of the plane waves. *Computer Physics Communications*, 211(??):54–60, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516301837`.

Grise:2011:SRU

[GMH11] Graziela Grise and Michael Meyer-Hermann. Surface reconstruction using Delaunay triangulation for applications in life sciences. *Computer Physics Communications*, 182(4):967–977, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510005308`.

Guo:2019:EFD

[GMHZ19] Shimin Guo, Liquan Mei, Yanren Hou, and Zhengqiang Zhang. An efficient finite difference/Hermite–Galerkin spectral method for time-fractional coupled sine-Gordon equations on multidimensional unbounded domains and its application in numerical simulations of vector solitons. *Computer*

Physics Communications, 237(??):110–128, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304028.

Gao:2015:TSG

[GML15] Yali Gao, Liquan Mei, and Rui Li. A time-splitting Galerkin finite element method for the Davey–Stewartson equations. *Computer Physics Communications*, 197(??):35–42, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500288X.

Glos:2019:QJJ

[GMO19] Adam Glos, Jaroslaw Adam Miszczak, and Mateusz Ostaszewski. QSWalk.jl: Julia package for quantum stochastic walks analysis. *Computer Physics Communications*, 235(??):414–421, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303151.

Galiana-Merino:2014:ECD

[GMPFC+14] J. J. Galiana-Merino, C. Pla, A. Fernandez-Cortes, S. Cuezva, J. Ortiz, and D. Benavente. EnvironmentalWaveletTool: Continuous and discrete wavelet analysis and filtering for environmental time series. *Computer Physics Communications*, 185(10):2758–2770, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400215X.

Galiana-Merino:2013:SCD

[GMRHRCME13] J. J. Galiana-Merino, J. L. Rosa-Herranz, S. Rosa-Cintas, and J. J. Martinez-Espla. SeismicWaveTool: Continuous and discrete wavelet analysis and filtering for multichannel seismic data. *Computer Physics Communications*, 184(1):162–171, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002639.

Gowrisankar:2014:RNS

[GN14] S. Gowrisankar and Srinivasan Natesan. Robust numerical scheme for singularly perturbed convection-diffusion parabolic initial-boundary-value problems on equidistributed grids. *Computer Physics Communications*, 185(7):2008–2019, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001271.

Glaser:2015:SSG

[GNA+15] Jens Glaser, Trung Dac Nguyen, Joshua A. Anderson, Pak Lui, Filippo Spiga, Jaime A. Millan, David C. Morse, and Sharon C. Glotzer. Strong scaling of general-purpose molecular dynamics simulations on GPUs. *Computer Physics Communications*, 192(??):97–107, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000867.

Gloster:2019:CBP

[GNP19] Andrew Gloster, Lennon Ó Náraigh, and Khang Ee Pang. cuPentBatch — a batched pentadiagonal solver for NVIDIA GPUs. *Computer Physics Communications*, 241(??):113–121, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300979.

Gyevi-Nagy:2017:SPA

[GNT17] László Gyevi-Nagy and Gyula Tasi. SYVA: a program to analyze symmetry of molecules based on vector algebra. *Computer Physics Communications*, 215(??):156–164, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300310.

Goraus:2019:NLL

[Gor19] Jerzy Goraus. Non-linear least squares fit of specific heat data within the Schotte–Schotte model using web page. *Computer Physics Communications*, 240(??):178–180, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300621.

Gao:2013:GGA

[GP13] Shuang Gao and Gregory D. Peterson. GASPRNG: GPU accelerated scalable parallel random number generator library. *Computer Physics Communications*, 184(4):1241–1249, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003979.

Golesorkhtabar:2013:ETC

[GPS+13] Rostam Golesorkhtabar, Pasquale Pavone, Jürgen Spitaler, Peter Puschnig, and Claudia Draxl. ElaStic: a tool for calculating second-order elastic constants from first principles. *Computer Physics Communications*, 184(8):1861–1873, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001070.

Gebhardt:2019:BDA

[GR19] Julian Gebhardt and Andrew M. Rappe. Big data approach for effective ionic radii. *Computer Physics Communications*, 237(??):238–243, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304065.

Green:2018:ASP

[Gre18] D. G. Green. ANTICOOL: Simulating positron cooling and annihilation in atomic gases. *Computer Physics Communications*, 224(??):362–370, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303958.

Grichine:2010:GHE

[Gri10] V. M. Grichine. Geant 4 hadron elastic diffuse model. *Computer Physics Communications*, 181(5):921–927, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000172.

Grigera:2011:GGL

[Gri11] Tomás S. Grigera. glsim: a general library for numerical simulation. *Computer Physics Communications*, 182(10):2122–2131, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001597.

Guo:2018:NMP

[GRLS18] Xiaohu Guo, Benedict D. Rogers, Steven Lind, and Peter K. Stansby. New massively parallel scheme for Incompressible Smoothed Particle Hydrodynamics (ISPH) for highly nonlinear and distorted flow. *Computer Physics Communications*, 233(??):16–28, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302145.

Glass:2014:IMS

[GRR+14] Colin W. Glass, Steffen Reiser, Gábor Rutkai, Stephan Deublein, Andreas Köster, Gabriela Guevara-Carrion, Amer Wafai, Martin Horsch, Martin Bernreuther, Thorsten Windmann, Hans Hasse, and Jadran Vrabec. ms2: a molecular simulation tool for thermodynamic properties, new version release. *Computer Physics Communications*, 185(12):3302–3306, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002550.

Gutierrez:2010:QCS

[GRTZ10] Eladio Gutiérrez, Sergio Romero, María A. Trenas, and Emilio L. Zapata. Quantum computer simulation using the CUDA programming model. *Computer Physics Communications*, 181(2):283–300, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003117.

Glazov:2010:FSS

[GRZ10] A. Glazov, N. Raicević, and A. Zhokin. Fast simulation of showers in the H1 calorimeter. *Computer Physics Communications*, 181(6):1008–1012, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000038X.

Greynat:2014:NAE

[GS14] David Greynat and Javier Sesma. A new approach to the epsilon expansion of generalized hypergeometric functions. *Computer Physics Communications*, 185(2):472–478, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300324X.

Gainullin:2015:HPP

[GS15] I. K. Gainullin and M. A. Sonkin. High-performance parallel solver for 3D time-dependent Schrödinger equation for large-scale nanosystems. *Computer Physics Communications*, 188(??):68–75, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003750.

Ghosh:2017:SAEb

[GS17a] Swarnava Ghosh and Phanish Suryanarayana. SPARC: Accurate and efficient finite-difference formulation and parallel implementation of density functional theory: Extended systems. *Computer Physics Communications*, 216(??):109–125, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300711.

Ghosh:2017:SAEa

[GS17b] Swarnava Ghosh and Phanish Suryanarayana. SPARC: Accurate and efficient finite-difference formulation and parallel implementation of Density Functional Theory: Isolated clusters. *Computer Physics Communications*, 212(??):189–204, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303046.

Golosio:2014:MCS

[GSB+14] Bruno Golosio, Tom Schoonjans, Antonio Brunetti, Piernicola Oliva, and Giovanni Luca Masala. Monte Carlo simulation of X-ray imaging and spectroscopy experiments using quadric geometry and variance reduction techniques. *Computer Physics Communications*, 185(3):1044–1052, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003834.

Guckenberger:2016:BAS

[GSC+16] Achim Guckenberger, Marcel P. Schraml, Paul G. Chen, Marc Leonetti, and Stephan Gekle. On the bending algorithms for soft objects in flows. *Computer Physics Communications*, 207(??):1–23, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301072.

Grimm-Strele:2014:CGW

[GSKM14] H. Grimm-Strele, F. Kupka, and H. J. Muthsam. Curvilinear grids for WENO methods in astrophysical simulations. *Computer Physics Communications*, 185(3):764–776, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003986.

Grimm-Strele:2015:AEN

[GSKM15] H. Grimm-Strele, F. Kupka, and H. J. Muthsam. Achievable efficiency of numerical methods for simulations of solar surface convection. *Computer Physics Communications*, 188(??):7–20, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003440.

Germanas:2017:HUP

[GSMK17] D. Germanas, A. Stepsys, S. Mickevicius, and R. K. Kalinauskas. HOTB update: Parallel code for calculation of three- and four-particle harmonic oscillator transformation brackets and their matrices using OpenMP. *Computer Physics Communications*, 215(??):259–264, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300401.

Gil:2012:IAF

[GST12] Amparo Gil, Javier Segura, and Nico M. Temme. An improved algorithm and a Fortran 90 module for computing the conical function $p^m_{1/2+i\tau}(x)$. *Computer Physics*

Communications, 183(3):794–799, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003936.

Gil:2015:GPI

[GST15] Amparo Gil, Javier Segura, and Nico M. Temme. GammaCHI: a package for the inversion and computation of the gamma and chi-square cumulative distribution functions (central and noncentral). *Computer Physics Communications*, 191(??):132–139, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000107.

Gil:2017:ECL

[GST17] Amparo Gil, Javier Segura, and Nico M. Temme. Efficient computation of Laguerre polynomials. *Computer Physics Communications*, 210(??):124–131, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302727.

Germaneau:2013:IMB

[GSZ13] Éric Germaneau, Gang Su, and Qing-Rong Zheng. Implementation of the modified Becke–Johnson meta-GGA functional in Quantum Espresso. *Computer Physics Communications*, 184(7):1697–1700, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000775.

Green:2019:DDM

[GT19] Adam Green and Philip Tanedo. DarkCapPy: Dark matter capture and annihilation. *Computer Physics Communications*, 242(??):120–131, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301237.

Gudmundsson:2011:TDM

[GTG+11] Vidar Gudmundsson, Chi-Shung Tang, Cosmin Mihai Gainar, Valeriu Moldoveanu, and Andrei Manolescu. Time-dependent magnetotransport in semiconductor nanostructures via the generalized master equation. *Computer Physics Communications*, 182(1):46–48, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002961.

Galler:2019:APV

[GTK+19a] Anna Galler, Patrik Thunström, Josef Kaufmann, Matthias Pickem, Jan M. Tomczaka, and Karsten Held. The AbinitioD Γ A Project v1.0: Non-local correlations beyond and susceptibilities within dynamical mean-field theory. *Computer Physics Communications*, 245(??):Article 106847, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302243.

Guzman:2019:EAM

[GTK+19b] Horacio V. Guzman, Nikita Tretyakov, Hideki Kobayashi, Aoife C. Fogarty, Karsten Kreis, Jakub Krajniak, Christoph Junghans, Kurt Kremer, and Torsten Stuehn. ESPResSo++ 2.0: Advanced methods for multiscale molecular simulation. *Computer Physics Communications*, 238(??):66–76, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304399.

Gonzalez:2011:EDA

[GTL11] S. González, A. R. Thornton, and S. Luding. An event-driven algorithm for fractal cluster formation. *Computer Physics Communications*, 182(9):1842–1845, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000456X.

Gao:2017:XRD

[GTL+17] Pengyue Gao, Qunchao Tong, Jian Lv, Yanchao Wang, and Yanming Ma. X-ray diffraction data-assisted structure searches. *Computer Physics Communications*, 213(??):40–45, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303617.

Garcia-Torano:2019:PMC

[GTPS19] E. García-Toraño, V. Peyres, and F. Salvat. PenNuc: Monte Carlo simulation of the decay of radionuclides. *Computer Physics Communications*, 245(??):Article 106849, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302267.

Galindo-Torres:2012:BPT

[GTPWL12] S. A. Galindo-Torres, D. M. Pedroso, D. J. Williams, and L. Li. Breaking processes in three-dimensional bonded granular materials with general shapes. *Computer Physics Communications*, 183(2):266–277, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003298.

Gomez:2014:SOT

[GTS14] Edgar A. Gómez, Saravana Prakash Thirumuruganandham, and Alejandro Santana. Split-operator technique for propagating phase space functions: Exploring chaotic, dissipative and relativistic dynamics. *Computer Physics Communications*, 185(1):136–143, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002981.

Galindo-Torres:2013:LBM

[GTSL+13] S. A. Galindo-Torres, A. Scheuermann, L. Li, D. M. Pedroso, and D. J. Williams. A Lattice Boltzmann model for studying transient effects during imbibition-drainage cycles in unsaturated soils. *Computer Physics Communications*, 184(4):1086–1093, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003918.

Godfrey:2015:INC

[GV15] Brendan B. Godfrey and Jean-Luc Vay. Improved numerical Cherenkov instability suppression in the generalized PSTD PIC algorithm. *Computer Physics Communications*, 196(??):221–225, November 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002532.

Garcia:2018:PFL

[GVPJ18] Alberto García, Matthieu J. Verstraete, Yann Pouillon, and Javier Junquera. The PSML format and library for norm-conserving pseudopotential data curation and interoperability. *Computer Physics Communications*, 227(??):51–71, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300390.

Gounley:2019:FCV

[GVR19] J. Gounley, M. Vardhan, and A. Randles. A framework for comparing vascular hemodynamics at different points in time. *Computer Physics Communications*, 235(??):1–8, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301772.

Gilmore:2015:EIC

[GVS+15] K. Gilmore, John Vinson, E. L. Shirley, D. Prendergast, C. D. Pemmaraju, J. J. Kas, F. D. Vila, and J. J. Rehr. Efficient implementation of core-excitation Bethe–Salpeter equation calculations. *Computer Physics Communications*, 197(??):109–117, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003008.

Gull:2011:CTQ

[GWF+11] Emanuel Gull, Philipp Werner, Sebastian Fuchs, Brigitte Surer, Thomas Pruschke, and Matthias Troyer. Continuous-time quantum Monte Carlo impurity solvers. *Computer Physics Communications*, 182(4):1078–1082, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000087.

Ge:2016:JII

[GWF+16] Xinmin Ge, Hua Wang, Yiren Fan, Yingchang Cao, Hua Chen, and Rui Huang. Joint inversion of $T_1 - T_2$ spectrum combining the iterative truncated singular value decomposition and the parallel particle swarm optimization algorithms. *Computer Physics Communications*, 198(??):59–70, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003410.

Gwizdalla:2012:HAS

[Gwi12] Tomasz M. Gwizdalla. The hybrid algorithm for the study of geometric configurations of 2D clusters of uniformly charged classical particles. *Computer Physics Communications*, 183(9):1899–1903, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001476.

Gabay:2017:SDE

[GWL+17] D. Gabay, X. Wang, V. Lomakin, A. Boag, M. Jain, and A. Natan. Size dependent electronic properties of silicon quantum dots — an analysis with hybrid, screened hybrid and local density functional theory. *Computer Physics Communications*, 221(??):95–101, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302485.

Giannotti:2013:MGI

[GWM13] M. Giannotti, M. Wise, and A. Mohammed. MESAFace, a graphical interface to analyze the MESA output. *Computer Physics Communications*, 184(4):1333–1338, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004298.

Guo:2015:SDP

[GX15] Z. Guo and S. M. Xiong. On solving the 3-D phase field equations by employing a parallel-adaptive mesh refinement (Para-AMR) algorithm. *Computer Physics Communications*, 190(??):89–97, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000363.

Gallicchio:2015:ARE

[GXF+15] Emilio Gallicchio, Junchao Xia, William F. Flynn, Baofeng Zhang, Sade Samlalsingh, Ahmet Mentes, and Ronald M. Levy. Asynchronous replica exchange software for grid and heterogeneous computing. *Computer Physics Communications*, 196(??):236–246, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002556`.

Guo:2010:REC

[GYW+10] Jian-You Guo, Miao Yu, Jing Wang, Bao-Mei Yao, and Peng Jiao. A relativistic extension of the complex scaling method using oscillator basis functions. *Computer Physics Communications*, 181(3):550–556, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003518`.

Gao:2014:ETL

[GZL14] Miao Gao, Gui-Ping Zhang, and Zhong-Yi Lu. Electronic transport of a large scale system studied by renormalized transfer matrix method: Application to armchair graphene nanoribbons between quantum wires. *Computer Physics Communications*, 185(3):856–861, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004189`.

Gong:2017:ESA

[GZW17] Yuezheng Gong, Jia Zhao, and Qi Wang. An energy stable algorithm for a quasi-incompressible hydrodynamic phase-field model of viscous fluid mixtures with variable densities and viscosities. *Computer Physics Communications*, 219(??):20–34, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301327`.

Gross:2018:MPM

[GZWJ18] Jonathan Gross, Johannes Zierenberg, Martin Weigel, and Wolfhard Janke. Massively parallel multicanonical simulations. *Computer Physics Communications*, 224(??):387–395, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303697.

Gou:2019:IMP

[GZZ19] Wenjin Gou, Shuai Zhang, and Yao Zheng. Implementation of the moving particle semi-implicit method for free-surface flows on GPU clusters. *Computer Physics Communications*, 244(??):13–24, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302218.

Hahn:2012:HEP

[Hah12] T. Hahn. The high-energy physicist's guide to MathLink. *Computer Physics Communications*, 183(3):460–469, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100350X.

Hopfer:2013:SGG

[HAH13] Markus Hopfer, Reinhard Alkofer, and Gundolf Haase. Solving the ghost-gluon system of Yang–Mills theory on GPUs. *Computer Physics Communications*, 184(4):1183–1190, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004109.

Hahn:2016:CC

[Hah16] T. Hahn. Concurrent Cuba. *Computer Physics Communications*, 207(??):341–349, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630128X.

Hirvijoki:2014:ASK

[HAK+14] E. Hirvijoki, O. Asunta, T. Koskela, T. Kurki-Suonio, J. Miettunen, S. Sipilä, A. Snicker, and S. Äkäslompolo. ASCOT: Solving the kinetic equation of minority particle species in tokamak plasmas. *Computer Physics Communications*, 185(4):1310–1321, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465514000277.

Hakel:2016:FFE

[Hak16] Peter Hakel. FESTR: Finite-Element Spectral Transfer of Radiation spectroscopic modeling and analysis code. *Computer Physics Communications*, 207(??):415–425, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301618.

Hakel:2019:FFE

[Hak19] Peter Hakel. FESTR: Finite-Element Spectral Transfer of Radiation spectroscopic modeling and analysis code (new version announcement). *Computer Physics Communications*, 242(??):156–157, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301225.

Hall:2017:SRD

[Hal17] D. C. Hall. Sampling random directions within an elliptical cone. *Computer Physics Communications*, 219(??):87–90, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301406.

Hamada:2011:GAI

[Ham11] Shoji Hamada. GPU-accelerated indirect boundary element method for voxel model analyses with fast multipole method. *Computer Physics Communications*, 182(5):1162–1168, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000403.

Howard:2016:ENL

[HAN+16] Michael P. Howard, Joshua A. Anderson, Arash Nikoubashman, Sharon C. Glotzer, and Athanassios Z. Panagiotopoulos. Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. *Computer Physics Communications*, 203(??):45–52, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300182.

Hasegawa:2011:PRG

[Has11] M. Hasegawa. Positive role of glassy dynamics in finite-time optimization by threshold algorithms. *Computer Physics Communications*, 182(1):229–231, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003048.

Hadjidoukas:2014:NVN

[HAV+14] P. E. Hadjidoukas, P. Angelikopoulos, C. Voglis, D. G. Papageorgiou, and I. E. Lagaris. NDL-v2.0: a new version of the numerical differentiation library for parallel architectures. *Computer Physics Communications*, 185(7):2217–2219, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001258.

Huber:2012:ADF

[HB12] Markus Q. Huber and Jens Braun. Algorithmic derivation of functional renormalization group equations and Dyson–Schwinger equations. *Computer Physics Communications*, 183(6):1290–1320, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200029X.

Huang:2013:ISN

[HB13] Beibei Huang and Vladimir A. Baulin. IPEC Solver: Numerical simulation tool to study inter-polyelectrolyte complexation. *Computer Physics Communications*, 184(9):2221–2229, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300163X.

Hadjidoukas:2010:PMC

[HBE10] P. Hadjidoukas, C. Bousis, and D. Emfietzoglou. Parallelization of a Monte Carlo particle transport simulation code. *Computer Physics Communications*, 181(5):928–936, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000184`.

Hu:2017:CMM

[HBH+17] Changjun Hu, He Bai, Xinfu He, Boyao Zhang, Ningming Nie, Xianmeng Wang, and Yingwen Ren. Crystal MD: the massively parallel molecular dynamics software for metal with BCC structure. *Computer Physics Communications*, 211(??):73–78, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551630193X`.

Halverson:2013:EMM

[HBL+13] Jonathan D. Halverson, Thomas Brandes, Olaf Lenz, Axel Arnold, Stas Bevc, Vitaliy Starchenko, Kurt Kremer, Torsten Stuehn, and Dirk Reith. ESPResSo++: a modern multiscale simulation package for soft matter systems. *Computer Physics Communications*, 184(4):1129–1149, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512004006`.

Hudspith:2015:FAC

[HbotRC15] R. J. Hudspith, On behalf of the RBC, and UKQCD Collaborations. Fourier accelerated conjugate gradient lattice gauge fixing. *Computer Physics Communications*, 187(??):115–119, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003634`.

Haskey:2014:CPM

[HBP14] S. R. Haskey, B. D. Blackwell, and D. G. Pretty. Clustering of periodic multichannel timeseries data with application to plasma fluctuations. *Computer Physics Communications*, 185(6):1669–1680, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000885`.

Hansel:2015:AGH

[HBP+15] R. A. Hansel, C. N. Brock, B. C. Paikoff, A. R. Tackett, and D. G. Walker. Automated generation of highly accurate, efficient and transferable pseudopotentials. *Computer Physics Communications*, 196(??):267–275, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002593.

Hung:2011:ETI

[HBS+11] R. F. Hung, D. Berco, I. Ya. Shapiro, B. Shapiro, and B. Rosenstein. Electrodynamics of type-II superconductor with periodic pinning array. *Computer Physics Communications*, 182(1):81–83, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002493.

He:2016:FAW

[HC16] Zi He and Ru-Shan Chen. Fast analysis of wide-band scattering from electrically large targets with time-domain parabolic equation method. *Computer Physics Communications*, 200(??):139–146, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004191.

He:2017:FDT

[HC17] Zi He and Ru-Shan Chen. Frequency-domain and time-domain solvers of parabolic equation for rotationally symmetric geometries. *Computer Physics Communications*, 220(??):181–187, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302102.

Ho:2014:TSE

[HCC14] I-Lin Ho, Chung-Hsien Chou, and Yia-Chung Chang. Theoretical study of electronic transport through quasicrystalline nanotubes using mesh inflation approach. *Computer Physics Communications*, 185(5):1383–1388, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400023X.

Hsieh:2016:EAC

[HCH16] Yu-Hsin Hsieh, Chi-Ning Chen, and Chin-Kun Hu. Efficient algorithm for computing exact partition functions of lattice polymer models. *Computer Physics Communications*, 209(??):27–33, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302363.

Hung:2011:DPI

[HCHW11] Chieh-Tsan Hung, Yuan-Ming Chiu, Feng-Nan Hwang, and Jong-Shinn Wu. Development of a parallel implicit solver of fluid modeling equations for gas discharges. *Computer Physics Communications*, 182(1):161–163, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001797.

Hutten:2019:CVR

[HCM19] Moritz Hütten, Céline Combet, and David Maurin. CLUMPY v3: γ-ray and ν signals from dark matter at all scales. *Computer Physics Communications*, 235(??):336–345, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303497.

Halder:2014:JAS

[HCRD14] P. Halder, A. Chakraborty, P. Deb Roy, and H. S. Das. Java application for the superposition T-matrix code to study the optical properties of cosmic dust aggregates. *Computer Physics Communications*, 185(9):2369–2379, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001532.

Hwang:2010:PNK

[HCSW10] Feng-Nan Hwang, Shang-Rong Cai, Yun-Long Shao, and Jong-Shinn Wu. Parallel Newton–Krylov–Schwarz algorithms for the three-dimensional Poisson–Boltzmann equation in numerical simulation of colloidal particle interactions. *Computer Physics Communications*, 181(9):1529–1537, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000144X.

Huang:2011:FRR

[HCT11] J. L. Huang, H. J. Chen, and H. C. Tseng. The flow of a reversible ratchet. *Computer Physics Communications*, 182(1):198–200, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003000.

Harvey:2011:STP

[HD11] M. J. Harvey and G. De Fabritiis. Swan: a tool for porting CUDA programs to OpenCL. *Computer Physics Communications*, 182(4):1093–1099, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000117.

Halder:2017:JSV

[HD17] Prithish Halder and Himadri Sekhar Das. JaSTA-2: Second version of the Java Superposition T-matrix Application. *Computer Physics Communications*, 221(??):421–422, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302667.

He:2019:FLA

[HDF+19] Z. He, M. Davidsaver, K. Fukushima, G. Shen, M. Ikegami, and J. Bengtsson. The fast linear accelerator modeling engine for FRIB online model service. *Computer Physics Communications*, 234(??):167–178, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302662.

Hynninen:2012:MDI

[HDM+12] T. Hynninen, C. L. Dias, A. Mkrtchyan, V. Heinonen, M. Karttunen, A. S. Foster, and T. Ala-Nissila. A molecular dynamics implementation of the 3D Mercedes–Benz water model. *Computer Physics Communications*, 183(2):363–369, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003262.

Hadade:2016:MMM

[HdM16] Ioan Hadade and Luca di Mare. Modern multicore and manycore architectures: Modelling, optimisation and benchmarking a multiblock CFD code. *Computer Physics Communications*, 205(??):32–47, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300959.

Hu:2014:MSM

[HDZ14] Weipeng Hu, Zichen Deng, and Yu Zhang. Multi-symplectic method for peakon–antipeakon collision of quasi-Degasperis–Procesi equation. *Computer Physics Communications*, 185(7):2020–2028, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001295.

Hadi:2013:CFA

[HE13] Mohammed F. Hadi and Seyed A. Esmaeili. CUDA Fortran acceleration for the finite-difference time-domain method. *Computer Physics Communications*, 184(5):1395–1400, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000118.

Hirayama:2011:TDN

[HEF+11] Naomi Hirayama, Akira Endo, Kazuhiro Fujita, Yasuhiro Hasegawa, Naomichi Hatano, Hiroaki Nakamura, and Ryoen Shirasaki. Temperature distribution in nano-devices under a strong magnetic field. *Computer Physics Communications*, 182(1):90–92, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002882.

Hlucha:2012:SPP

[HEF12] H. Hluchá, H. Eberl, and W. Frisch. SFOLD — a program package for calculating two-body sfermion decays at full one-loop level in the MSSM. *Computer Physics Communications*, 183(10):2307–2312, October 2012. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002007.

Heinasmaki:2012:IAA

[Hei12] Sami Heinäsmäki. IONIS: Approximate atomic photoionization intensities. *Computer Physics Communications*, 183(2):431–437, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003390.

Homola:2013:SUH

[HEPW13] P. Homola, R. Engel, A. Pysz, and H. Wilczyński. Simulation of ultra-high energy photon propagation with PRESHOWER 2.0. *Computer Physics Communications*, 184(5):1468–1475, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000325.

Honda:2016:DFT

[HF16] Mitsuru Honda and Atsushi Fukuyama. Development of the fluid-type transport code on the flux coordinates in a tokamak. *Computer Physics Communications*, 208(??):117–134, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302387.

Harvey:2015:PIL

[HFOPF15] Daniel G. Harvey, Alexander G. Fletcher, James M. Osborne, and Joe Pitt-Francis. A parallel implementation of an off-lattice individual-based model of multicellular populations. *Computer Physics Communications*, 192(??):130–137, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001046.

Hischenhuber:2012:MCM

[HFSK12] B. Hischenhuber, F. Frommlet, W. Schreiner, and B. Knapp. MH^2 c: Characterization of major histocompatibility α-helices — an information criterion approach. *Computer Physics Communications*, 183(7):1481–1490, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000616.

Hoefling:2013:SFS

[HG13] Martin Hoefling and Helmut Grubmüller. In silico FRET from simulated dye dynamics. *Computer Physics Communications*, 184(3):841–852, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200361X.

Hernandez-Garcia:2015:CAS

[HGCARM15] L. F. Hernández-García, V. Cabrera-Arenas, and L. M. Reséndiz-Mendoza. On the convergence of the algorithm for simulating organic solar cells. *Computer Physics Communications*, 196(??):372–379, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002751.

Hsiao:2011:ARE

[HH11a] Ju-Tang Hsiao and Keh-Ning Huang. Applications of the relativistic equation of motion to photoionization of Mg-like ions. *Computer Physics Communications*, 182(1):136–139, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001712.

Hung:2011:CRN

[HH11b] Yao-Chen Hung and Chin-Kun Hu. Constructive role of noise in p53 regulatory network. *Computer Physics Communications*, 182(1):249–250, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002250.

Huang:2010:MTF

[HHC+10] Zhen-Ting Huang, Huan-Chun Hsu, Chau-Lyan Chang, Chin-Tien Wu, and T. F. Jiang. Momentum-time flux conservation method for one-dimensional wave equations. *Computer Physics Communications*, 181(3):473–480, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003397.

Hsieh:2016:IAU

[HHC16] Chi-Ti Hsieh, Tung-Han Hsieh, and Shu-Wei Chang. Improving accuracy using subpixel smoothing for multiband effective-mass Hamiltonians of semiconductor nanostructures. *Computer Physics Communications*, 201(??):63–76, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004567.

Hunt:2015:PCN

[HHM+15] Martin Hunt, Benjamin Haley, Michael McLennan, Marisol Koslowski, Jayathi Murthy, and Alejandro Strachan. PUQ: a code for non-intrusive uncertainty propagation in computer simulations. *Computer Physics Communications*, 194(??):97–107, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001435.

Hoschele:2014:MMP

[HHP+14] Maik Höschele, Jens Hoff, Alexey Pak, Matthias Steinhauser, and Takahiro Ueda. MT: a Mathematica package to compute convolutions. *Computer Physics Communications*, 185(2):528–539, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003354.

Hynninen:2016:OOP

[HHP+16] T. Hynninen, L. Himanen, V. Parkkinen, T. Musso, J. Corander, and A. S. Foster. An object oriented Python interface for atomistic simulations. *Computer Physics Communications*, 198(??):230–237, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003483.

Hung:2010:IPP

[HHS+10] Linda Hung, Chen Huang, Ilgyou Shin, Gregory S. Ho, Vincent L. Lignères, and Emily A. Carter. Introducing PRO-

FESS 2.0: a parallelized, fully linear scaling program for orbital-free density functional theory calculations. *Computer Physics Communications*, 181(12):2208–2209, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003462.

Huang:2014:OTE

[HHT14] Yi-An Huang, Yu-Ting Hung, and Snow H. Tseng. An optical target to eliminate impinging light in a light scattering simulation. *Computer Physics Communications*, 185(10):2504–2509, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400201X.

Hinde:2011:QMD

[Hin11] Robert J. Hinde. QSATS: MPI-driven quantum simulations of atomic solids at zero temperature. *Computer Physics Communications*, 182(11):2339–2349, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001615.

Hirel:2015:ATM

[Hir15] Pierre Hirel. Atomsk: a tool for manipulating and converting atomic data files. *Computer Physics Communications*, 197(??):212–219, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002817.

Hook:2014:CSS

[HJ14] L. J. Höök and T. Johnson. Composition schemes for the stochastic differential equation describing collisional pitch-angle diffusion. *Computer Physics Communications*, 185(2):590–594, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003676.

Hormann:2019:SSS

[HJE+19] Lukas Hörmann, Andreas Jeindl, Alexander T. Egger, Michael Scherbela, and Oliver T. Hofmann. SAM-

PLE: Surface structure search enabled by coarse graining and statistical learning. *Computer Physics Communications*, 244(??):143–155, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301973.

Hu:2018:DRU

[HJGL18] Shuyao Hu, Chongwen Jiang, Zhenxun Gao, and Chun-Hian Lee. Disturbance region update method for steady compressible flows. *Computer Physics Communications*, 229 (??):68–86, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301000.

Hu:2019:ZDR

[HJGL19] Shuyao Hu, Chongwen Jiang, Zhenxun Gao, and Chun-Hian Lee. Zonal disturbance region update method for steady compressible viscous flows. *Computer Physics Communications*, 244(??):97–116, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302024.

Haddadi:2017:CEC

[HJH17] Bahram Haddadi, Christian Jordan, and Michael Harasek. Cost efficient CFD simulations: Proper selection of domain partitioning strategies. *Computer Physics Communications*, 219(??):121–134, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730156X.

Huang:2014:CAA

[HJL+14] Yunbao Huang, Shaoen Jiang, Haiyan Li, Qifu Wang, and Liping Chen. Compressive analysis applied to radiation symmetry evaluation and optimization for laser-driven inertial confinement fusion. *Computer Physics Communications*, 185(2):459–471, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300297X.

Hirai:2012:NSE

[HK12] M. Hirai and S. Kumano. Numerical solution of Q^2 evolution equations for fragmentation functions. *Computer Physics Communications*, 183(4):1002–1013, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004103.

Hornyak:2015:ACP

[HK15] I. Hornyak and A. T. Kruppa. An algorithm for the calculation of the partial wave expansion of the Coulomb-distorted plane wave. *Computer Physics Communications*, 197(??):291–297, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003045.

Hamiaz:2012:FVT

[HKF+12] Adnane Hamiaz, Rudy Klein, Xavier Ferrieres, Olivier Pascal, Jean-Pierre Boeuf, and Jean-Rene Poirier. Finite Volume Time Domain modelling of microwave breakdown and plasma formation in a metallic aperture. *Computer Physics Communications*, 183(8):1634–1640, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000938.

Heikkinen:2012:IMC

[HKJ+12] J. A. Heikkinen, T. Korpilo, S. J. Janhunen, T. P. Kiviniemi, S. Leerink, and F. Ogando. Interpolation for momentum conservation in 3D toroidal gyrokinetic particle simulation of plasmas. *Computer Physics Communications*, 183(8):1719–1727, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200118X.

Hwang:2011:LSD

[HKK11] Soonwook Hwang, Hangi Kim, and Seyong Kim. Large-scale deployment of two-color QCD simulations on the grid using Ganga. *Computer Physics Communications*, 182(1):277–279, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002304.

Heylmun:2019:QBM

[HKPF19] J. C. Heylmun, B. Kong, A. Passalacqua, and R. O. Fox. A quadrature-based moment method for polydisperse bubbly flows. *Computer Physics Communications*, 244(??):187–204, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301924.

Hammerling:2010:NSS

[HKSW10] Robert Hammerling, Othmar Koch, Christa Simon, and Ewa B. Weinmüller. Numerical solution of singular ODE eigenvalue problems in electronic structure computations. *Computer Physics Communications*, 181(9):1557–1561, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001475.

Hornikx:2016:OOS

[HKvH16] Maarten Hornikx, Thomas Krijnen, and Louis van Harten. openPSTD: the open source pseudospectral time-domain method for acoustic propagation. *Computer Physics Communications*, 203(??):298–308, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300443.

Hulsmann:2010:GGB

[HKVR10] Marco Hülsmann, Thorsten Köddermann, Jadran Vrabec, and Dirk Reith. GROW: a gradient-based optimization workflow for the automated development of molecular models. *Computer Physics Communications*, 181(3):499–513, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003452.

Haar:2017:APF

[HKZN17] Taylor Haar, Waseem Kamleh, James Zanotti, and Yoshifumi Nakamura. Applying polynomial filtering to mass preconditioned Hybrid Monte Carlo. *Computer Physics Communications*, 215(??):113–127, June 2017. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300723.

Haar:2019:SFO

[HKZN19] Taylor Haar, Waseem Kamleh, James Zanotti, and Yoshifumi Nakamura. Single flavour optimisations to Hybrid Monte Carlo. *Computer Physics Communications*, 238 (??):111–123, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304259.

Huang:2013:NNE

[HL13] Zhi-Wei Huang and Jueping Liu. NumExp: Numerical epsilon expansion of hypergeometric functions. *Computer Physics Communications*, 184(8):1973–1980, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001136.

Homann:2018:SGC

[HL18] Holger Homann and François Laenen. SoAx: a generic C++ structure of arrays for handling particles in HPC codes. *Computer Physics Communications*, 224(??):325–332, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303983.

Hedin:2019:GPF

[HL19a] Florent Hédin and Tony Lelièvre. gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems. *Computer Physics Communications*, 239(??):311–324, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300062.

Hutson:2019:BNF

[HL19b] Jeremy M. Hutson and C. Ruth Le Sueur. `bound` and `field`: Programs for calculating bound states of interacting pairs of atoms and molecules. *Computer Physics Communications*, 241(??):1–8, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465519300694.

Hutson:2019:MPN

[HL19c] Jeremy M. Hutson and C. Ruth Le Sueur. molscat: a program for non-reactive quantum scattering calculations on atomic and molecular collisions. *Computer Physics Communications*, 241(??):9–18, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300669.

Hu:2013:PSG

[HLD13] HanPing Hu, LingFeng Liu, and NaiDa Ding. Pseudorandom sequence generator based on the Chen chaotic system. *Computer Physics Communications*, 184(3):765–768, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003931.

Hao:2013:NIV

[HLL13] Wenrui Hao, Zhenzhou Lu, and Luyi Li. A new interpretation and validation of variance based importance measures for models with correlated inputs. *Computer Physics Communications*, 184(5):1401–1413, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300012X.

He:2016:OSA

[HLLH16] Yu-Xuan He, Liang Li, Stéphane Lanteri, and Ting-Zhu Huang. Optimized Schwarz algorithms for solving time-harmonic Maxwell's equations discretized by a hybridizable discontinuous Galerkin method. *Computer Physics Communications*, 200(??):176–181, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004336.

Harlander:2013:SPC

[HLM13] Robert V. Harlander, Stefan Liebler, and Hendrik Mantler. SusHi: a program for the calculation of Higgs production in gluon fusion and bottom-quark annihilation in the Standard Model and the MSSM. *Computer Physics Communications*, 184(6):1605–1617, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000507.

Harlander:2017:SBB

[HLM17] Robert V. Harlander, Stefan Liebler, and Hendrik Mantler. SusHi Bento: Beyond NNLO and the heavy-top limit. *Computer Physics Communications*, 212(??):239–257, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303344.

Hadzibeganovic:2012:ETM

[HLS12] Tarik Hadzibeganovic, F. Welington S. Lima, and Dietrich Stauffer. Evolution of tag-mediated altruistic behavior in one-shot encounters on large-scale complex networks. *Computer Physics Communications*, 183(11):2315–2321, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001890.

Halliday:2017:IMC

[HLS+17] I. Halliday, S. V. Lishchuk, T. J. Spencer, K. Burgin, and T. Schenkel. Interfacial micro-currents in continuum-scale multi-component lattice Boltzmann equation hydrodynamics. *Computer Physics Communications*, 219(??):286–296, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730187X.

Huang:2019:HEG

[HLTW19] Tsung-Ming Huang, Wen-Wei Lin, Hsinhan Tsai, and Weichung Wang. Highly efficient GPU eigensolver for three-dimensional photonic crystal band structures with any Bravais lattice. *Computer Physics Communications*, 245 (??):Article 106841, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302188.

Huang:2016:HJD

[HLW16] Tsung-Ming Huang, Wen-Wei Lin, and Weichung Wang. A hybrid Jacobi–Davidson method for interior cluster eigenvalues with large null-space in three dimensional lossless Drude dispersive metallic photonic crystals. *Computer Physics Communications*, 207(??):221–231, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301825.

Hou:2013:MDS

[HLZ+13] Qing Hou, Min Li, Yulu Zhou, Jiechao Cui, Zhenguo Cui, and Jun Wang. Molecular dynamics simulations with many-body potentials on multiple GPUs-the implementation, package and performance. *Computer Physics Communications*, 184(9):2091–2101, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001367.

Huber:2010:BSP

[HM10] Gary A. Huber and J. Andrew McCammon. Browndye: a software package for Brownian dynamics. *Computer Physics Communications*, 181(11):1896–1905, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002559.

Heltemes:2012:BVF

[HM12a] T. A. Heltemes and G. A. Moses. BADGER v1.0: a Fortran equation of state library. *Computer Physics Communications*, 183(12):2629–2646, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200238X.

Huber:2012:CFS

[HM12b] Markus Q. Huber and Mario Mitter. CrasyDSE: a framework for solving Dyson–Schwinger equations. *Computer Physics Communications*, 183(11):2441–2457, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001889.

Huber:2012:HEH

[HM12c] Tobias Huber and Daniel Maître. HypExp 2, expanding hypergeometric functions about half-integer parameters. *Computer Physics Communications*, 183(4):1060, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551100378X`.

Humeniuk:2017:DSP

[HM17] Alexander Humeniuk and Roland Mitrić. DFTBaby: a software package for non-adiabatic molecular dynamics simulations based on long-range corrected tight-binding TD-DFT(B). *Computer Physics Communications*, 221(??):174–202, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302576`.

Humeniuk:2018:BJM

[HM18] Alexander Humeniuk and Roland Mitrić. A block Jacobi method for complex skew-symmetric matrices with applications in the time-dependent variational principle. *Computer Physics Communications*, 231(??):187–197, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301425`.

Hu:2011:NSG

[HML11] Feiming Hu, Tianxing Ma, and Hai-Qing Lin. Numerical study of geometrical frustration: From square to triangular lattices. *Computer Physics Communications*, 182(1):74–76, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003036`.

Hoffmann:2014:KLK

[HMR14] Max J. Hoffmann, Sebastian Matera, and Karsten Reuter. `kmos`: a lattice kinetic Monte Carlo framework. *Computer Physics Communications*, 185(7):2138–2150, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551400126X`.

Hewitt:2019:OPF

[HMR+19] Sam Hewitt, Lee Margetts, Alistair Revell, Pankaj Pankaj, and Francesc Levrero-Florencio. OpenFPCI: a parallel fluid-structure interaction framework. *Computer Physics Communications*, 244(??):469–482, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301742.

Hasegawa:2010:AAG

[HMU10] K. Hasegawa, S. Moch, and P. Uwer. AutoDipole — automated generation of dipole subtraction terms. *Computer Physics Communications*, 181(10):1802–1817, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002535.

Hariri:2013:FCI

[HO13] F. Hariri and M. Ottaviani. A flux-coordinate independent field-aligned approach to plasma turbulence simulations. *Computer Physics Communications*, 184(11):2419–2429, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001999.

Hohenester:2014:OMT

[Hoh14a] Ulrich Hohenester. OCTBEC — a Matlab toolbox for optimal quantum control of Bose–Einstein condensates. *Computer Physics Communications*, 185(1):194–216, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003172.

Hohenester:2014:SEE

[Hoh14b] Ulrich Hohenester. Simulating electron energy loss spectroscopy with the MNPBEM toolbox. *Computer Physics Communications*, 185(3):1177–1187, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004220.

Hohenester:2018:MSM

[Hoh18] Ulrich Hohenester. Making simulations with the MNPBEM toolbox big: Hierarchical matrices and iterative solvers. *Computer Physics Communications*, 222(??):209–228, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302552.

Holzwarth:2019:UCP

[Hol19] N. A. W. Holzwarth. Updated comments on projector augmented wave (PAW) implementations within various electronic structure code packages. *Computer Physics Communications*, 243(??):25–29, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301584.

Honda:2010:STF

[Hon10] M. Honda. Simulation technique of free-boundary equilibrium evolution in plasma ramp-up phase. *Computer Physics Communications*, 181(9):1490–1500, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001372.

Honda:2018:AGA

[Hon18] Mitsuru Honda. Application of genetic algorithms to modelings of fusion plasma physics. *Computer Physics Communications*, 231(??):94–106, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301413.

Hsu:2011:FMC

[HP11] Hsiao-Ping Hsu and Wolfgang Paul. A fast Monte Carlo algorithm for studying bottle-brush polymers. *Computer Physics Communications*, 182(10):2115–2121, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001585.

Hammer:2014:SGL

[HP14] René Hammer and Walter Pötz. Staggered grid leap-frog scheme for the $(2+1)D$ Dirac equation. *Computer Physics Communications*, 185(1):40–52, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002750`.

Hahn:2017:IIM

[HP17] Thomas Hahn and Sebastian Paßehr. Implementation of the $\mathcal{O}(\alpha_t^2)$ MSSM Higgs-mass corrections in FeynHiggs. *Computer Physics Communications*, 214(??):91–97, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300383`.

Hinz:2015:PBS

[HPKF15] Denis F. Hinz, Alexander Panchenko, Tae-Yeon Kim, and Eliot Fried. Particle-based simulations of self-motile suspensions. *Computer Physics Communications*, 196(??):45–57, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001940`.

Howard:2018:EMH

[HPN18] Michael P. Howard, Athanassios Z. Panagiotopoulos, and Arash Nikoubashman. Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. *Computer Physics Communications*, 230(??):10–20, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301218`.

Horst:2011:CPA

[HR11] Christoph Horst and Jürgen Reuter. CleGo: a package for automated computation of Clebsch–Gordan coefficients in tensor product representations for Lie algebras *A*–*G*. *Computer Physics Communications*, 182(7):1543–1565, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001184`.

Ho:2011:GFM

[HRC11] Tak-San Ho, Herschel Rabitz, and Shih-I Chu. A general formulation of monotonically convergent algorithms in the control of quantum dynamics beyond the linear dipole interaction. *Computer Physics Communications*, 182(1):14–17, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002833.

Hansen:2011:P

[HS11] Alex Hansen and Asle Sudbø. Preface. *Computer Physics Communications*, 182(9):1755, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001536.

Henke:2014:MSP

[HS14a] Steven F. Henke and Sachin Shanbhag. Mesh sensitivity in peridynamic simulations. *Computer Physics Communications*, 185(1):181–193, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003111.

Howell:2014:SGS

[HS14b] E. C. Howell and C. R. Sovinec. Solving the Grad–Shafranov equation with spectral elements. *Computer Physics Communications*, 185(5):1415–1421, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400040X.

Hosek:2016:MVF

[HS16] Petr Hosek and Vojtech Spiwok. Metadyn View: Fast web-based viewer of free energy surfaces calculated by metadynamics. *Computer Physics Communications*, 198(??):222–229, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003367.

Herren:2018:VRC

[HS18] Florian Herren and Matthias Steinhauser. Version 3 of RunDec and CRunDec. *Computer Physics Com-*

munications, 224(??):333–345, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303971.

Hayen:2019:BSG

[HS19] L. Hayen and N. Severijns. Beta spectrum generator: High precision allowed β spectrum shapes. *Computer Physics Communications*, 240(??):152–164, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300645.

Hill:2017:DBC

[HSD17] Peter Hill, Brendan Shanahan, and Ben Dudson. Dirichlet boundary conditions for arbitrary-shaped boundaries in stellarator-like magnetic fields for the Flux-Coordinate Independent method. *Computer Physics Communications*, 213(??):9–18, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303587.

Horgue:2015:OST

[HSF+15] P. Horgue, C. Soulaine, J. Franc, R. Guibert, and G. Debenest. An open-source toolbox for multiphase flow in porous media. *Computer Physics Communications*, 187(??):217–226, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003403.

Hammerschmidt:2019:BPT

[HSF+19] T. Hammerschmidt, B. Seiser, M. E. Ford, A. N. Ladines, S. Schreiber, N. Wang, J. Jenke, Y. Lysogorskiy, C. Teijeiro, M. Mrovec, M. Cak, E. R. Margine, D. G. Pettifor, and R. Drautz. BOPfox program for tight-binding and analytic bond-order potential calculations. *Computer Physics Communications*, 235(??):221–233, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303096.

Hirvijoki:2012:AEN

[HSK+12] E. Hirvijoki, A. Snicker, T. Korpilo, P. Lauber, E. Poli, M. Schneller, and T. Kurki-Suonio. Alfvén eigenmodes and neoclassical tearing modes for orbit-following implementations. *Computer Physics Communications*, 183 (12):2589–2593, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002378.

Hayashi:2011:TCM

[HST+11] Keiji Hayashi, Tomoki Shiraishi, Kazuho Toyoda, Fumiya Tanaka, Taiga Mori, and Takumi Hata. Temperature-controlled molecular dynamics study on velocity-dependent threshold behavior of dynamic nano-friction. *Computer Physics Communications*, 182(9):2032–2035, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000622.

Hsu:2011:P

[Hsu11a] James J. Y. Hsu. Preface. *Computer Physics Communications*, 182(1):1, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003875.

Hsu:2011:RTM

[Hsu11b] Jang-Yu Hsu. Relativistic theory of mode conversion at plasma frequency — the finite difference time domain simulation. *Computer Physics Communications*, 182(1):155–157, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000319X.

Hohenester:2012:MMT

[HT12] Ulrich Hohenester and Andreas Trügler. MNPBEM — a Matlab toolbox for the simulation of plasmonic nanoparticles. *Computer Physics Communications*, 183(2):370–381, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003274.

Hariri:2016:PPA

[HTJ+16] F. Hariri, T. M. Tran, A. Jocksch, E. Lanti, J. Progsch, P. Messmer, S. Brunner, C. Gheller, and L. Villard. A portable platform for accelerated PIC codes and its application to GPUs using OpenACC. *Computer Physics Communications*, 207(??):69–82, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516301242`.

Hollis:2013:TRT

[HTT13] M. D. J. Hollis, M. Tessenyi, and G. Tinetti. `tau`: a 1D radiative transfer code for transmission spectroscopy of extrasolar planet atmospheres. *Computer Physics Communications*, 184(10):2351–2361, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001719`.

Hollis:2014:TRT

[HTT14] M. D. J. Hollis, M. Tessenyi, and G. Tinetti. `tau`: a 1D radiative transfer code for transmission spectroscopy of extrasolar planet atmospheres. *Computer Physics Communications*, 185(2):695, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003184`.

Huang:2017:LLC

[HTY17] Xiaoyuan Huang, Yue-Lin Sming Tsai, and Qiang Yuan. LikeDM: Likelihood calculator of dark matter detection. *Computer Physics Communications*, 213(??):252–263, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303940`.

Huang:2017:IQV

[Hua17] Li Huang. iQIST v0.7: an open source continuous-time quantum Monte Carlo impurity solver toolkit. *Computer Physics Communications*, 221(??):423–424, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302898`.

Haelterman:2015:ACT

[HV15] R. Haelterman and D. Van Eester. Accelerating the convergence of a tokamak modeling code with Aitken's method. *Computer Physics Communications*, 196(??):70–79, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001988.

Honkonen:2013:PGL

[HvAS+13] I. Honkonen, S. von Alfthan, A. Sandroos, P. Janhunen, and M. Palmroth. Parallel grid library for rapid and flexible simulation development. *Computer Physics Communications*, 184(4):1297–1309, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004237.

Hulsmann:2010:ANO

[HVMR10] Marco Hülsmann, Jadran Vrabec, Astrid Maaß, and Dirk Reith. Assessment of numerical optimization algorithms for the development of molecular models. *Computer Physics Communications*, 181(5):887–905, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000147.

Hawkes:2019:CMM

[HVP+19] J. Hawkes, G. Vaz, A. B. Phillips, C. M. Klaij, S. J. Cox, and S. R. Turnock. Chaotic multigrid methods for the solution of elliptic equations. *Computer Physics Communications*, 237(??):26–36, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303916.

Hehn:2017:HTS

[HvWT17] Andreas Hehn, Natalija van Well, and Matthias Troyer. High-temperature series expansion for spin-1/2 Heisenberg models. *Computer Physics Communications*, 212(??):180–188, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302739.

Huang:2011:NSL

[HW11] B. J. Huang and Ten-Ming Wu. Numerical studies for localization-delocalization transition in vibrational spectra. *Computer Physics Communications*, 182(1):213–215, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000247X.

Hutchinson:2012:VGA

[HW12] M. Hutchinson and M. Widom. VASP on a GPU: Application to exact-exchange calculations of the stability of elemental boron. *Computer Physics Communications*, 183(7):1422–1426, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000707.

Hadade:2019:SUO

[HWCdM19] Ioan Hadade, Feng Wang, Mauro Carnevale, and Luca di Mare. Some useful optimisations for unstructured computational fluid dynamics codes on multicore and manycore architectures. *Computer Physics Communications*, 235(??):305–323, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302492.

Huang:2011:ESC

[HWCH11] Chih-Hsien Huang, Jing-Nuo Wu, Szu-Cheng Cheng, and Wen-Feng Hsieh. The evolution of solitons in coupled resonator optical waveguides and photonic-crystal waveguides. *Computer Physics Communications*, 182(1):232–236, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001633.

Hafermann:2013:EIC

[HWG13] Hartmut Hafermann, Philipp Werner, and Emanuel Gull. Efficient implementation of the continuous-time hybridization expansion quantum impurity solver. *Computer Physics Communications*, 184(4):1280–1286, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004092.

Hu:2017:KOS

[HWL+17] Changjun Hu, Xianmeng Wang, Jianjiang Li, Xinfu He, Shigang Li, Yangde Feng, Shaofeng Yang, and He Bai. Kernel optimization for short-range molecular dynamics. *Computer Physics Communications*, 211(??):31–40, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301928.

Huang:2015:IOS

[HWM+15] Li Huang, Yilin Wang, Zi Yang Meng, Liang Du, Philipp Werner, and Xi Dai. iQIST: an open source continuous-time quantum Monte Carlo impurity solver toolkit. *Computer Physics Communications*, 195(??):140–160, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001629.

Held:2016:TDG

[HWS16] M. Held, M. Wiesenberger, and A. Stegmeir. Three discontinuous Galerkin schemes for the anisotropic heat conduction equation on non-aligned grids. *Computer Physics Communications*, 199(??):29–39, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003896.

Holmes:2010:EBA

[HWT10] David W. Holmes, John R. Williams, and Peter Tilke. An events based algorithm for distributing concurrent tasks on multi-core architectures. *Computer Physics Communications*, 181(2):341–354, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003221.

Huang:2012:DCC

[HWW12] Gui-Yang Huang, Chong-Yu Wang, and Jian-Tao Wang. Detailed check of the $LDA+U$ and $GGA+U$ corrected method for defect calculations in wurtzite ZnO. *Computer Physics Communications*, 183(8):1749–1752, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465512001221.

Hou:2013:EGA

[HXW+13] Chaofeng Hou, Ji Xu, Peng Wang, Wenlai Huang, and Xiaowei Wang. Efficient GPU-accelerated molecular dynamics simulation of solid covalent crystals. *Computer Physics Communications*, 184(5):1364–1371, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000064.

Hoshino:2011:PIS

[HYM11] K. Hoshino, T. Yoshikawa, and S. Munejiri. Pressure-induced structural change from low-density to high-density amorphous ice by molecular-dynamics simulations. *Computer Physics Communications*, 182(1):49–51, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002845.

Hu:2011:CFD

[HZ11] Xiuling Hu and Luming Zhang. A compact finite difference scheme for the fourth-order fractional diffusion-wave system. *Computer Physics Communications*, 182(8):1645–1650, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001445.

Huang:2019:CCN

[HZC19] Jianqing Huang, Jianan Zhao, and Weiwei Cai. Compressing convolutional neural networks using POD for the reconstruction of nonlinear tomographic absorption spectroscopy. *Computer Physics Communications*, 241(??):33–39, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301018.

Huang:2016:FGI

[HZW+16] C.-K. Huang, Y. Zeng, Y. Wang, M. D. Meyers, S. Yi, and B. J. Albright. Finite grid instability and spectral fidelity of the electrostatic particle-in-cell algorithm. *Computer Physics Communications*, 207(??):123–135, October 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630145X.

Ho:2019:MLP

[HZW+19] Minh Tuan Ho, Lianhua Zhu, Lei Wu, Peng Wang, Zhaoli Guo, Zhi-Hui Li, and Yonghao Zhang. A multi-level parallel solver for rarefied gas flows in porous media. *Computer Physics Communications*, 234(??):14–25, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303047.

Ilyushin:2011:APF

[IB11] Ya. A. Ilyushin and V. P. Budak. Analysis of the propagation of the femtosecond laser pulse in the scattering medium. *Computer Physics Communications*, 182(4):940–945, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005242.

Ismailov:2018:TDP

[IBB18] Mansur I. Ismailov, Fermín S. V. Bazán, and Luciano Bedin. Time-dependent perfusion coefficient estimation in a bioheat transfer problem. *Computer Physics Communications*, 230(??):50–58, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301358.

Iniguez:2011:MOF

[IBKK11] Gerardo Iñiguez, Rafael A. Barrio, János Kertész, and Kimmo K. Kaski. Modelling opinion formation driven communities in social networks. *Computer Physics Communications*, 182(9):1866–1869, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004662.

Innocenti:2015:ITS

[IBP+15] M. E. Innocenti, A. Beck, T. Ponweiser, S. Markidis, and G. Lapenta. Introduction of temporal sub-stepping in the Multi-Level Multi-Domain semi-implicit Particle-In-Cell code Parsek2D-MLMD. *Computer Physics Communications*, 189(??):47–59, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400410X.

Moxley:2013:GFD

[ICD13] Frederick Ira Moxley III, David T. Chuss, and Weizhong Dai. A generalized finite-difference time-domain scheme for solving nonlinear Schrödinger equations. *Computer Physics Communications*, 184(8):1834–1841, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001033.

Ito:2016:VBI

[ICPD16] Keiichi Ito, Ivo Couckuyt, Silvia Poles, and Tom Dhaene. Variance-based interaction index measuring heteroscedasticity. *Computer Physics Communications*, 203(??):152–161, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300479.

Iskakov:2018:EDL

[ID18] Sergei Iskakov and Michael Danilov. Exact diagonalization library for quantum electron models. *Computer Physics Communications*, 225(??):128–139, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304216.

Ito:2018:IRE

[IFOI18] Shingo Ito, Dmitri G. Fedorov, Yuko Okamoto, and Stephan Irle. Implementation of replica-exchange umbrella sampling in GAMESS. *Computer Physics Communications*, 228(??):152–162, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300274.

Ibanez:2011:SDM

[IH11] Javier Ibáñez and Vicente Hernández. Solving differential matrix Riccati equations by a piecewise-linearized method based on diagonal Padé approximants. *Computer Physics Communications*, 182(3):669–678, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004704.

Ihnatsenka:2012:CEQ

[Ihn12] S. Ihnatsenka. Computation of electron quantum transport in graphene nanoribbons using GPU. *Computer Physics Communications*, 183(3):543–546, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100381X.

Ito:2016:IRE

[IIO16] Shingo Ito, Stephan Irle, and Yuko Okamoto. Implementation of replica-exchange umbrella sampling in the DFTB+ semiempirical quantum chemistry package. *Computer Physics Communications*, 204(??):1–10, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630025X.

Ikeno:2018:MLF

[Ike18] Hidekazu Ikeno. mxpfit: A library for finding optimal multi-exponential approximations. *Computer Physics Communications*, 230(??):135–144, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301310.

Iserles:2019:CSL

[IKS19] Arieh Iserles, Karolina Kropielnicka, and Pranav Singh. Compact schemes for laser–matter interaction in Schrödinger equation based on effective splittings of Magnus expansion. *Computer Physics Communications*, 234(??):195–201, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302601.

Incardona:2019:OSO

[ILZ+19] Pietro Incardona, Antonio Leo, Yaroslav Zaluzhnyi, Rajesh Ramaswamy, and Ivo F. Sbalzarini. OpenFPM: a scalable open framework for particle and particle-mesh codes on parallel computers. *Computer Physics Communications*, 241(??):155–177, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300852.

Nomura:2015:ELS

[iNSK+15] Ken ichi Nomura, Patrick E. Small, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta. An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations. *Computer Physics Communications*, 192(??):91–96, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000818.

Idesman:2014:AFE

[IP14] A. Idesman and D. Pham. Accurate finite element modeling of acoustic waves. *Computer Physics Communications*, 185(7):2034–2045, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001325.

Satake:2011:SPC

[iSSMI11] Shin ichi Satake, Gaku Sorimachi, Nobuyuki Masuda, and Tomoyoshi Ito. Special-purpose computer for Particle Image Velocimetry. *Computer Physics Communications*, 182(5):1178–1182, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000427.

Satake:2012:OGA

[iSYS12] Shin ichi Satake, Hajime Yoshimori, and Takayuki Suzuki. Optimizations of a GPU accelerated heat conduction equation by a programming of CUDA Fortran from an analysis of a PTX file. *Computer Physics Communications*, 183(11):2376–2385, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002068.

Tadaki:2011:EFN

[iT11] Shin ichi Tadaki. Effects of fast noises on long-range correlations. *Computer Physics Communications*, 182(1):237–239, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002821.

Ishizuka:2013:PEM

[IUM13] Hiroaki Ishizuka, Masafumi Udagawa, and Yukitoshi Motome. Polynomial expansion Monte Carlo study of frustrated itinerant electron systems: Application to a spin-ice type Kondo lattice model on a pyrochlore lattice. *Computer Physics Communications*, 184(12):2684–2692, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002373.

Izaac:2015:PCT

[IW15] Josh A. Izaac and Jingbo B. Wang. pyCTQW: a continuous-time quantum walk simulator on distributed memory computers. *Computer Physics Communications*, 186(??):81–92, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003166.

Ixaru:2010:NNM

[Ixa10] L. Gr. Ixaru. New numerical method for the eigenvalue problem of the 2D Schrödinger equation. *Computer Physics Communications*, 181(10):1738–1742, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002080.

Ixaru:2012:RKM

[Ixa12] L. Gr. Ixaru. Runge–Kutta method with equation dependent coefficients. *Computer Physics Communications*, 183(1):63–69, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003018.

Ixaru:2016:NAS

[Ixa16] L. Gr. Ixaru. Numerical approach of some three-body problems. *Computer Physics Communications*, 209(??):48–57, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302429.

Isakov:2015:OSA

[IZRT15] S. V. Isakov, I. N. Zintchenko, T. F. Rønnow, and M. Troyer. Optimised simulated annealing for Ising spin glasses. *Computer Physics Communications*, 192(??):265–271, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000727.

Javadi:2017:KMC

[JA17] Mohammad Javadi and Yaser Abdi. Kinetic Monte Carlo simulation of single-electron multiple-trapping transport in disordered media. *Computer Physics Communications*, 221(??):282–289, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302862.

Jablonski:2012:EAC

[Jab12] A. Jablonski. An effective algorithm for calculating the Chandrasekhar function. *Computer Physics Communications*, 183(8):1773–1782, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000847.

Jablonski:2013:IAC

[Jab13] A. Jablonski. Improved algorithm for calculating the Chandrasekhar function. *Computer Physics Communications*, 184(2):440–442, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200286X.

Jablonski:2015:CFR

[Jab15] A. Jablonski. The Chandrasekhar function revisited. *Computer Physics Communications*, 196(??):416–428, November

2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001903.

Jablonski:2017:MES

[Jab17] A. Jablonski. Multiple elastic scattering of electrons in condensed matter. *Computer Physics Communications*, 210(??):92–102, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630248X.

Jablonski:2019:CFM

[Jab19] A. Jablonski. The Chandrasekhar function for modeling photoelectron transport in solids. *Computer Physics Communications*, 235(??):489–501, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302546.

Jacobse:2019:MMP

[Jac19] Peter H. Jacobse. MathemaTB: a Mathematica package for tight-binding calculations. *Computer Physics Communications*, 244(??):392–408, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301821.

Jalilian:2010:NPS

[Jal10] R. Jalilian. Non-polynomial spline method for solving Bratu's problem. *Computer Physics Communications*, 181(11):1868–1872, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002912.

Jang:2010:SLN

[Jan10] Bongsoo Jang. Solving linear and nonlinear initial value problems by the projected differential transform method. *Computer Physics Communications*, 181(5):848–854, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004123.

Junghans:2017:CEA

[JAS17] Christoph Junghans, Animesh Agarwal, and Luigi Delle Site. Computational efficiency and Amdahl's law for the adaptive resolution simulation technique. *Computer Physics Communications*, 215(??):20–25, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300425.

Javanainen:2017:SA

[Jav17] Juha Javanainen. The software atom. *Computer Physics Communications*, 212(??):1–7, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302880.

Jarema:2016:BSG

[JBG+16] D. Jarema, H. J. Bungartz, T. Görler, F. Jenko, T. Neckel, and D. Told. Block-structured grids for Eulerian gyrokinetic simulations. *Computer Physics Communications*, 198(??):105–117, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003458.

Jarema:2017:BSG

[JBG+17] D. Jarema, H. J. Bungartz, T. Görler, F. Jenko, T. Neckel, and D. Told. Block-structured grids in full velocity space for Eulerian gyrokinetic simulations. *Computer Physics Communications*, 215(??):49–62, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300474.

Jamali:2015:GIA

[JBKM15] Safa Jamali, Arman Boromand, Shaghayegh Khani, and Joao Maia. Gaussian-inspired auxiliary non-equilibrium thermostat (GIANT) for dissipative particle dynamics simulations. *Computer Physics Communications*, 197(??):27–34, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002878.

Jefferson:2013:AAS

[JC13] G. F. Jefferson and J. Carminati. ASP: Automated symbolic computation of approximate symmetries of differential equations. *Computer Physics Communications*, 184(3): 1045–1063, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003888.

Jefferson:2014:FAS

[JC14] G. F. Jefferson and J. Carminati. FracSym: Automated symbolic computation of Lie symmetries of fractional differential equations. *Computer Physics Communications*, 185(1):430–441, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003202.

Jaeken:2016:SCE

[JC16] Jan W. Jaeken and Stefaan Cottenier. Solving the Christoffel equation: Phase and group velocities. *Computer Physics Communications*, 207(??):445–451, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301795.

Jezequel:2010:NVC

[JCL10] Fabienne Jézéquel, Jean-Marie Chesneaux, and Jean-Luc Lamotte. A new version of the CADNA library for estimating round-off error propagation in Fortran programs. *Computer Physics Communications*, 181(11):1927–1928, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002419.

Jiang:2018:ESS

[JCL+18] Tao Jiang, Zhen-Chao Chen, Wei-Gang Lu, Jin-Yun Yuan, and Deng-Shan Wang. An efficient split-step and implicit pure mesh-free method for the 2D/3D nonlinear Gross–Pitaevskii equations. *Computer Physics Communications*, 231(??):19–30, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301607.

Jia:2013:APW

[JCW+13] Weile Jia, Zongyan Cao, Long Wang, Jiyun Fu, Xuebin Chi, Weiguo Gao, and Lin-Wang Wang. The analysis of a plane wave pseudopotential density functional theory code on a GPU machine. *Computer Physics Communications*, 184(1):9–18, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200255X.

Julia-Diaz:2012:SEA

[JDG12] Bruno Juliá-Díaz and Tobias Graß. Strongdeco: Expansion of analytical, strongly correlated quantum states into a many-body basis. *Computer Physics Communications*, 183(3):737–745, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003791.

Jara:2012:NVJ

[JEC+12] Carlos A. Jara, Francisco Esquembre, Wolfgang Christian, Francisco A. Candelas, Fernando Torres, and Sebastián Dormido. A new 3D visualization Java framework based on physics principles. *Computer Physics Communications*, 183(2):231–244, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002797.

Jelinek:2014:LSP

[JEFP14] Bohumir Jelinek, Mohsen Eshraghi, Sergio Felicelli, and John F. Peters. Large-scale parallel lattice Boltzmann-cellular automaton model of two-dimensional dendritic growth. *Computer Physics Communications*, 185(3):939–947, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003147.

Jiang:2012:NMC

[JFC12] R.-L. Jiang, C. Fang, and P.-F. Chen. A new MHD code with adaptive mesh refinement and parallelization for astrophysics. *Computer Physics Communications*, 183(8):1617–1633, August 2012. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000926.

Ji:2019:LIC

[JFHA19] Zhe Ji, Lin Fu, Xiangyu Y. Hu, and Nikolaus A. Adams. A Lagrangian inertial centroidal Voronoi particle method for dynamic load balancing in particle-based simulations. *Computer Physics Communications*, 239(??):53–63, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300177.

Jensen:2016:DTA

[JG16] Kristian Ejlebjerg Jensen and Gerard Gorman. Details of tetrahedral anisotropic mesh adaptation. *Computer Physics Communications*, 201(??):135–143, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004397.

Jiang:2013:FGC

[JGAL+13] Hong Jiang, Ricardo I. Gómez-Abal, Xin-Zheng Li, Christian Meisenbichler, Claudia Ambrosch-Draxl, and Matthias Scheffler. FHI-gap: a *GW* code based on the all-electron augmented plane wave method. *Computer Physics Communications*, 184(2):348–366, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003049.

Jonsson:2013:NVG

[JGB+13] P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I. P. Grant. New version: Grasp 2 K relativistic atomic structure package. *Computer Physics Communications*, 184(9):2197–2203, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000738.

Jucker:2011:IMI

[JGC+11] M. Jucker, J. P. Graves, W. A. Cooper, N. Mellet, T. Johnson, and S. Brunner. Integrated modeling for ion cyclotron resonant heating in toroidal systems. *Computer Physics Communications*, 182(4):912–925, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510005217`.

Jelinek:2011:CHV

[JH11] Petr Jelínek and Gerhard Hensler. The collisions of high-velocity clouds with the galactic halo. *Computer Physics Communications*, 182(9):1784–1789, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000439`.

Jiao:2015:CTE

[JH15] Li Guang Jiao and Yew Kam Ho. Computation of two-electron screened Coulomb potential integrals in Hylleraas basis sets. *Computer Physics Communications*, 188(??):140–147, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514004020`.

Jamshidi:2019:SPF

[JHH+19] F. Jamshidi, H. Heimel, M. Hasert, X. Cai, O. Deutschmann, H. Marschall, and M. Wörner. On suitability of phase-field and algebraic volume-of-fluid OpenFOAM(R) solvers for gas-liquid microfluidic applications. *Computer Physics Communications*, 236(??):72–85, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303631`.

Jiang:2014:NMM

[JHJG14] Rui Jiang, Mao-Bin Hu, Bin Jia, and Zi-You Gao. A new mechanism for metastability of under-saturated traffic responsible for time-delayed traffic breakdown at the signal. *Computer Physics Communications*, 185(5):1439–1442, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000435`.

Jolliet:2015:NAP

[JHL+15] S. Jolliet, F. D. Halpern, J. Loizu, A. Mosetto, F. Riva, and P. Ricci. Numerical approach to the parallel gradient operator in tokamak scrape-off layer turbulence simulations and application to the GBS code. *Computer Physics Communications*, 188(??):21–32, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400366X.

Jia:2018:NVF

[Jia18] Shouqing Jia. New version of FDTD with GFM program in Schwarzschild space-time. *Computer Physics Communications*, 232(??):264–265, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302133.

Jiwari:2012:HWQ

[Jiw12] Ram Jiwari. A Haar wavelet quasilinearization approach for numerical simulation of Burgers' equation. *Computer Physics Communications*, 183(11):2413–2423, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200210X.

Jiwari:2015:HNS

[Jiw15a] Ram Jiwari. A hybrid numerical scheme for the numerical solution of the Burgers' equation. *Computer Physics Communications*, 188(??):59–67, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003749.

Jiwari:2015:LIM

[Jiw15b] Ram Jiwari. Lagrange interpolation and modified cubic B-spline differential quadrature methods for solving hyperbolic partial differential equations with Dirichlet and Neumann boundary conditions. *Computer Physics Communications*, 193(??):55–65, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001204.

Jo:2015:GIR

[JJ15] Sunhwan Jo and Wei Jiang. A generic implementation of replica exchange with solute tempering (REST2) algorithm in NAMD for complex biophysical simulations. *Computer Physics Communications*, 197(??):304–311, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500329X.

Junghans:2011:HNT

[JJB11] Christoph Junghans, Wolfhard Janke, and Michael Bachmann. Hierarchies in nucleation transitions. *Computer Physics Communications*, 182(9):1937–1940, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004613.

Januszewski:2010:ANS

[JK10] M. Januszewski and M. Kostur. Accelerating numerical solution of stochastic differential equations with CUDA. *Computer Physics Communications*, 181(1):183–188, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002999.

Johnson:2013:NDP

[JK13] Chris Johnson and A. D. Kennedy. Numerical determination of partial spectrum of Hermitian matrices using a Lánczos method with selective reorthogonalization. *Computer Physics Communications*, 184(3):689–697, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003797.

Januszewski:2014:SFM

[JK14] M. Januszewski and M. Kostur. Sailfish: a flexible multi-GPU implementation of the lattice Boltzmann method. *Computer Physics Communications*, 185(9):2350–2368, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001520.

Jeong:2019:FAA

[JK19] Darae Jeong and Junseok Kim. Fast and accurate adaptive finite difference method for dendritic growth. *Computer Physics Communications*, 236(??):95–103, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303680.

Joung:2018:CSA

[JKG+18] InSuk Joung, Jong Yun Kim, Steven P. Gross, Keehyoung Joo, and Jooyoung Lee. Conformational Space Annealing explained: a general optimization algorithm, with diverse applications. *Computer Physics Communications*, 223(??):28–33, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303351.

Jung:2016:PIF

[JKIS16] Jaewoon Jung, Chigusa Kobayashi, Toshiyuki Imamura, and Yuji Sugita. Parallel implementation of 3D FFT with volumetric decomposition schemes for efficient molecular dynamics simulations. *Computer Physics Communications*, 200(??):57–65, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004063.

Jiang:2010:ASF

[JL10] Wei Jiang and Yingzhen Lin. Approximate solution of the fractional advection-dispersion equation. *Computer Physics Communications*, 181(3):557–561, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900352X.

Jentschura:2012:NCB

[JL12] U. D. Jentschura and E. Lötstedt. Numerical calculation of Bessel, Hankel and Airy functions. *Computer Physics Communications*, 183(3):506–519, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003729.

Jia:2019:FRT

[JL19] Weile Jia and Lin Lin. Fast real-time time-dependent hybrid functional calculations with the parallel transport gauge and the adaptively compressed exchange formulation. *Computer Physics Communications*, 240(??):21–29, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930061X`.

Jansen:2014:QMC

[JLA+14] K. Jansen, H. Leovey, A. Ammon, A. Griewank, and M. Müller-Preussker. Quasi-Monte Carlo methods for lattice systems: a first look. *Computer Physics Communications*, 185(3):948–959, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003391`.

Jia:2018:NSE

[JLM18] Shouqing Jia, Dongsheng La, and Xuelian Ma. Numerical simulation of electromagnetic waves in Schwarzschild space-time by finite difference time domain method and Green function method. *Computer Physics Communications*, 225(??):166–173, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517304149`.

Jiang:2013:SBF

[JLW13] Xiang-Wei Jiang, Shu-Shen Li, and Lin-Wang Wang. A small box Fast Fourier Transformation method for fast Poisson solutions in large systems. *Computer Physics Communications*, 184(12):2693–2702, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002385`.

Jonsson:2017:EDM

[JMG+17] Thorsteinn H. Jonsson, Andrei Manolescu, Hsi-Sheng Goan, Nzar Rauf Abdullah, Anna Sitek, Chi-Shung Tang, and Vidar Gudmundsson. Efficient determination of the Markovian time-evolution towards a steady-state of a complex open quantum system. *Computer Physics Communications*, 220(??):81–90, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730200X.

Johansson:2012:QOS

[JNN12] J. R. Johansson, P. D. Nation, and Franco Nori. QuTiP: an open-source Python framework for the dynamics of open quantum systems. *Computer Physics Communications*, 183(8):1760–1772, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000835.

Johansson:2013:QPF

[JNN13] J. R. Johansson, P. D. Nation, and Franco Nori. QuTiP 2: a Python framework for the dynamics of open quantum systems. *Computer Physics Communications*, 184(4): 1234–1240, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003955.

Johnson:2013:FLS

[JOK13] Calvin W. Johnson, W. Erich Ormand, and Plamen G. Krastev. Factorization in large-scale many-body calculations. *Computer Physics Communications*, 184(12):2761–2774, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002518.

Jiang:2012:MCS

[JOR+12] Tao Jiang, Jie Ouyang, Jin-Lian Ren, Bin-Xin Yang, and Xiao-Yang Xu. A mixed corrected symmetric SPH (MC–SSPH) method for computational dynamic problems. *Computer Physics Communications*, 183(1):50–62, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003006.

Junghans:2010:RIA

[JP10] Christoph Junghans and Simón Poblete. A reference implementation of the adaptive resolution scheme in ESPResSo.

Computer Physics Communications, 181(8):1449–1454, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001244.

Jenkins:2011:AAE

[JP11] David D. Jenkins and Gregory D. Peterson. AESS: Accelerated exact stochastic simulation. *Computer Physics Communications*, 182(12):2580–2586, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002608.

Januszewski:2015:GBA

[JPCG15] Michal Januszewski, Andrzej Ptok, Dawid Crivelli, and Bartlomiej Gardas. GPU-based acceleration of free energy calculations in solid state physics. *Computer Physics Communications*, 192(??):220–227, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000697.

Jiang:2014:GSM

[JPH+14] Wei Jiang, James C. Phillips, Lei Huang, Mikolai Fajer, Yilin Meng, James C. Gumbart, Yun Luo, Klaus Schulten, and Benoît Roux. Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. *Computer Physics Communications*, 185(3):908–916, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004268.

Joulaian:2012:NAS

[JPK+12] M. Joulaian, A. Pishevar, S. Khajepor, F. Schmid, and Y. Afshar. A new algorithm for simulating flows of conducting fluids in the presence of electric fields. *Computer Physics Communications*, 183(11):2405–2412, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002093.

Jiwari:2012:NST

[JPM12] Ram Jiwari, Sapna Pandit, and R. C. Mittal. Numerical simulation of two-dimensional sine–Gordon solitons by differential quadrature method. *Computer Physics Communications*, 183(3):600–616, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003894`.

Jadach:2010:MMC

[JPSS10] S. Jadach, W. Placzek, M. Skrzypek, and P. Stoklosa. Markovian Monte Carlo program EvolFMC v.2 for solving QCD evolution equations. *Computer Physics Communications*, 181(2):393–412, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003178`.

Jourdan:2016:ASS

[JSLM16] T. Jourdan, G. Stoltz, F. Legoll, and L. Monasse. An accurate scheme to solve cluster dynamics equations using a Fokker–Planck approach. *Computer Physics Communications*, 207(??):170–178, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551630162X`.

Jollet:2014:GPA

[JTH14] François Jollet, Marc Torrent, and Natalie Holzwarth. Generation of Projector Augmented-Wave atomic data: a 71 element validated table in the XML format. *Computer Physics Communications*, 185(4):1246–1254, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004359`.

Jenista:2011:CNS

[JTN$^+$11] Jirí Jenista, Hidemasa Takana, Hideya Nishiyama, Milada Bartlová, Vladimír Aubrecht, Petr Krenek, Viktor Sember, and Alan Masláni. A comparative numerical study of hybrid-stabilized argon-water electric arc. *Computer Physics Communications*, 182(9):1776–1783, September 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000269.

Jiao:2015:RDA

[JTP15] A. S. M. Jiao, P. W. M. Tsang, and T.-C. Poon. Restoration of digital off-axis Fresnel hologram by exemplar and search based image inpainting with enhanced computing speed. *Computer Physics Communications*, 193(??):30–37, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001174.

Jin:2011:IHM

[JTT11] Ying-Jun Jin, Xiao-Min Tong, and Nobuyuki Toshima. Ionization of hydrogen molecular ions in an intense laser field via a resonant state. *Computer Physics Communications*, 182(1):146–148, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002018.

Jing:2017:MHP

[JTW+17] Weipeng Jing, Danyu Tong, Yangang Wang, Jingyuan Wang, Yaqiu Liu, and Peng Zhao. MaMR: High-performance MapReduce programming model for material cloud applications. *Computer Physics Communications*, 211(??):79–87, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301977.

Jones:2017:ECT

[JU17] Adam Jones and Sergey Utyuzhnikov. Efficient computation of turbulent flow in ribbed passages using a non-overlapping near-wall domain decomposition method. *Computer Physics Communications*, 217(??):1–10, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300760.

Jamil:2016:HCC

[JuIAM16] Khalid Jamil, Siraj ul Islam Ahmad, and Shahid Manzoor. HIBRA: a computer code for heavy ion binary reaction analysis employing ion track detectors. *Computer Physics Communications*, 198(??):216–221, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003355.

Jin:2017:NCC

[JvOK17] Wenjie Jin, J. Ruud van Ommen, and Chris R. Kleijn. A new cut-cell algorithm for DSMC simulations of rarefied gas flows around immersed moving objects. *Computer Physics Communications*, 212(??):146–151, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303423.

Jorissen:2012:HPS

[JVR12] K. Jorissen, F. D. Vila, and J. J. Rehr. A high performance scientific cloud computing environment for materials simulations. *Computer Physics Communications*, 183(9):1911–1919, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200149X.

Jeng:2013:TPC

[JWC13] B.-W. Jeng, Y.-S. Wang, and C.-S. Chien. A two-parameter continuation algorithm for vortex pinning in rotating Bose–Einstein condensates. *Computer Physics Communications*, 184(3):493–508, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003335.

Jaschke:2018:OSM

[JWC18] Daniel Jaschke, Michael L. Wall, and Lincoln D. Carr. Open source matrix product states: Opening ways to simulate entangled many-body quantum systems in one dimension. *Computer Physics Communications*, 225(??):59–91, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304204.

Jia:2017:GIL

[JWCW17] Weile Jia, Jue Wang, Xuebin Chi, and Lin-Wang Wang. GPU implementation of the linear scaling three dimensional fragment method for large scale electronic structure calculations. *Computer Physics Communications*, 211(??):8–15, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301850.

Jakubczyk:2012:CIK

[JWJL12] P. Jakubczyk, A. Wal, D. Jakubczyk, and T. Lulek. Computer implementation of the Kerov–Kirillov–Reshetikhin algorithm. *Computer Physics Communications*, 183(6):1354–1362, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000549.

Jiang:2013:NSG

[JWL13] Wei Jiang, Hanquan Wang, and Xianggui Li. A numerical study of the ground state and dynamics of atomic-molecular Bose–Einstein condensates. *Computer Physics Communications*, 184(11):2396–2407, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300194X.

Jia:2018:PPH

[JWM$^+$18] C. J. Jia, Y. Wang, C. B. Mendl, B. Moritz, and T. P. Devereaux. Paradeisos: a perfect hashing algorithm for many-body eigenvalue problems. *Computer Physics Communications*, 224(??):81–89, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303946.

Ji:2016:LSW

[JXTS16] Zhe Ji, Fei Xu, Akiyuki Takahashi, and Yu Sun. Large scale water entry simulation with smoothed particle hydrodynamics on single- and multi-GPU systems. *Computer Physics Communications*, 209(??):1–12, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301400.

Ji:2018:AAB

[JYPA18] Songsong Ji, Yibo Yang, Gang Pang, and Xavier Antoine. Accurate artificial boundary conditions for the semi-discretized linear Schrödinger and heat equations on rectangular domains. *Computer Physics Communications*, 222(??):84–93, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303247.

Jiang:2018:ATE

[JZJ18] Tongsong Jiang, Zhaozhong Zhang, and Ziwu Jiang. Algebraic techniques for eigenvalues and eigenvectors of a split quaternion matrix in split quaternionic mechanics. *Computer Physics Communications*, 229(??):1–7, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300936.

Jiao:2019:ACS

[JZZ+19] Li Guang Jiao, Li Rong Zan, Lin Zhu, Jia Ma, and Yew Kam Ho. Accurate computation of screened Coulomb potential integrals in numerical Hartree–Fock programs. *Computer Physics Communications*, 244(??):217–227, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301791.

Koretsune:2017:EMC

[KA17] Takashi Koretsune and Ryotaro Arita. Efficient method to calculate the electron-phonon coupling constant and superconducting transition temperature. *Computer Physics Communications*, 220(??):239–242, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302308.

Keaveney:2018:EEA

[KAH18] James Keaveney, Charles S. Adams, and Ifan G. Hughes. ElecSus: Extension to arbitrary geometry magneto-optics. *Computer Physics Communications*, 224(??):311–324, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304009.

Khoromskaia:2012:FAT

[KAK12] V. Khoromskaia, D. Andrae, and B. N. Khoromskij. Fast and accurate 3D tensor calculation of the Fock operator in a general basis. *Computer Physics Communications*, 183(11):2392–2404, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002081.

Kant:2014:FLD

[Kan14] Philipp Kant. Finding linear dependencies in integration-by-parts equations: a Monte Carlo approach. *Computer Physics Communications*, 185(5):1473–1476, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000307.

Kaneko:2018:CNF

[Kan18] T. Kaneko. Counting the number of Feynman graphs in QCD. *Computer Physics Communications*, 226(??):104–113, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300018.

Kaprzyk:2012:AFI

[Kap12a] S. Kaprzyk. An algebraic formulation and implementation of the tetrahedron linear method for the Brillouin zone integration of spectral functions. *Computer Physics Communications*, 183(2):347–362, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003109.

Kaprzyk:2012:AFS

[Kap12b] S. Kaprzyk. An algebraic formulation of the simplex linear method for multiple integrals over the d-dimensional domain. *Computer Physics Communications*, 183(1):20–25, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002785.

Kappl:2016:SCS

[Kap16] Rolf Kappl. SOLARPROP: Charge-sign dependent solar modulation for everyone. *Computer Physics Communications*, 207(??):386–399, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630159X.

Khan:2015:STP

[KAR+15] Banaras Khan, H. A. Rahnamaye Aliabad, N. Razghandi, M. Maqbool, S. Jalali Asadabadi, and Iftikhar Ahmad. Structural and thermoelectric properties of pure and La, Y doped $HoMnO_3$ for their use as alternative energy materials. *Computer Physics Communications*, 187(??):1–7, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400321X.

Kosti:2012:OER

[KAS12] A. A. Kosti, Z. A. Anastassi, and T. E. Simos. An optimized explicit Runge–Kutta–Nyström method for the numerical solution of orbital and related periodical initial value problems. *Computer Physics Communications*, 183(3):470–479, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100364X.

Kaspar:2014:EEE

[Kas14] J. Kaspar. Elegent — an elastic event generator. *Computer Physics Communications*, 185(3):1081–1084, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004098.

Kaushik:2013:IAA

[Kau13] Aditya Kaushik. Iterative analytic approximation to nonlinear convection dominated systems. *Computer Physics Communications*, 184(9):2061–2069, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001343.

Knap:2011:PPJ

[KAvdL11] Michael Knap, Enrico Arrigoni, and Wolfgang von der Linden. Polaritonic properties of the Jaynes–Cummings lattice model in two dimensions. *Computer Physics Communications*, 182(9):2036–2040, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000634.

Kunes:2010:WLA

[KAW+10] Jan Kunes, Ryotaro Arita, Philipp Wissgott, Alessandro Toschi, Hiroaki Ikeda, and Karsten Held. Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions. *Computer Physics Communications*, 181(11):1888–1895, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002948.

Kawamura:2019:FFS

[Kaw19] Mitsuaki Kawamura. FermiSurfer: Fermi-surface viewer providing multiple representation schemes. *Computer Physics Communications*, 239(??):197–203, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300347.

Kabin:2015:MCP

[KB15a] K. Kabin and G. Bonner. Motion of a charged particle in an axisymmetric longitudinal magnetic field that is inversely proportional to the radius. *Computer Physics Communications*, 189(??):155–161, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004068.

Kittelmann:2015:PNS

[KB15b] T. Kittelmann and M. Boin. Polycrystalline neutron scattering for Geant4: NXSG4. *Computer Physics Communications*, 189(??):114–118, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003816.

Kahl:2019:APH

[KB19] E. V. Kahl and J. C. Berengut. AMBiT: a programme for high-precision relativistic atomic structure calculations. *Computer Physics Communications*, 238(??):232–243, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304302.

Kjaergaard:2017:MPL

[KBB+17] Thomas Kjærgaard, Pablo Baudin, Dmytro Bykov, Janus Juul Eriksen, Patrick Ettenhuber, Kasper Kristensen, Jeff Larkin, Dmitry Liakh, Filip Pawlowski, Aaron Vose, Yang Min Wang, and Poul Jørgensen. Massively parallel and linear-scaling algorithm for second-order Møller–Plesset perturbation theory applied to the study of supramolecular wires. *Computer Physics Communications*, 212(??):152–160, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303447.

Kundu:2018:PPA

[KBLJ18] Sudipta Kundu, Satadeep Bhattacharjee, Seung-Cheol Lee, and Manish Jain. PASTA: Python Algorithms for Searching Transition stAtes. *Computer Physics Communications*, 233(??):261–268, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302583.

Kopp:2012:SDE

[KBSP12] A. Kopp, I. Büsching, R. D. Strauss, and M. S. Potgieter. A stochastic differential equation code for multidimensional Fokker–Planck type problems. *Computer Physics Communications*, 183(3):530–542, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003766.

Koval:2019:PNE

[KBSP19] Peter Koval, Marc Barbry, and Daniel Sánchez-Portal. PySCF-NAO: an efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals. *Computer Physics Communications*, 236(??):188–204, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302996.

Kratzer:2014:FRE

[KBT+14] Kai Kratzer, Joshua T. Berryman, Aaron Taudt, Johannes Zeman, and Axel Arnold. The Flexible Rare Event Sampling Harness System (FRESHS). *Computer Physics Communications*, 185(7):1875–1885, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000939.

Khankhoje:2014:MRS

[KC14] Uday K. Khankhoje and Thomas A. Cwik. A mesh reconfiguration scheme for speeding up Monte Carlo simulations of electromagnetic scattering by random rough surfaces. *Computer Physics Communications*, 185(2):445–447, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001021.

Khaziev:2018:HSE

[KC18] Rinat Khaziev and Davide Curreli. hPIC: A scalable electrostatic Particle-in-Cell for plasma-material interactions. *Computer Physics Communications*, 229(??):87–98, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301012.

Knuth:2015:AEF

[KCA+15] Franz Knuth, Christian Carbogno, Viktor Atalla, Volker Blum, and Matthias Scheffler. All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. *Computer Physics Communications*, 190(??):33–50, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000090.

Kim:2011:PPP

[KCL11] Doo Hwan Kim, Moon-Yong Cha, and Jae Woo Lee. The persistence probability and the price-price correlation functions in the Korean stock market. *Computer Physics Communications*, 182(1):243–244, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002274.

Kassar:2018:CCV

[KCN18] Bruno B. M. Kassar, João N. E. Carneiro, and Angela O. Nieckele. Curvature computation in volume-of-fluid method based on point-cloud sampling. *Computer Physics Communications*, 222(??):189–208, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303417.

Kulikov:2015:ACC

[KCS+15] I. M. Kulikov, I. G. Chernykh, A. V. Snytnikov, B. M. Glinskiy, and A. V. Tutukov. AstroPhi: a code for complex simulation of the dynamics of astrophysical objects using hybrid supercomputers. *Computer Physics Communications*, 186(??):71–80, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003099.

Karasiev:2015:IAR

[KCT15] Valentin V. Karasiev, Debajit Chakraborty, and S. B. Trickey. Improved analytical representation of combinations of Fermi–Dirac integrals for finite-temperature density functional calculations. *Computer Physics Communications*, 192(??):114–123, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000880.

Kupczynski:2016:BSI

[KD16] Marian Kupczynski and Hans De Raedt. Breakdown of statistical inference from some random experiments. *Computer Physics Communications*, 200(??):168–175, March 2016.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004324.

Kiesewetter:2017:AIS

[KD17] Simon Kiesewetter and Peter D. Drummond. Algorithms for integration of stochastic differential equations using parallel optimized sampling in the Stratonovich calculus. *Computer Physics Communications*, 212(??):25–38, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303083.

Kong:2011:IVG

[KDM11] Ling Ti Kong, Colin Denniston, and Martin H. Müser. An improved version of the Green's function molecular dynamics method. *Computer Physics Communications*, 182(2):540–541, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003851.

Karimi:2017:PNO

[KDM17] M. Karimi, H. Droghetti, and D. L. Marchisio. PUFoam: a novel open-source CFD solver for the simulation of polyurethane foams. *Computer Physics Communications*, 217(??):138–148, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300978.

Kuijpers:2014:OLD

[KdMvO14] Kasper R. Kuijpers, Lilian de Martín, and J. Ruud van Ommen. Optimizing off-lattice Diffusion-Limited Aggregation. *Computer Physics Communications*, 185(3):841–846, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004153.

Kauzlaric:2014:SSP

[KDP+14] David Kauzlarić, Marek Dynowski, Lars Pastewka, Andreas Greiner, and Jan G. Korvink. SYMPLER: SYMbolic ParticLE simulatoR with grid-computing interface. *Computer*

Physics Communications, 185(3):1085–1099, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004104.

Kalantzis:2012:UST

[KEH12] Georgios Kalantzis, Dimitrios Emfietzoglou, and Panagiotis Hadjidoukas. A unified spatio-temporal parallelization framework for accelerated Monte Carlo radiobiological modeling of electron tracks and subsequent radiation chemistry. *Computer Physics Communications*, 183(8):1683–1695, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001130.

Kerby:2017:EDN

[Ker17] Leslie M. Kerby. An energy-dependent numerical model for the condensation probability, γ_j. *Computer Physics Communications*, 213(??):29–39, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303605.

Kim:2016:CGS

[KFF+16] Jaewook Kim, M. F. J. Fox, A. R. Field, Y. U. Nam, and Y.-C. Ghim. Conditions for generating synthetic data to investigate characteristics of fluctuating quantities. *Computer Physics Communications*, 204(??):152–158, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300935.

Koehne:2013:PTP

[KFS+13] J.-H. Koehne, K. Frantzen, M. Schmitz, T. Fuchs, W. Rhode, D. Chirkin, and J. Becker Tjus. PROPOSAL: a tool for propagation of charged leptons. *Computer Physics Communications*, 184(9):2070–2090, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001355.

Kachman:2017:NIM

[KFS17] Tal Kachman, Shmuel Fishman, and Avy Soffer. Numerical implementation of the multiscale and averaging methods for quasi periodic systems. *Computer Physics Communications*, 221(??):235–245, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302643`.

Khayyer:2018:EIS

[KGFS18] Abbas Khayyer, Hitoshi Gotoh, Hosein Falahaty, and Yuma Shimizu. An enhanced ISPH–SPH coupled method for simulation of incompressible fluid-elastic structure interactions. *Computer Physics Communications*, 232(??):139–164, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301759`.

Korpilo:2016:GFT

[KGG+16] T. Korpilo, A. D. Gurchenko, E. Z. Gusakov, J. A. Heikkinen, S. J. Janhunen, T. P. Kiviniemi, S. Leerink, P. Niskala, and A. A. Perevalov. Gyrokinetic full-torus simulations of ohmic tokamak plasmas in circular limiter configuration. *Computer Physics Communications*, 203(??):128–137, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300364`.

Kunze:2010:LTM

[KGNS10] T. Kunze, S. Gemming, S. Numazawa, and M. Schreiber. Low-temperature modeling for degenerate and frustrated Heisenberg systems with anisotropy. *Computer Physics Communications*, 181(4):806–812, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509004056`.

Kroger:2010:ASC

[KH10] Martin Kröger and Markus Hütter. Automated symbolic calculations in nonequilibrium thermodynamics. *Computer Physics Communications*, 181(12):2149–2157, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003176.

Kar:2011:RSP

[KH11] Sabyasachi Kar and Y. K. Ho. Resonance states of Ps^- using correlated wave functions. *Computer Physics Communications*, 182(1):119–121, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001888.

Kleiber:2012:PMF

[KH12] R. Kleiber and R. Hatzky. A partly matrix-free solver for the gyrokinetic field equation in three-dimensional geometry. *Computer Physics Communications*, 183(2):305–308, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003365.

Krivenko:2019:TSI

[KH19] Igor Krivenko and Malte Harland. TRIQS/SOM: Implementation of the stochastic optimization method for analytic continuation. *Computer Physics Communications*, 239(??):166–183, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300402.

Karpenko:2014:IDV

[KHB14] Iu. Karpenko, P. Huovinen, and M. Bleicher. A 3 + 1 dimensional viscous hydrodynamic code for relativistic heavy ion collisions. *Computer Physics Communications*, 185(11):3016–3027, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002537.

Kallenborn:2019:MPC

[KHBS19] Felix Kallenborn, Christian Hundt, Sebastian Böser, and Bertil Schmidt. Massively parallel computation of atmospheric neutrino oscillations on CUDA-enabled accelerators. *Computer Physics Communications*, 234(??):235–244, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302790.

Kleiber:2011:ICV

[KHK+11] R. Kleiber, R. Hatzky, A. Könies, K. Kauffmann, and P. Helander. An improved control-variate scheme for particle-in-cell simulations with collisions. *Computer Physics Communications*, 182(4):1005–1012, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005382.

Kramer:2014:API

[KHKR14] Andreas Krämer, Marco Hülsmann, Thorsten Köddermann, and Dirk Reith. Automated parameterization of intermolecular pair potentials using global optimization techniques. *Computer Physics Communications*, 185(12):3228–3239, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003038.

Kunaseth:2019:SCN

[KHN19] Manaschai Kunaseth, Supa Hannongbua, and Aiichiro Nakano. Shift/collapse on neighbor list (SC-NBL): Fast evaluation of dynamic many-body potentials in molecular dynamics simulations. *Computer Physics Communications*, 235(??):88–94, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303448.

Kielbik:2018:ANL

[KHZ+18] Rafał Kiełbik, Krzysztof Hałagan, Witold Zatorski, Jarosław Jung, Jacek Ulański, Andrzej Napieralski, Kamil Rudnicki, Piotr Amrozik, Grzegorz Jabłoński, Dominik Stożek, Piotr Polanowski, Zbigniew Mudza, Joanna Kupis, and Przemysław Panek. ARUZ — large-scale, massively parallel FPGA-based analyzer of real complex systems. *Computer Physics Communications*, 232(??):22–34, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302182.

Ki:2010:LSM

[Ki10] Hyungson Ki. Level set method for two-phase incompressible flows under magnetic fields. *Computer Physics Communications*, 181(6):999–1007, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000226.

Kitajima:2011:MSR

[KI11] Akimasa Kitajima and Yukito Iba. Multicanonical sampling of rare trajectories in chaotic dynamical systems. *Computer Physics Communications*, 182(1):251–253, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002900.

Kirby:2010:CRP

[Kir10] P. Kirby. Calculation of radial prolate spheroidal wave functions of the second kind. *Computer Physics Communications*, 181(3):514–519, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003476.

Kamali:2013:IMF

[KK13] Reza Kamali and Ali Kharazmi. Investigation of multiscale fluid flow characteristics based on a hybrid atomistic-continuum method. *Computer Physics Communications*, 184(10):2316–2320, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001781.

Khoromskaia:2014:MPM

[KK14a] V. Khoromskaia and B. N. Khoromskij. Møller–Plesset (MP2) energy correction using tensor factorization of the grid-based two-electron integrals. *Computer Physics Communications*, 185(1):2–10, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002658.

Khoromskaia:2014:GBL

[KK14b] Venera Khoromskaia and Boris N. Khoromskij. Grid-based lattice summation of electrostatic potentials by assembled rank-structured tensor approximation. *Computer Physics Communications*, 185(12):3162–3174, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002938.

Kafri:2016:BPN

[KK16a] H. Q. Kafri and S. A. Khuri. Bratu's problem: a novel approach using fixed-point iterations and Green's functions. *Computer Physics Communications*, 198(??):97–104, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003446. See corrigendum [Ano20].

Kennes:2016:ERR

[KK16b] D. M. Kennes and C. Karrasch. Extending the range of real time density matrix renormalization group simulations. *Computer Physics Communications*, 200(??):37–43, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004002.

Kozynchenko:2017:AIE

[KK17] Alexander I. Kozynchenko and Sergey A. Kozynchenko. About improving efficiency of the P^3M algorithms when computing the inter-particle forces in beam dynamics. *Computer Physics Communications*, 212(??):47–54, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303113.

Kim:2019:ODF

[KKCC19] Hyun-Seok Kim, Jae-Hyun Kim, Song-Hyun Cha, and Seonho Cho. Optimal determination of force field parameters for reduced molecular dynamics model. *Computer Physics Communications*, 236(??):86–94, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303679.

Kempf:2015:PSC

[KKG+15] Andreas Kempf, Patrick Kilian, Urs Ganse, Cedric Schreiner, and Felix Spanier. PICPANTHER: a simple, concise implementation of the relativistic moment implicit particle-in-cell method. *Computer Physics Communications*, 188(??):198–207, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003828.

Kant:2015:HST

[KKK+15] P. Kant, O. M. Kind, T. Kintscher, T. Lohse, T. Martini, S. Mölbitz, P. Rieck, and P. Uwer. HatHor for single top-quark production: Updated predictions and uncertainty estimates for single top-quark production in hadronic collisions. *Computer Physics Communications*, 191(??):74–89, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000454.

Kittelmann:2017:MCP

[KKK+17] T. Kittelmann, E. Klinkby, E. B. Knudsen, P. Willendrup, X. X. Cai, and K. Kanaki. Monte Carlo particle lists: MCPL. *Computer Physics Communications*, 218(??):17–42, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301261.

Kim:2018:KSA

[KKL+18] Jaewook Kim, Sungwoo Kang, Jaechang Lim, Sang-Yeon Hwang, and Woo Youn Kim. Kohn–Sham approach for fast hybrid density functional calculations in real-space numerical grid methods. *Computer Physics Communications*, 230(??):21–26, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830122X.

Kozynchenko:2019:DCT

[KKO19] A. I. Kozynchenko, S. A. Kozynchenko, and A. D. Ovsyannikov. Development of the C++ three-dimensional reference simulation model of the wedge-shaped beam dynamics.

Computer Physics Communications, 244(??):86–96, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465519302061`.

Kim:2011:PAO

[KKP11] Ki-Hwan Kim, KyoungHo Kim, and Q-Han Park. Performance analysis and optimization of three-dimensional FDTD on GPU using roofline model. *Computer Physics Communications*, 182(6):1201–1207, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000452`.

Korol:2018:PST

[KKS18] Roman Korol, Michael Kilgour, and Dvira Segal. ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Büttiker's probes. *Computer Physics Communications*, 224(??):396–404, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465517303454`.

Kanemura:2018:HCP

[KKSY18] Shinya Kanemura, Mariko Kikuchi, Kodai Sakurai, and Kei Yagyu. H-COUP: a program for one-loop corrected Higgs boson couplings in non-minimal Higgs sectors. *Computer Physics Communications*, 233(??):134–144, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302200`.

Kleefeld:2011:NLM

[KL11] Andreas Kleefeld and Tzu-Chu Lin. The nonlinear Landweber method applied to an inverse scattering problem for sound-soft obstacles in 3D. *Computer Physics Communications*, 182(12):2550–2560, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002724`.

Kuo:2014:TLO

[KL14] Yueh-Cheng Kuo and Tsung-Lin Lee. Tracking local optimality for cost parameterized optimization problems. *Computer Physics Communications*, 185(2):572–577, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003652.

Kim:2017:NCV

[KL17] Junseok Kim and Hyun Geun Lee. A new conservative vector-valued Allen–Cahn equation and its fast numerical method. *Computer Physics Communications*, 221(??):102–108, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302497.

Kao:2011:DAB

[KLKR11] H. C. Kao, M. Lewkowicz, Y. Korniyenko, and B. Rosenstein. Dynamical approach to ballistic transport in graphene. *Computer Physics Communications*, 182(1):112–114, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002626.

Kumar:2019:FOP

[KLM+19] Ramavarmaraja Kishor Kumar, Vladimir Loncar, Paulsamy Muruganandam, Sadhan K. Adhikari, and Antun Balaz. C and Fortran OpenMP programs for rotating Bose–Einstein condensates. *Computer Physics Communications*, 240(??):74–82, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300827.

Krieg:2019:AHM

[KLO+19] Stefan Krieg, Thomas Luu, Johann Ostmeyer, Philippos Papaphilippou, and Carsten Urbach. Accelerating Hybrid Monte Carlo simulations of the Hubbard model on the hexagonal lattice. *Computer Physics Communications*, 236(??):15–25, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303564.

Kosower:2015:FFB

[KLV15] David A. Kosower and J. J. Lopez-Villarejo. Flowgen: Flowchart-based documentation for C++ codes. *Computer Physics Communications*, 196(??):497–505, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500209X.

Khanna:2010:NMG

[KM10] Gaurav Khanna and Justin McKennon. Numerical modeling of gravitational wave sources accelerated by OpenCL. *Computer Physics Communications*, 181(9):1605–1611, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001682.

Kohno:2017:FEP

[KM17] H. Kohno and J. R. Myra. A finite element procedure for radio-frequency sheath-plasma interactions based on a sheath impedance model. *Computer Physics Communications*, 220(??):129–142, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302072.

Kuchelmeister:2012:GBF

[KMA+12] Daniel Kuchelmeister, Thomas Müller, Marco Ament, Günter Wunner, and Daniel Weiskopf. GPU-based four-dimensional general-relativistic ray tracing. *Computer Physics Communications*, 183(10):2282–2290, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001798.

Kohno:2012:FEP

[KMD12] H. Kohno, J. R. Myra, and D. A. D'Ippolito. A finite element procedure for radio-frequency sheath-plasma interactions in the ion cyclotron range of frequencies. *Computer Physics Communications*, 183(10):2116–2127, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200183X.

Krasilnikov:2011:FPD

[KME+11] V. Krasilnikov, D. Marocco, B. Esposito, M. Riva, and Yu. Kaschuck. Fast pulse detection algorithms for digitized waveforms from scintillators. *Computer Physics Communications*, 182(3):735–738, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004182.

Kroonblawd:2016:GCC

[KMJS16] Matthew P. Kroonblawd, Nithin Mathew, Shan Jiang, and Thomas D. Sewell. A generalized crystal-cutting method for modeling arbitrarily oriented crystals in 3D periodic simulation cells with applications to crystal–crystal interfaces. *Computer Physics Communications*, 207(??):232–242, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301898.

Kaur:2013:HWA

[KMM13] Harpreet Kaur, R. C. Mittal, and Vinod Mishra. Haar wavelet approximate solutions for the generalized Lane–Emden equations arising in astrophysics. *Computer Physics Communications*, 184(9):2169–2177, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001598.

Kim:2019:SGS

[KMM+19] Minjung Kim, Subhasish Mandal, Eric Mikida, Kavitha Chandrasekar, Eric Bohm, Nikhil Jain, Qi Li, Raghavendra Kanakagiri, Glenn J. Martyna, Laxmikant Kale, and Sohrab Ismail-Beigi. Scalable GW software for quasiparticle properties using OpenAtom. *Computer Physics Communications*, 244(??):427–441, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S001046551930178X.

Kachelriess:2019:AIR

[KMO19] M. Kachelrieß, I. V. Moskalenko, and S. Ostapchenko. AAfrag: Interpolation routines for Monte Carlo results on secondary production in proton–proton, proton–nucleus and nucleus–nucleus interactions. *Computer Physics Communications*, 245(??):Article 106846, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302231.

Kalogiratou:2014:FOM

[KMS14] Z. Kalogiratou, Th. Monovasilis, and T. E. Simos. A fourth order modified trigonometrically fitted symplectic Runge–Kutta–Nyström method. *Computer Physics Communications*, 185(12):3151–3155, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002914.

Klimenkova:2019:VSL

[KMS19] Olga Klimenkova, Anton Yu. Menshutin, and Lev N. Shchur. Variable-step-length algorithms for a random walk: Hitting probability and computation performance. *Computer Physics Communications*, 241(??):28–32, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930102X.

Kohno:2013:NML

[KN13] Haruhiko Kohno and Jean-Christophe Nave. A new method for the level set equation using a hierarchical-gradient truncation and remapping technique. *Computer Physics Communications*, 184(6):1547–1554, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000465.

Klein:2017:SMC

[KNS+17] Spencer R. Klein, Joakim Nystrand, Janet Seger, Yuri Gorbunov, and Joey Butterworth. STARlight: a Monte Carlo simulation program for ultra-peripheral collisions of relativistic ions. *Computer Physics Communications*, 212(??):258–268, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303356.

Komura:2012:GBS

[KO12] Yukihiro Komura and Yutaka Okabe. GPU-based Swendsen–Wang multi-cluster algorithm for the simulation of two-dimensional classical spin systems. *Computer Physics Communications*, 183(6):1155–1161, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551200032X`.

Komura:2013:MGB

[KO13] Yukihiro Komura and Yutaka Okabe. Multi-GPU-based Swendsen–Wang multi-cluster algorithm for the simulation of two-dimensional q-state Potts model. *Computer Physics Communications*, 184(1):40–44, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002597`.

Kitsunezaki:2014:HOC

[KO14a] Naofumi Kitsunezaki and Atsushi Okabe. Higher-order correction to the FDTD method based on the integral form of Maxwell's equations. *Computer Physics Communications*, 185(6):1582–1588, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000666`.

Komura:2014:CPG

[KO14b] Yukihiro Komura and Yutaka Okabe. CUDA programs for the GPU computing of the Swendsen–Wang multi-cluster spin flip algorithm: 2D and 3D Ising, Potts, and XY models. *Computer Physics Communications*, 185(3):1038–1043, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003743`.

Komura:2016:ICP

[KO16] Yukihiro Komura and Yutaka Okabe. Improved CUDA programs for GPU computing of Swendsen–Wang multi-cluster spin flip algorithm: 2D and 3D Ising, Potts, and XY models. *Computer Physics Communications*, 200(??):400–401, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003689.

Kobus:2013:FDH

[Kob13] Jacek Kobus. A finite difference Hartree–Fock program for atoms and diatomic molecules. *Computer Physics Communications*, 184(3):799–811, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003311.

Kelling:2017:SCM

[KÓG17] Jeffrey Kelling, Géza Ódor, and Sibylle Gemming. Suppressing correlations in massively parallel simulations of lattice models. *Computer Physics Communications*, 220(??):205–211, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302175.

Kohno:2015:EHO

[Koh15] Haruhiko Kohno. An efficient, high-order finite element method using the nodal averaging technique for incompressible fluid flows. *Computer Physics Communications*, 195(??):68–76, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500168X.

Kutepov:2017:LSC

[KOK17] A. L. Kutepov, V. S. Oudovenko, and G. Kotliar. Linearized self-consistent quasiparticle GW method: Application to semiconductors and simple metals. *Computer Physics Communications*, 219(??):407–414, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301947.

Kolodziej:2014:CVP

[Kol14] Karol Kolodziej. carlomat, version 2 of the program for automatic computation of lowest order cross sections. *Computer Physics Communications*, 185(1):323–329, January

2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002968.

Kolodziej:2015:CAT

[Kol15] Karol Kolodziej. carlomat_3.0, an automatic tool for the electron-positron annihilation into hadrons at low energies. *Computer Physics Communications*, 196(??):563–568, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002581.

Komura:2015:GBC

[Kom15a] Yukihiro Komura. GPU-based cluster-labeling algorithm without the use of conventional iteration: Application to the Swendsen–Wang multi-cluster spin flip algorithm. *Computer Physics Communications*, 194(??):54–58, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001472.

Komura:2015:MGB

[Kom15b] Yukihiro Komura. Multi-GPU-based Swendsen–Wang multi-cluster algorithm with reduced data traffic. *Computer Physics Communications*, 195(??):84–94, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001708.

Komura:2015:OPS

[Kom15c] Yukihiro Komura. OpenACC programs of the Swendsen–Wang multi-cluster spin flip algorithm. *Computer Physics Communications*, 197(??):298–303, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003197.

Kong:2011:PDM

[Kon11] Ling Ti Kong. Phonon dispersion measured directly from molecular dynamics simulations. *Computer Physics Communications*, 182(10):2201–2207, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465511001500. See corrigendum [Sco13].

Kachelriess:2012:EMC

[KOT12] M. Kachelrieß, S. Ostapchenko, and R. Tomàs. ELMAG: a Monte Carlo simulation of electromagnetic cascades on the extragalactic background light and in magnetic fields. *Computer Physics Communications*, 183(4):1036–1043, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004255.

Kamleh:2012:PFH

[KP12a] Waseem Kamleh and Mike Peardon. Polynomial filtered HMC — an algorithm for lattice QCD with dynamical quarks. *Computer Physics Communications*, 183(9):1993–2000, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001695.

Kim:2012:OCC

[KP12b] Ki-Hwan Kim and Q-Han Park. Overlapping computation and communication of three-dimensional FDTD on a GPU cluster. *Computer Physics Communications*, 183(11):2364–2369, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002044.

Kumar:2014:CNS

[KP14] Manoj Kumar and Sapna Pandit. A composite numerical scheme for the numerical simulation of coupled Burgers' equation. *Computer Physics Communications*, 185(3):809–817, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004050.

Khorshidi:2016:AMA

[KP16] Alireza Khorshidi and Andrew A. Peterson. Amp: a modular approach to machine learning in atomistic simulations.

Computer Physics Communications, 207(??):310–324, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301266.

Khan:2013:MTO

[KPA13] I. M. Khan, M. Poursina, and K. S. Anderson. Model transitions and optimization problem in multi-flexible-body systems: Application to modeling molecular systems. *Computer Physics Communications*, 184(7):1717–1728, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000829.

King:2019:GAP

[KPA+19] J. R. King, I. V. Pogorelov, K. M. Amyx, M. Borland, and R. Soliday. GPU acceleration and performance of the particle-beam-dynamics code Elegant. *Computer Physics Communications*, 235(??):346–355, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830345X.

Kirsanskas:2017:QOS

[KPK+17] Gediminas Kirsanskas, Jonas Nyvold Pedersen, Olov Karlström, Martin Leijnse, and Andreas Wacker. QmeQ 1.0: an open-source Python package for calculations of transport through quantum dot devices. *Computer Physics Communications*, 221(??):317–342, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302515.

Kramer:2018:QJJ

[KPOR18] Sebastian Krämer, David Plankensteiner, Laurin Ostermann, and Helmut Ritsch. QuantumOptics.jl: A Julia framework for simulating open quantum systems. *Computer Physics Communications*, 227(??):109–116, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300328.

Kumar:2013:PGS

[KPPC13] D. Kumar, A. K. Patra, E. B. Pitman, and H. Chi. Parallel Godunov smoothed particle hydrodynamics (SPH) with improved treatment of boundary conditions and an application to granular flows. *Computer Physics Communications*, 184(10):2277–2286, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001744.

Kozlov:2015:CMP

[KPST15] M. G. Kozlov, S. G. Porsev, M. S. Safronova, and I. I. Tupitsyn. CI–MBPT: a package of programs for relativistic atomic calculations based on a method combining configuration interaction and many-body perturbation theory. *Computer Physics Communications*, 195(??):199–213, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500185X.

Kniehl:2016:MCL

[KPV16] Bernd A. Kniehl, Andrey F. Pikelner, and Oleg L. Veretin. mr: a C++ library for the matching and running of the Standard Model parameters. *Computer Physics Communications*, 206(??):84–96, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301060.

Kuipers:2013:IMH

[KPVvdH13] J. Kuipers, A. Plaat, J. A. M. Vermaseren, and H. J. van den Herik. Improving multivariate Horner schemes with Monte Carlo tree search. *Computer Physics Communications*, 184(11):2391–2395, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001689.

Kwon:2017:ITT

[KQYH17] Jae-Min Kwon, Lei Qi, S. Yi, and T. S. Hahm. ITG–TEM turbulence simulation with bounce-averaged kinetic electrons in tokamak geometry. *Computer Physics Communications*, 215(??):81–90, June 2017. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300619.

Kumar:2014:NAM

[KR14] Sunil Kumar and Mohammad Mehdi Rashidi. New analytical method for gas dynamics equation arising in shock fronts. *Computer Physics Communications*, 185(7):1947–1954, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001052.

Kylanpaa:2016:EES

[KR16] Ilkka Kylänpää and Esa Räsänen. Extended Ewald summation technique. *Computer Physics Communications*, 206(??):64–68, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301217.

Krawczyk:2010:ADE

[Kra10] Małgorzata J. Krawczyk. Application of the differential equations method for identifying communities in sparse networks. *Computer Physics Communications*, 181(10):1702–1706, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001931.

Kramida:2011:PLL

[Kra11] A. E. Kramida. The program LOPT for least-squares optimization of energy levels. *Computer Physics Communications*, 182(2):419–434, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003784.

Kramida:2017:CIC

[Kra17] Alexander Kramida. Configuration interactions of class 11: an error in Cowan's atomic structure theory. *Computer Physics Communications*, 215(??):47–48, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300450. See correction [Kra18a].

Kramida:2018:CCI

[Kra18a] Alexander Kramida. Corrigendum to "Configuration interactions of class 11: an error in Cowan's atomic structure theory" [Comput. Phys. Commun. 215 (2017) 47–48]. *Computer Physics Communications*, 232(??):266–267, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830211X. See [Kra17].

Krasnopolsky:2018:AAI

[Kra18b] Boris I. Krasnopolsky. An approach for accelerating incompressible turbulent flow simulations based on simultaneous modelling of multiple ensembles. *Computer Physics Communications*, 229(??):8–19, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830095X.

Kourtzanidis:2015:AFM

[KRB15] Konstantinos Kourtzanidis, François Rogier, and Jean-Pierre Boeuf. ADI–FDTD modeling of microwave plasma discharges in air towards fully three-dimensional simulations. *Computer Physics Communications*, 195(??):49–60, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001502.

Kurchin:2019:BTA

[KRB19] Rachel Kurchin, Giuseppe Romano, and Tonio Buonassisi. Bayesim: a tool for adaptive grid model fitting with Bayesian inference. *Computer Physics Communications*, 239(??):161–165, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300414.

Krivec:2012:NRK

[Kri12] R. Krivec. Numerical regularization of Klauder effect in QLM. *Computer Physics Communications*, 183(12):2601–2607, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002512.

Kasilov:2016:GIC

[KRK16] S. V. Kasilov, A. M. Runov, and W. Kernbichler. Geometric integrator for charged particle orbits in axisymmetric fusion devices. *Computer Physics Communications*, 207(??):282–286, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302077.

Kapil:2019:PUF

[KRM+19] Venkat Kapil, Mariana Rossi, Ondrej Marsalek, Riccardo Petraglia, Yair Litman, Thomas Spura, Bingqing Cheng, Alice Cuzzocrea, Robert H. Meißner, David M. Wilkins, Benjamin A. Helfrecht, Przemysław Juda, Sébastien P. Bienvenue, Wei Fang, Jan Kessler, Igor Poltavsky, Steven Vandenbrande, Jelle Wieme, Clemence Corminboeuf, Thomas D. Kühne, David E. Manolopoulos, Thomas E. Markland, Jeremy O. Richardson, Alexandre Tkatchenko, Gareth A. Tribello, Veronique Van Speybroeck, and Michele Ceriotti. i-PI 2.0: a universal force engine for advanced molecular simulations. *Computer Physics Communications*, 236(??):214–223, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303436.

Krogel:2016:NMW

[Kro16] Jaron T. Krogel. Nexus: a modular workflow management system for quantum simulation codes. *Computer Physics Communications*, 198(??):154–168, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002982.

Kroger:2019:EHA

[Krö19] Martin Kröger. Efficient hybrid algorithm for the dynamic creation of wormlike chains in solutions, brushes, melts and glasses. *Computer Physics Communications*, 241(??):178–179, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300876.

Kersevan:2013:MCE

[KRW13] Borut Paul Kersevan and Elzbieta Richter-Was. The Monte Carlo event generator AcerMC versions 2.0 to 3.8 with interfaces to PYTHIA 6.4, HERWIG 6.5 and ARIADNE 4.1. *Computer Physics Communications*, 184(3):919–985, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200375X.

Kondayya:2012:FHF

[KS12] Gundra Kondayya and Alok Shukla. A Fortran 90 Hartree–Fock program for one-dimensional periodic π-conjugated systems using Pariser–Parr–Pople model. *Computer Physics Communications*, 183(3):677–689, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003687.

Kroonblawd:2015:SNU

[KS15] Matthew P. Kroonblawd and Thomas D. Sewell. Strategies for non-uniform sampling of molecular dynamics phase space trajectories of relaxation phenomena. *Computer Physics Communications*, 196(??):143–148, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002064.

Khorasanizade:2016:TDS

[KS16a] Sh. Khorasanizade and J. M. M. Sousa. A two-dimensional Segmented Boundary Algorithm for complex moving solid boundaries in smoothed particle hydrodynamics. *Computer Physics Communications*, 200(??):66–75, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004075.

Kiviniemi:2016:ESS

[KS16b] T. P. Kiviniemi and U. Sauerwein. The effects of spatial sampling on random noise for gyrokinetic PIC simulations in real space. *Computer Physics Communications*, 203(??):162–167, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300583.

Kashyap:2019:PDS

[KS19] Rahul Kashyap and Surajit Sen. PULSEDYN — a dynamical simulation tool for studying strongly nonlinear chains. *Computer Physics Communications*, 239(??):134–149, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930044X`.

Kesselheim:2011:AID

[KSH11] Stefan Kesselheim, Marcello Sega, and Christian Holm. Applying ICC* to DNA translocation: Effect of dielectric boundaries. *Computer Physics Communications*, 182 (1):33–35, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551000305X`.

Koenka:2014:IOS

[KSH14] Israel Joel Koenka, Jorge Sáiz, and Peter C. Hauser. Instrumentino: an open-source modular Python framework for controlling Arduino based experimental instruments. *Computer Physics Communications*, 185(10):2724–2729, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002112`.

Kirchner:2011:WCC

[KSL$^+$11] Barbara Kirchner, Christian Spickermann, Sebastian B. C. Lehmann, Eva Perlt, Johanna Langner, Michael von Domaros, Patricia Reuther, Frank Uhlig, Miriam Kohagen, and Marc Brüssel. What can clusters tell us about the bulk?: Peacemaker: Extended quantum cluster equilibrium calculations. *Computer Physics Communications*, 182(7):1428–1446, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000890`.

Kilian:2018:APC

[KSS18] Patrick Kilian, Cedric Schreiner, and Felix Spanier. Afterlive: A performant code for Vlasov-hybrid simulations. *Computer Physics Communications*, 230(??):121–134, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301309`.

Karasiev:2014:FTO

[KST14a] Valentin V. Karasiev, Travis Sjostrom, and S. B. Trickey. Finite-temperature orbital-free DFT molecular dynamics: Coupling Profess and Quantum Espresso. *Computer Physics Communications*, 185(12):3240–3249, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551400304X`.

Koyama:2014:IDL

[KST+14b] Yukinobu Koyama, Atsuki Shinbori, Yoshimasa Tanaka, Tomoaki Hori, Masahito Nosé, and Satoshi Oimatsu. An Interactive Data Language software package to calculate ionospheric conductivity by using numerical models. *Computer Physics Communications*, 185(12):3398–3405, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002781`.

Kim:2015:FCC

[KSTR15] Jong Soo Kim, Daniel Schmeier, Jamie Tattersall, and Krzysztof Rolbiecki. A framework to create customised LHC analyses within CheckMATE. *Computer Physics Communications*, 196(??):535–562, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002477`.

Kuo:2012:RQP

[KSW12] Yueh-Cheng Kuo, Shih-Feng Shieh, and Weichung Wang. Rotational quotient procedure: a tracking control continuation method for PDEs on radially symmetric domains. *Computer Physics Communications*, 183(4):998–1001, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000112`.

Kroninger:2015:IMC

[KSW15] Kevin Kröninger, Steffen Schumann, and Benjamin Willenberg. $(MC)^3$ — a multi-channel Markov chain Monte Carlo algorithm for phase-space sampling. *Computer Physics Communications*, 186(??):1–10, January 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003051.

Kwon:2017:PMT

[KSY17] Deuk-Chul Kwon, Sung-Sik Shin, and Dong-Hun Yu. A parallelization method for time periodic steady state in simulation of radio frequency sheath dynamics. *Computer Physics Communications*, 219(??):297–302, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301881.

Kwon:2013:FBC

[KSYY13] Deuk-Chul Kwon, Mi-Young Song, Jung-Sik Yoon, and Nam-Sik Yoon. A feed-back control approach for global simulation of high density plasma discharges. *Computer Physics Communications*, 184(10):2251–2256, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001628.

Koval:2010:USB

[KT10] Peter Koval and J. D. Talman. Update of spherical Bessel transform: FFTW and OpenMP. *Computer Physics Communications*, 181(12):2212–2213, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003188.

Karasiev:2012:ICO

[KT12] V. V. Karasiev and S. B. Trickey. Issues and challenges in orbital-free density functional calculations. *Computer Physics Communications*, 183(12):2519–2527, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002287.

Kucherenko:2012:EGS

[KTA12] S. Kucherenko, S. Tarantola, and P. Annoni. Estimation of global sensitivity indices for models with dependent variables. *Computer Physics Communications*, 183(4):937–946, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004085.

Karsai:2017:ILO

[KTB17] Ferenc Karsai, Fabien Tran, and Peter Blaha. On the importance of local orbitals using second energy derivatives for d and f electrons. *Computer Physics Communications*, 220(??):230–238, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302151.

Knight:2012:CGT

[KTE+12] P. J. Knight, A. Thyagaraja, T. D. Edwards, J. Hein, M. Romanelli, and K. G. McClements. CENTORI: a global toroidal electromagnetic two-fluid plasma turbulence code. *Computer Physics Communications*, 183(11):2346–2363, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002032.

Kaneko:2010:GMS

[KU10] Toshiaki Kaneko and Takahiro Ueda. A geometric method of sector decomposition. *Computer Physics Communications*, 181(8):1352–1361, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001116.

Kuipers:2015:COF

[KUV15] J. Kuipers, T. Ueda, and J. A. M. Vermaseren. Code optimization in FORM. *Computer Physics Communications*, 189(??):1–19, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002756.

Kuipers:2013:FV

[KUVV13] J. Kuipers, T. Ueda, J. A. M. Vermaseren, and J. Vollinga. FORM version 4.0. *Computer Physics Communications*, 184(5):1453–1467, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000052.

Koleva:2010:TGQ

[KV10a] Miglena N. Koleva and Lubin G. Vulkov. Two-grid quasilinearization approach to ODEs with applications to model problems in physics and mechanics. *Computer Physics Communications*, 181(3):663–670, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003907.

Kosmas:2010:PFD

[KV10b] O. T. Kosmas and D. S. Vlachos. Phase-fitted discrete Lagrangian integrators. *Computer Physics Communications*, 181(3):562–568, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003531.

Kornyik:2019:MCW

[KV19] M. Kornyik and A. Vukics. The Monte Carlo wave-function method: a robust adaptive algorithm and a study in convergence. *Computer Physics Communications*, 238(??):88–101, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304314.

Kleiss:2011:CCL

[KvdO11] R. Kleiss and G. van den Oord. CAMORRA: a C++ library for recursive computation of particle scattering amplitudes. *Computer Physics Communications*, 182(2):435–447, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003796.

Kallala:2019:GMP

[KVV19] Haithem Kallala, Jean-Luc Vay, and Henri Vincenti. A generalized massively parallel ultra-high order FFT-based Maxwell solver. *Computer Physics Communications*, 244 (??):25–34, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302206.

Korzec:2011:PWA

[KVW11] Tomasz Korzec, Ingmar Vierhaus, and Ulli Wolff. Performance of a worm algorithm in ϕ^4 theory at finite quartic coupling. *Computer Physics Communications*, 182(7):1477–1480, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100110X.

Kageyama:2014:AEV

[KY14] Akira Kageyama and Tomoki Yamada. An approach to exascale visualization: Interactive viewing of in-situ visualization. *Computer Physics Communications*, 185(1):79–85, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002804.

Kim:2015:CDV

[KYKN15a] YoungJin Kim, Min-Gu Yoo, S. H. Kim, and Yong-Su Na. Corrigendum to "Development of vector following mesh generator for analysis of two dimensional tokamak plasma transport" [comput. phys. comm. **186** (2015) 31–38]. *Computer Physics Communications*, 189(??):220, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004160. See [KYKN15b].

Kim:2015:DVF

[KYKN15b] YoungJin Kim, Min-Gu Yoo, S. H. Kim, and Yong-Su Na. Development of vector following mesh generator for analysis of two-dimensional tokamak plasma transport. *Computer Physics Communications*, 186(??):31–38, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003142. See corrigendum [KYKN15a].

Kawamura:2017:QLM

[KYM+17] Mitsuaki Kawamura, Kazuyoshi Yoshimi, Takahiro Misawa, Youhei Yamaji, Synge Todo, and Naoki Kawashima. Quantum lattice model solver $H\Phi$. *Computer Physics Communications*, 217(??):180–192, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465517301200.

Kumar:2015:FPT

[KYSV+15] R. Kishor Kumar, Luis E. Young-S., Dusan Vudragović, Antun Balaz, Paulsamy Muruganandam, and S. K. Adhikari. Fortran and C programs for the time-dependent dipolar Gross–Pitaevskii equation in an anisotropic trap. *Computer Physics Communications*, 195(??):117–128, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001344.

Keren-Zur:2011:HIE

[KZ11] Boaz Keren-Zur. HidSecSOFTSUSY: Incorporating effects from hidden sectors in the numerical computation of the MSSM spectrum. *Computer Physics Communications*, 182(2):477–484, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003863.

Kristensen:2014:BUQ

[KZ14] Jesper Kristensen and Nicholas J. Zabaras. Bayesian uncertainty quantification in the evaluation of alloy properties with the cluster expansion method. *Computer Physics Communications*, 185(11):2885–2892, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002562.

Kong:2010:SES

[KZC+10] Linghua Kong, Jingjing Zhang, Ying Cao, Yali Duan, and Hong Huang. Semi-explicit symplectic partitioned Runge–Kutta Fourier pseudo-spectral scheme for Klein–Gordon–Schrödinger equations. *Computer Physics Communications*, 181(8):1369–1377, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000113X.

Lapelosa:2013:TPT

[LA13] Mauro Lapelosa and Cameron F. Abrams. Transition-path theory calculations on non-uniform meshes in two and three dimensions using finite elements. *Computer Physics Communications*, 184(10):2310–2315, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300177X.

Lazic:2010:JJN

[LAA+10] Predrag Lazić, Nicolae Atodiresei, Mojtaba Alaei, Vasile Caciuc, Stefan Blügel, and Radovan Brako. JuNoLo — Jülich nonlocal code for parallel post-processing evaluation of vdW–DF correlation energy. *Computer Physics Communications*, 181(2):371–379, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003063.

Lozano:2017:ECA

[LAG+17] Lorena Lozano, Ma Jesús Algar, Eliseo García, Iván González, and Felipe Cátedra. Efficient combination of acceleration techniques applied to high frequency methods for solving radiation and scattering problems. *Computer Physics Communications*, 221(??):28–41, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302333.

Lanzafame:2013:IIS

[Lan13] G. Lanzafame. Implicit integrations for SPH in semi-Lagrangian approach: Application to the accretion disc modeling in a microquasar. *Computer Physics Communications*, 184(3):671–688, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003773.

Locans:2017:RTC

[LAS+17] Uldis Locans, Andreas Adelmann, Andreas Suter, Jannis Fischer, Werner Lustermann, Günther Dissertori, and Qiulin Wang. Real-time computation of parameter fitting and image reconstruction using graphical processing units. *Computer Physics Communications*, 215(??):71–80, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300498`.

Law:2019:ICD

[Law19] Everest Law. Identifying clusters on a discrete periodic lattice via machine learning. *Computer Physics Communications*, 243(??):106–109, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301535`.

Lazic:2015:CCT

[Laz15] Predrag Lazić. CellMatch: Combining two unit cells into a common supercell with minimal strain. *Computer Physics Communications*, 197(??):324–334, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003379`.

Liverts:2010:TEA

[LB10a] Evgeny Z. Liverts and Nir Barnea. The two-electron atomic systems. *S*-states. *Computer Physics Communications*, 181(1):206–212, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003026`.

Lorin:2010:MST

[LB10b] Emmanuel Lorin and A. D. Bandrauk. Multiresolution scheme for time-dependent Schrödinger equation. *Computer Physics Communications*, 181(3):626–638, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003877`.

Liverts:2011:SHL

[LB11] Evgeny Z. Liverts and Nir Barnea. *S*-states of helium-like ions. *Computer Physics Communications*, 182(9):1790–1795, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004844`.

Liverts:2012:SHL

[LB12] Evgeny Z. Liverts and Nir Barnea. *S*-states of helium-like ions. *Computer Physics Communications*, 183(3):844–845, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003638.

Liverts:2013:TBS

[LB13] Evgeny Z. Liverts and Nir Barnea. Three-body systems with Coulomb interaction. bound and quasi-bound *S*-states. *Computer Physics Communications*, 184(11):2596–2603, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002075.

Loncar:2016:CPS

[LBB+16] Vladimir Loncar, Antun Balaz, Aleksandar Bogojević, Srdjan Skrbić, Paulsamy Muruganandam, and Sadhan K. Adhikari. CUDA programs for solving the time-dependent dipolar Gross–Pitaevskii equation in an anisotropic trap. *Computer Physics Communications*, 200(??):406–410, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004361.

Larentzos:2014:PII

[LBM+14] James P. Larentzos, John K. Brennan, Joshua D. Moore, Martin Lísal, and William D. Mattson. Parallel implementation of isothermal and isoenergetic Dissipative Particle Dynamics using Shardlow-like splitting algorithms. *Computer Physics Communications*, 185(7):1987–1998, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400109X.

Lulli:2015:HOS

[LBP15] M. Lulli, M. Bernaschi, and G. Parisi. Highly optimized simulations on single- and multi-GPU systems of the 3D Ising spin glass model. *Computer Physics Communications*, 196(??):290–303, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002647.

Longshaw:2018:MAM

[LBR+18] S. M. Longshaw, M. K. Borg, S. B. Ramisetti, J. Zhang, D. A. Lockerby, D. R. Emerson, and J. M. Reese. mdFoam+: Advanced molecular dynamics in OpenFOAM. *Computer Physics Communications*, 224(??):1–21, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465517303363`.

Lee:2015:EFA

[LC15] Jungpyo Lee and Antoine Cerfon. ECOM: a fast and accurate solver for toroidal axisymmetric MHD equilibria. *Computer Physics Communications*, 190(??):72–88, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000351`.

Le:2013:GBF

[LCC13] Hai P. Le, Jean-Luc Cambier, and Lord K. Cole. GPU-based flow simulation with detailed chemical kinetics. *Computer Physics Communications*, 184(3):596–606, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003463`.

Li:2011:SCM

[LCCC11] Z.-C. Li, S.-Y. Chen, C.-S. Chien, and H.-S. Chen. A spectral collocation method for a rotating Bose–Einstein condensation in optical lattices. *Computer Physics Communications*, 182(6):1215–1234, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000610`.

Lee:2013:CUT

[LCE+13] J. S. Lee, M. Carena, J. Ellis, A. Pilaftsis, and C. E. M. Wagner. CPsuperH2.3: an updated tool for phenomenology in the MSSM with explicit CP violation. *Computer Physics Communications*, 184(4):1220–1233, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003827`.

Li:2011:QHS

[LCH11] Yiming Li, Hui-Wen Cheng, and Ming-Hung Han. Quantum hydrodynamic simulation of discrete-dopant fluctuated physical quantities in nanoscale FinFET. *Computer Physics Communications*, 182(1):96–98, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000250X.

Lu:2010:AAF

[LCHM10] Benzhuo Lu, Xiaolin Cheng, Jingfang Huang, and J. Andrew McCammon. AFMPB: An adaptive fast multipole Poisson–Boltzmann solver for calculating electrostatics in biomolecular systems. *Computer Physics Communications*, 181(6):1150–1160, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000548.

Lu:2013:AAF

[LCHM13] Benzhuo Lu, Xiaolin Cheng, Jingfang Huang, and J. Andrew McCammon. AFMPB: an adaptive fast multipole Poisson–Boltzmann solver for calculating electrostatics in biomolecular systems. *Computer Physics Communications*, 184(11):2618–2619, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001720.

Lamotte:2010:CVC

[LCJ10] Jean-Luc Lamotte, Jean-Marie Chesneaux, and Fabienne Jézéquel. CADNA_C: a version of CADNA for use with C or C++ programs. *Computer Physics Communications*, 181(11):1925–1926, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002353.

Li:2014:SSB

[LCKM14] Wu Li, Jesús Carrete, Nebil A. Katcho, and Natalio Mingo. ShengBTE: a solver of the Boltzmann transport equation for phonons. *Computer Physics Communications*, 185(6):1747–1758, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000484.

Lin:2011:HBS

[LCL+11] Huey-Wen Lin, Saul D. Cohen, Liuming Liu, Nilmani Mathur, Kostas Orginos, and Andre Walker-Loud. Heavy-baryon spectroscopy from lattice QCD. *Computer Physics Communications*, 182(1):24–26, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002316.

Li:2018:MDL

[LCQF18] Junpu Li, Wen Chen, Qinghua Qin, and Zhuojia Fu. A modified dual-level fast multipole boundary element method for large-scale three-dimensional potential problems. *Computer Physics Communications*, 233(??):51–61, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302467.

Lundberg:2010:LDC

[LCRL10] J. Lundberg, J. Conrad, W. Rolke, and A. Lopez. Limits, discovery and cut optimization for a Poisson process with uncertainty in background and signal efficiency: TRolke 2.0. *Computer Physics Communications*, 181(3):683–686, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900349X.

Lee:2011:LEE

[LCY+11] C. H. Lee, S. C. Chen, C. K. Yang, W. S. Su, and M. F. Lin. Low-energy electronic structures of nanotube-nanoribbon hybrid systems. *Computer Physics Communications*, 182(1):68–70, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002614.

Lakestani:2010:CFD

[LD10a] Mehrdad Lakestani and Mehdi Dehghan. Collocation and finite difference-collocation methods for the solution of nonlinear Klein–Gordon equation. *Computer Physics Com-*

munications, 181(8):1392–1401, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001177.

Lakestani:2010:NSR

[LD10b] Mehrdad Lakestani and Mehdi Dehghan. Numerical solution of Riccati equation using the cubic B-spline scaling functions and Chebyshev cardinal functions. *Computer Physics Communications*, 181(5):957–966, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000378.

Langr:2019:EAR

[LDD+19] Daniel Langr, Tomás Dytrych, Jerry P. Draayer, Kristina D. Launey, and Pavel Tvrdík. Efficient algorithm for representations of U(3) in U(N). *Computer Physics Communications*, 244(??):442–447, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301766.

Loureiro:2016:VFH

[LDF+16] N. F. Loureiro, W. Dorland, L. Fazendeiro, A. Kanekar, A. Mallet, M. S. Vilelas, and A. Zocco. Viriato: a Fourier–Hermite spectral code for strongly magnetized fluid–kinetic plasma dynamics. *Computer Physics Communications*, 206(??):45–63, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301205.

Leddy:2017:NFF

[LDR+17] J. Leddy, B. Dudson, M. Romanelli, B. Shanahan, and N. Walkden. A novel flexible field-aligned coordinate system for tokamak edge plasma simulation. *Computer Physics Communications*, 212(??):59–68, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303150.

Lerner:2013:SDO

[LDW13] Edan Lerner, Gustavo Düring, and Matthieu Wyart. Simulations of driven overdamped frictionless hard spheres. *Computer Physics Communications*, 184(3):628–637, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003633`.

Lee:2018:TMA

[Lee18] Julian Lee. Transfer matrix algorithm for computing the exact partition function of a square lattice polymer. *Computer Physics Communications*, 228(??):11–21, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300948`.

Leon:2012:EMS

[Leó12] Alejandro León. An efficient model for studying the dynamics of frustrated systems. *Computer Physics Communications*, 183(10):2089–2097, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001804`.

Lesur:2016:MSI

[Les16] Maxime Lesur. Method- and scheme-independent entropy production in turbulent kinetic simulations. *Computer Physics Communications*, 200(??):182–189, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515004385`.

Levy:2019:DCD

[Lev19] Edmond Levy. Decay chain differential equations: Solutions through matrix analysis. *Computer Physics Communications*, 234(??):188–194, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302613`.

Liu:2012:FES

[LF12] Victor Liu and Shanhui Fan. S^4: a free electromagnetic solver for layered periodic structures. *Computer Physics*

Communications, 183(10):2233–2244, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001658`.

Li:2014:KFB

[LFG14] Bo Li, Keisuke Fujii, and Yuanning Gao. Kalman-filter-based track fitting in non-uniform magnetic field with segment-wise helical track model. *Computer Physics Communications*, 185(3):754–761, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003846`.

Lambert:2018:ICF

[LFKD18] H. Lambert, Adam Fekete, J. R. Kermode, and A. De Vita. Imeall: a computational framework for the calculation of the atomistic properties of grain boundaries. *Computer Physics Communications*, 232(??):256–263, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518301450`.

LeGrand:2013:SSC

[LGW13] Scott Le Grand, Andreas W. Götz, and Ross C. Walker. SPFP: Speed without compromise — a mixed precision model for GPU accelerated molecular dynamics simulations. *Computer Physics Communications*, 184(2):374–380, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003098`.

Lin:2011:PEH

[LH11] C. Y. Lin and Y. K. Ho. The photoionization of excited hydrogen atom in plasmas. *Computer Physics Communications*, 182(1):125–129, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001906`.

Liu:2018:BBA

[LH18] Cheng Liu and Changhong Hu. Block-based adaptive mesh refinement for fluid-structure interactions in incompressible flows. *Computer Physics Communications*, 232(??):104–123, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301784.

Luk:2019:CFM

[LHB+19] O. O. Luk, O. Hoenen, A. Bottino, B. D. Scott, and D. P. Coster. ComPat framework for multiscale simulations applied to fusion plasmas. *Computer Physics Communications*, 239(??):126–133, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300074.

Lambert:2012:TRT

[LHC+12] Dean Lambert, Alasdair C. Hamilton, George Constable, Harsh Snehanshu, Sharvil Talati, and Johannes Courtial. TIM, a ray-tracing program for METATOY research and its dissemination. *Computer Physics Communications*, 183(3):711–732, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003730.

Li:2013:SDE

[LHC+13] Liang Li, Ting-Zhu Huang, Guang-Hui Cheng, Yan-Fei Jing, Zhi-Gang Ren, and Hou-Biao Li. Solution to 3-D electromagnetic problems discretized by a hybrid FEM/MOM method. *Computer Physics Communications*, 184(1):73–78, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002834.

Lopez:2019:VAV

[LHG+19] Joaquín López, Julio Hernández, Pablo Gómez, Claudio Zanzi, and Rosendo Zamora. VOFTools 3.2: Added VOF functionality to initialize the liquid volume fraction in general convex cells. *Computer Physics Communications*, 245(??):Article 106859, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930236X.

Lopez:2018:VIS

[LHGF18] J. López, J. Hernández, P. Gómez, and F. Faura. VOFTools — a software package of calculation tools for volume of fluid methods using general convex grids. *Computer Physics Communications*, 223(??):45–54, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303430.

Lin:2012:PHN

[LHH+12a] K.-M. Lin, M.-H. Hu, C.-T. Hung, J.-S. Wu, F.-N. Hwang, Y.-S. Chen, and G. Cheng. A parallel hybrid numerical algorithm for simulating gas flow and gas discharge of an atmospheric-pressure plasma jet. *Computer Physics Communications*, 183(12):2550–2560, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002329.

Lin:2012:DPS

[LHH+12b] K.-M. Lin, C.-T. Hung, F.-N. Hwang, M. R. Smith, Y.-W. Yang, and J.-S. Wu. Development of a parallel semi-implicit two-dimensional plasma fluid modeling code using finite-volume method. *Computer Physics Communications*, 183(6):1225–1236, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000501.

Li:2015:ECA

[LHJ+15] Haiyan Li, Yunbao Huang, Shaoen Jiang, Longfei Jing, and Yongkun Ding. An efficient computational approach for evaluating radiation flux for laser driven inertial confinement fusion targets. *Computer Physics Communications*, 193(??):49–54, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001198.

Li:2010:AIC

[LHJZ10] Liang Li, Ting-Zhu Huang, Yan-Fei Jing, and Yong Zhang. Application of the incomplete Cholesky factorization preconditioned Krylov subspace method to the vector finite element method for 3-D electromagnetic scattering problems. *Computer Physics Communications*, 181(2):271–276, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003099.

Lorca:2011:GJT

[LHL11] Alejandro Lorca, Eduardo Huedo, and Ignacio M. Llorente. The Grid[Way] Job Template Manager, a tool for parameter sweeping. *Computer Physics Communications*, 182(4): 1047–1060, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005345.

Li:2016:AOT

[LHL16] Qing-Xiao Li, Rong-Qiang He, and Zhong-Yi Lu. Accelerating optimization by tracing valley. *Computer Physics Communications*, 203(??):168–177, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300601.

Lin:2014:SEB

[LHSL14] Ken-Ming Lin, Yu-Hui Huang, W. S. Su, and T. C. Leung. Strain effects on the band gap and work function of zigzag single-walled carbon nanotubes and graphene: a comparative study. *Computer Physics Communications*, 185(5):1422–1428, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000411.

Liu:2016:PAA

[LHWL16] Zhong-Li Liu, Qian-Ku Hu, Hai-Yan Wang, and Xiao-Feng Li. Phasego 3.0: Automatic analysis of synthesis and decomposition conditions for compounds. *Computer Physics Communications*, 209(??):197–198, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302296.

Liu:2011:EPI

[LHZ11] Yali Liu, Changjun Hu, and Chongchong Zhao. Efficient parallel implementation of Ewald summation in molecular dynamics simulations on multi-core platforms. *Computer Physics Communications*, 182(5):1111–1119, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000270`.

Lin:2013:PCS

[Lin13] Bin Lin. Parametric cubic spline method for the solution of the nonlinear Schrödinger equation. *Computer Physics Communications*, 184(1):60–65, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002652`.

Litsarev:2013:DCC

[Lit13] Mikhail S. Litsarev. The DEPOSIT computer code: Calculations of electron-loss cross-sections for complex ions colliding with neutral atoms. *Computer Physics Communications*, 184(2):432–439, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003153`.

Liu:2011:GMT

[Liu11] Jun Liu. A general method for testing validity of one-particle spectral functions. *Computer Physics Communications*, 182(8):1585–1588, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001214`.

Liu:2013:LSB

[Liu13] Jun Liu. Least square based method for obtaining one-particle spectral functions from temperature Green functions. *Computer Physics Communications*, 184(2):367–373, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003050`.

Liu:2014:MMA

[Liu14] Zhong-Li Liu. Muse: Multi-algorithm collaborative crystal structure prediction. *Computer Physics Communications*, 185(7):1893–1900, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000976.

Liu:2015:PCF

[Liu15a] Zhong-Li Liu. Phasego 2.0: Counting full anharmonic effects from high-temperature phonon density of states. *Computer Physics Communications*, 197(??):341–342, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003239.

Liu:2015:PTA

[Liu15b] Zhong-Li Liu. Phasego: a toolkit for automatic calculation and plot of phase diagram. *Computer Physics Communications*, 191(??):150–158, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000430.

Lv:2016:OSM

[LJB+16] Q. Z. Lv, D. J. Jennings, J. Betke, Q. Su, and R. Grobe. Optimized spatial matrix representations of quantum Hamiltonians. *Computer Physics Communications*, 198(??):31–40, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003331.

Liu:2019:ICF

[LJD+19] Jian-Xiao Liu, Lu Ju, Peng Du, Yu-Jie Liu, and Hong-Wei Yang. An improved cascaded SO-FDTD method for high temperature magnetized plasma. *Computer Physics Communications*, 235(??):153–158, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303254.

Lee:2011:GWB

[LJE11] W. W. Lee, T. G. Jenkins, and S. Ethier. A generalized weight-based particle-in-cell simulation scheme. *Computer Physics Communications*, 182(3):564–569, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000408X.

Lee:2011:TDS

[LJSW11] Y.-M. Lee, T.-F. Jiang, Z.-Y. Su, and J.-S. Wu. Three-dimensional simulation of the femto-second pulsed laser interacting with a nitrogen molecule. *Computer Physics Communications*, 182(1):140–142, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001943.

Lin:2011:LRR

[LJWK11] Zhiwei Lin, Shaoen Jiang, Shunchao Wu, and Longyu Kuang. A local rezoning and remapping method for unstructured mesh. *Computer Physics Communications*, 182(6):1361–1376, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000762.

Lin:2018:MRR

[LJZ+18] Zhiwei Lin, Shaoen Jiang, Lu Zhang, Longyu Kuang, and Hang Li. Maxis — a rezoning and remapping code in two dimensional cylindrical geometry. *Computer Physics Communications*, 227(??):148–149, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300341.

Lee:2012:EAN

[LK12] Hyun Geun Lee and Junseok Kim. An efficient and accurate numerical algorithm for the vector-valued Allen–Cahn equations. *Computer Physics Communications*, 183(10):2107–2115, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001828.

Liu:2015:LIV

[LK15] Liang-Chun Liu and Jer-Lai Kuo. A LAMMPS implementation of volume-temperature replica exchange molecular dynamics. *Computer Physics Communications*, 189(??):119–127, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004044.

Lehe:2016:SQC

[LKA+16] Rémi Lehe, Manuel Kirchen, Igor A. Andriyash, Brendan B. Godfrey, and Jean-Luc Vay. A spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm. *Computer Physics Communications*, 203(??):66–82, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300224.

Lee:2011:PAC

[LKL11] Jae Hwan Lee, Seung-Yeon Kim, and Julian Lee. Parallel algorithm for calculation of the exact partition function of a lattice polymer. *Computer Physics Communications*, 182(4):1027–1033, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000130.

Laptyeva:2016:CFS

[LKM+16] T. V. Laptyeva, E. A. Kozinov, I. B. Meyerov, M. V. Ivanchenko, S. V. Denisov, and P. Hänggi. Calculating Floquet states of large quantum systems: a parallelization strategy and its cluster implementation. *Computer Physics Communications*, 201(??):85–94, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000059.

Li:2019:VPV

[LKPH19] Gang Li, Anna Kauch, Petra Pudleiner, and Karsten Held. The *victory* project v1.0: an efficient parquet equations solver. *Computer Physics Communications*, 241(??):146–154, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465519300864.

Loft:2016:CCL

[LKT+16] N. J. S. Loft, L. B. Kristensen, A. E. Thomsen, A. G. Volosniev, and N. T. Zinner. CONAN — the cruncher of local exchange coefficients for strongly interacting confined systems in one dimension. *Computer Physics Communications*, 209(??):171–182, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302545.

Lo:2011:MHS

[LKW11] Ying-Yi Lo, Chung-Ming Ko, and Chih-Yueh Wang. 3D magneto-hydrodynamic simulations of Parker instability with cosmic rays. *Computer Physics Communications*, 182(1):177–179, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001761.

Lu:2012:SPM

[LL12] Haokai Lu and Peng Li. Stochastic projective methods for simulating stiff chemical reacting systems. *Computer Physics Communications*, 183(7):1427–1442, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200080X.

Lou:2015:MNF

[LL15] Tak Pui Lou and Bernhard Ludewigt. MMAPDNG: a new, fast code backed by a memory-mapped database for simulating delayed γ-ray emission with MCNPX package. *Computer Physics Communications*, 194(??):10–17, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001368.

Li:2019:ECS

[LL19] Wanshan Li and Dong Liang. The energy conservative splitting FDTD scheme and its energy identities for metamaterial electromagnetic Lorentz system. *Computer Physics*

Communications, 239(??):94–111, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300049.

Lemaire:2018:VPT

[LLE+18] Matthieu Lemaire, Hyunsuk Lee, Bamidele Ebiwonjumi, Chidong Kong, Wonkyeong Kim, Yunki Jo, Jinsu Park, and Deokjung Lee. Verification of photon transport capability of UNIST Monte Carlo code MCS. *Computer Physics Communications*, 231(??):1–18, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301619.

Levy:2017:IME

[LLG17] Ryan Levy, J. P. F. LeBlanc, and Emanuel Gull. Implementation of the maximum entropy method for analytic continuation. *Computer Physics Communications*, 215(??):149–155, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300309.

Lai:2011:DSM

[LLHC11] S. K. Lai, Yu-Ting Lin, P. J. Hsu, and S. A. Cheong. Dynamical study of metallic clusters using the statistical method of time series clustering. *Computer Physics Communications*, 182(4):1013–1026, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000038.

Lin:2012:SCA

[LLL12] Yezhi Lin, Yinping Liu, and Zhibin Li. Symbolic computation of analytic approximate solutions for nonlinear differential equations with initial conditions. *Computer Physics Communications*, 183(1):106–117, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002736.

Lin:2013:SCA

[LLL13] Yezhi Lin, Yinping Liu, and Zhibin Li. Symbolic computation of analytic approximate solutions for nonlinear fractional differential equations. *Computer Physics Communications*, 184(1):130–141, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002615.

Li:2017:HDG

[LLMW17] Liang Li, Stéphane Lanteri, N. Asger Mortensen, and Martijn Wubs. A hybridizable discontinuous Galerkin method for solving nonlocal optical response models. *Computer Physics Communications*, 219(??):99–107, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301546.

Li:2015:CLW

[LLP15] Liang Li, Stéphane Lanteri, and Ronan Perrussel. A class of locally well-posed hybridizable discontinuous Galerkin methods for the solution of time-harmonic Maxwell's equations. *Computer Physics Communications*, 192(??):23–31, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000740.

Lan:2019:TDG

[LLQX19] Ting Lan, Jian Liu, Hong Qin, and Lin Li Xu. Time-domain global similarity method for automatic data cleaning for multi-channel measurement systems in magnetic confinement fusion devices. *Computer Physics Communications*, 234(??):159–166, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302674.

Lee:2017:PFS

[LLSK17] Seunggyu Lee, Yibao Li, Jaemin Shin, and Junseok Kim. Phase-field simulations of crystal growth in a two-dimensional cavity flow. *Computer Physics Communications*, 216(??):84–94, July 2017. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300814.

Liao:2014:NSF

[lLsSZ14] Hong lin Liao, Han sheng Shi, and Ying Zhao. Numerical study of fourth-order linearized compact schemes for generalized NLS equations. *Computer Physics Communications*, 185(8):2240–2249, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001556.

Luo:2014:FCM

[LLX14a] Xiaopeng Luo, Zhenzhou Lu, and Xin Xu. A fast computational method for moment-independent uncertainty importance measure. *Computer Physics Communications*, 185(1):19–27, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002671.

Luo:2014:RKT

[LLX14b] Xiaopeng Luo, Zhenzhou Lu, and Xin Xu. Reproducing kernel technique for high dimensional model representations (HDMR). *Computer Physics Communications*, 185(12):3099–3108, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002641.

Li:2016:CFO

[LLXK16] Yibao Li, Hyun Geun Lee, Binhu Xia, and Junseok Kim. A compact fourth-order finite difference scheme for the three-dimensional Cahn–Hilliard equation. *Computer Physics Communications*, 200(??):108–116, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004178.

Liu:2017:DAC

[LLZ+17] Zhong-Li Liu, Rui Li, Xiu-Lu Zhang, Nuo Qu, and Ling-Cang Cai. Direct anharmonic correction method by molecular dynamics. *Computer Physics Communications*, 213(??):122–

129, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303964.

Li:2012:MBF

[LM12] Xuesong Li and Lin Ma. Minimizing binary functions with simulated annealing algorithm with applications to binary tomography. *Computer Physics Communications*, 183(2):309–315, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003432.

Lee:2016:ISP

[LM16] Roman N. Lee and Kirill T. Mingulov. Introducing SummerTime: a package for high-precision computation of sums appearing in DRA [1] method. *Computer Physics Communications*, 203(??):255–267, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300339.

Lai:2019:EOA

[LM19] S. K. Lai and Wafa Maftuhin. An efficient optimization algorithm that hybridizes DFTB and DFT theories both operated within the modified basin hopping method. *Computer Physics Communications*, 236(??):164–175, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303758.

Lu:2016:KCC

[LMAB16] Hongliang Lü, Anthony Marchix, Yasuhisa Abe, and David Boilley. KEWPIE2: a cascade code for the study of dynamical decay of excited nuclei. *Computer Physics Communications*, 200(??):381–399, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004415.

Laburta:2015:NMN

[LMRC15] M. P. Laburta, J. I. Montijano, L. Rández, and M. Calvo. Numerical methods for non conservative perturbations of conservative problems. *Computer Physics Communications*, 187(??):72–82, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003476.

Li:2016:MCB

[LN16] Xuesong Li and William F. Northrop. A Markov Chain-based quantitative study of angular distribution of photons through turbid slabs via isotropic light scattering. *Computer Physics Communications*, 201(??):77–84, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004580.

Lv:2017:CDS

[LNP+17] Q. Z. Lv, S. Norris, R. Pelphrey, Q. Su, and R. Grobe. Computation of diverging sums based on a finite number of terms. *Computer Physics Communications*, 219(??):1–10, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301303.

Lopez:2015:CSJ

[LNSD15] Alejandro López, William Nicholls, Matthew T. Stickland, and William M. Dempster. CFD study of jet impingement test erosion using Ansys Fluent$^($$R$) and OpenFOAM$^($$R$). *Computer Physics Communications*, 197(??):88–95, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002945.

Litsarev:2014:DCC

[LO14] Mikhail S. Litsarev and Ivan V. Oseledets. The DEPOSIT computer code based on the low rank approximations. *Computer Physics Communications*, 185(10):2801–2802, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002173.

Lee:2016:IMD

[LOK+16] In-Ho Lee, Young Jun Oh, Sunghyun Kim, Jooyoung Lee, and K. J. Chang. Ab initio materials design using conformational space annealing and its application to searching for direct band gap silicon crystals. *Computer Physics Communications*, 203(??):110–121, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300261.

Liu:2018:ASE

[LOK+18] Xiaoxing Liu, Ryusei Ogawa, Masatsugu Kato, Koji Morita, and Shuai Zhang. Accuracy and stability enhancements in the incompressible finite-volume-particle method for multiphase flow simulations. *Computer Physics Communications*, 230(??):59–69, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830136X.

Laguna:2018:FIF

[LOL+18] A. Alvarez Laguna, N. Ozak, A. Lani, H. Deconinck, and S. Poedts. Fully-implicit finite volume method for the ideal two-fluid plasma model. *Computer Physics Communications*, 231(??):31–44, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301590.

Lyakhov:2013:NDE

[LOSZ13] Andriy O. Lyakhov, Artem R. Oganov, Harold T. Stokes, and Qiang Zhu. New developments in evolutionary structure prediction algorithm USPEX. *Computer Physics Communications*, 184(4):1172–1182, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004055.

Lyakhov:2010:HPV

[LOV10] Andriy O. Lyakhov, Artem R. Oganov, and Mario Valle. How to predict very large and complex crystal structures. *Computer Physics Communications*, 181(9):1623–1632, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001840.

Levine:2015:FMM

[LP15] Zachary H. Levine and Adam L. Pintar. A fixed-memory moving, expanding window for obtaining scatter corrections in X-ray CT and other stochastic averages. *Computer Physics Communications*, 196(??):455–459, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500199X.

Landau:2011:MPE

[LPBH11] Rubin H. Landau, Manuel J. Paez, Cristian Bordeianu, and Sally Haerer. Making physics education more relevant and accessible via computation and eTextBooks. *Computer Physics Communications*, 182(9):2071–2075, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004522.

Lauricella:2015:JSP

[LPC+15] Marco Lauricella, Giuseppe Pontrelli, Ivan Coluzza, Dario Pisignano, and Sauro Succi. JETSPIN: a specific-purpose open-source software for simulations of nanofiber electrospinning. *Computer Physics Communications*, 197(??):227–238, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002994.

Ladutenko:2017:MCE

[LPRPR17] Konstantin Ladutenko, Umapada Pal, Antonio Rivera, and Ovidio Peña-Rodríguez. Mie calculation of electromagnetic near-field for a multilayered sphere. *Computer Physics Communications*, 214(??):225–230, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300292.

Liu:2018:SMP

[LQ18] Zhicong Liu and Ji Qiang. Symplectic multi-particle tracking on GPUs. *Computer Physics Communications*, 226(??):10–17, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300298.

Li:2013:TSS

[LQZ+13] Jin-Chun Li, Ping Qian, Zhen-Feng Zhang, Ying Liu, Xiao-Jian Yuan, Jiang Shen, and Nan-Xian Chen. Theoretical study of structure and lattice vibrations of $R_3Co_{11-x}Fe_xB_4$ (R = Nd, Gd). *Computer Physics Communications*, 184(2):342–347, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003037`.

Luukko:2013:ITP

[LR13] P. J. J. Luukko and E. Räsänen. Imaginary time propagation code for large-scale two-dimensional eigenvalue problems in magnetic fields. *Computer Physics Communications*, 184(3):769–776, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551200327X`. See corrigendum [LR16].

Luukko:2016:CIT

[LR16] P. J. J. Luukko and E. Räsänen. Corrigendum to “Imaginary time propagation code for large-scale two-dimensional eigenvalue problems in magnetic fields” [comput. phys. comm. **184**(3) (2013) 769–776]. *Computer Physics Communications*, 198(??):262, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551500363X`. See [LR13].

Larsen:2018:MMPa

[LR18a] Kasper J. Larsen and Robbert Rietkerk. MultivariateResidues: a Mathematica package for computing multivariate residues. *Computer Physics Communications*, 222(??):250–262, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302886`.

Larsen:2018:MMPb

[LR18b] Kasper J. Larsen and Robbert Rietkerk. MultivariateResidues: a Mathematica package for computing multivariate residues. *Computer Physics Communications*, 233(??):269–270, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302212.

Li:2011:GTR

[LRC+11] Dingping Li, B. Rosenstein, Shou Chen, H. H. Lin, and D. Berco. Glass transition and the replica symmetry breaking in vortex matter: MC study. *Computer Physics Communications*, 182(1):55–57, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002869.

Luo:2013:IMM

[LRK13] L. Luo, T. Rafiq, and A. H. Kritz. Improved multi-mode anomalous transport module for tokamak plasmas. *Computer Physics Communications*, 184(10):2267–2276, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001732.

Lopez:2015:DNV

[LRR+15] Rafael López, Jaime Fernández Rico, Guillermo Ramírez, Ignacio Ema, and David Zorrilla. DAMQT 2.0: a new version of the DAMQT package for the analysis of electron density in molecules. *Computer Physics Communications*, 192(??):289–294, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000855.

Lopez:2017:TME

[LRR+17] Rafael López, Jaime Fernández Rico, Guillermo Ramírez, Ignacio Ema, David Zorrilla, Anmol Kumar, Sachin D. Yeole, and Shridhar R. Gadre. Topology of molecular electron density and electrostatic potential with DAMQT. *Computer Physics Communications*, 214(??):207–215, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300243.

Lujan:2019:LTG

[LRSS19] E. Luján, M. S. Rosito, A. Soba, and C. Suárez. LibreGrowth: a tumor growth code based on reaction–diffusion equations using shared memory. *Computer Physics Communications*, 243(??):97–105, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301547.

Levchenko:2015:HFL

[LRW+15] Sergey V. Levchenko, Xinguo Ren, Jürgen Wieferink, Rainer Johanni, Patrick Rinke, Volker Blum, and Matthias Scheffler. Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, 192(??):60–69, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500079X.

Londero:2011:VPV

[LS11] Elisa Londero and Elsebeth Schröder. Vanadium pentoxide (V_2O_5): a van der Waals density functional study. *Computer Physics Communications*, 182(9):1805–1809, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005291.

Li:2012:NMS

[LS12a] Haochen Li and Jianqiang Sun. A new multi-symplectic scheme for the generalized Kadomtsev–Petviashvili equation. *Computer Physics Communications*, 183(9):1956–1965, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001579.

Lindner:2012:SXR

[LS12b] Benjamin Lindner and Jeremy C. Smith. Sassena — X-ray and neutron scattering calculated from molecular dynamics trajectories using massively parallel computers. *Computer Physics Communications*, 183(7):1491–1501, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200063X.

Luscher:2013:LQO

[LS13] Martin Lüscher and Stefan Schaefer. Lattice QCD with open boundary conditions and twisted-mass reweighting. *Computer Physics Communications*, 184(3):519–528, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003359.

Leetmaa:2014:KGF

[LS14] Mikael Leetmaa and Natalia V. Skorodumova. KMCLib: a general framework for lattice kinetic Monte Carlo (KMC) simulations. *Computer Physics Communications*, 185(9):2340–2349, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001519.

Leetmaa:2015:KER

[LS15a] Mikael Leetmaa and Natalia V. Skorodumova. KMCLib 1.1: Extended random number support and technical updates to the KMCLib general framework for kinetic Monte-Carlo simulations. *Computer Physics Communications*, 196(??):611–613, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002611.

Leetmaa:2015:MSD

[LS15b] Mikael Leetmaa and Natalia V. Skorodumova. Mean square displacements with error estimates from non-equidistant time-step kinetic Monte Carlo simulations. *Computer Physics Communications*, 191(??):119–124, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500051X.

Linaro:2016:BLB

[LS16] Daniele Linaro and Marco Storace. BAL: a library for the brute-force analysis of dynamical systems. *Computer Physics Communications*, 201(??):126–134, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004142.

Lv:2017:MDS

[LS17a] Guocai Lv and Yanjing Su. Molecular dynamics simulation and first principles calculations of radiation-induced Cu clusters in Fe-3 at.% Cu alloy. *Computer Physics Communications*, 211(??):41–44, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301849.

Lyonnet:2017:PPT

[LS17b] F. Lyonnet and I. Schienbein. PyR@TE 2: a Python tool for computing RGEs at two-loop. *Computer Physics Communications*, 213(??):181–196, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630368X.

Levchenko:2019:CRO

[LS19] Sergey V. Levchenko and Matthias Scheffler. Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. *Computer Physics Communications*, 237(??):42–46, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303965.

Li:2011:LSM

[LSCZ11] Jun Li, Yi Sun, Zhiwei Cui, and Fanlin Zeng. Least square method for the calculation of elastic constants. *Computer Physics Communications*, 182(7):1447–1451, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000907.

Lopez:2018:CSF

[LSD18] Alejandro López, Matthew T. Stickland, and William M. Dempster. CFD study of fluid flow changes with erosion. *Computer Physics Communications*, 227(??):27–41, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300304.

Launey:2014:PSC

[LSDD14] K. D. Launey, S. Sarbadhicary, T. Dytrych, and J. P. Draayer. Program in C for studying characteristic properties of two-body interactions in the framework of spectral distribution theory. *Computer Physics Communications*, 185(1):254–267, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002683.

Landreman:2014:NCR

[LSF14] Matt Landreman, Adam Stahl, and Tünde Fülöp. Numerical calculation of the runaway electron distribution function and associated synchrotron emission. *Computer Physics Communications*, 185(3):847–855, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004165.

Leidi:2012:CEP

[LSG+12] Tiziano Leidi, Giulio Scocchi, Loris Grossi, Simone Pusterla, Claudio D'Angelo, Jean-Philippe Thiran, and Alberto Ortona. Computing effective properties of random heterogeneous materials on heterogeneous parallel processors. *Computer Physics Communications*, 183(11):2424–2433, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002111.

Lopez:2013:ISP

[LSJ13] R. López and J. F. San-Juan. Astrody$^{\mathrm{Web}}_{\mathrm{tools}}$: an e-science project in astrodynamics and celestial mechanics fields. *Computer Physics Communications*, 184(5):1381–1386, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000088.

Lin:2013:TDR

[LSK+13] Y.-J. Lin, M. R. Smith, F.-A. Kuo, H. M. Cave, J.-C. Huang, and J.-S. Wu. A true-direction reconstruction of the quiet direct simulation method for inviscid gas flows. *Computer Physics Communications*, 184(11):2378–2390, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001677`.

Lourderaj:2014:VNS

[LSK+14] Upakarasamy Lourderaj, Rui Sun, Swapnil C. Kohale, George L. Barnes, Wibe A. de Jong, Theresa L. Windus, and William L. Hase. The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. *Computer Physics Communications*, 185(3):1074–1080, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004049`.

Lichtenstein:2017:HPF

[LSR+17] J. Lichtenstein, D. Sánchez de la Peña, D. Rohe, E. Di Napoli, C. Honerkamp, and S. A. Maier. High-performance functional Renormalization Group calculations for interacting fermions. *Computer Physics Communications*, 213 (??):100–110, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303927`.

Lyonnet:2014:PRG

[LSSW14] F. Lyonnet, I. Schienbein, F. Staub, and A. Wingerter. PyR@TE: Renormalization group equations for general gauge theories. *Computer Physics Communications*, 185(3): 1130–1152, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004141`.

Li:2015:SSO

[LST15] Leonard Z. Li, Hai-Wei Sun, and Sik-Chung Tam. A spatial sixth-order alternating direction implicit method for two-dimensional cubic nonlinear Schrödinger equations. *Computer Physics Communications*, 187(??):38–48, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003439`.

Lu:2012:PEH

[LSYZ12] Fengshun Lu, Junqiang Song, Fukang Yin, and Xiaoqian Zhu. Performance evaluation of hybrid programming patterns for large CPU/GPU heterogeneous clusters. *Computer Physics Communications*, 183(6):1172–1181, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000343.

Levitt:2015:PEP

[LT15] Antoine Levitt and Marc Torrent. Parallel eigensolvers in plane-wave Density Functional Theory. *Computer Physics Communications*, 187(??):98–105, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003531.

Liu:2012:AEP

[LTL+12] Mingzhe Liu, Xianguo Tuo, Zhe Li, Jianbo Yang, and Yang Gao. Asymmetric exclusion process for modeling of information flow. *Computer Physics Communications*, 183(2):316–319, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003456.

Luu:2016:VPM

[LTP16] Phuc T. Luu, T. Tückmantel, and A. Pukhov. Voronoi particle merging algorithm for PIC codes. *Computer Physics Communications*, 202(??):165–174, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551600028X.

Little:2017:TPD

[LTP+17] Duncan A. Little, Jonathan Tennyson, Martin Plummer, Clifford J. Noble, and Andrew G. Sunderland. TIMEDELn: a programme for the detection and parametrization of overlapping resonances using the time-delay method. *Computer Physics Communications*, 215(??):137–148, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730005X.

Lutsyshyn:2015:FQM

[Lut15] Y. Lutsyshyn. Fast quantum Monte Carlo on a GPU. *Computer Physics Communications*, 187(??):162–174, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003221`.

Ledoux:2010:SSL

[LV10] V. Ledoux and M. Van Daele. Solving Sturm–Liouville problems by piecewise perturbation methods, revisited. *Computer Physics Communications*, 181(8):1335–1345, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000974`.

Ledoux:2013:ACQ

[LV13] V. Ledoux and M. Van Daele. Automatic computation of quantum-mechanical bound states and wavefunctions. *Computer Physics Communications*, 184(4):1287–1296, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512004225`.

Ledoux:2014:ANS

[LV14] V. Ledoux and M. Van Daele. The accurate numerical solution of the Schrödinger equation with an explicitly time-dependent Hamiltonian. *Computer Physics Communications*, 185(6):1589–1594, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000678`.

Lee:2015:EPM

[LV15] P. Lee and J.-L. Vay. Efficiency of the perfectly matched layer with high-order finite difference and pseudo-spectral Maxwell solvers. *Computer Physics Communications*, 194(??):1–9, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001356`.

Lee:2019:CNL

[LV19] P. Lee and J.-L. Vay. Convergence in nonlinear laser wakefield accelerators modeling in a Lorentz-boosted frame. *Com-*

puter Physics Communications, 238(??):102–110, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304296.

Loke:2011:EQC

[LW11] T. Loke and J. B. Wang. An efficient quantum circuit analyser on qubits and qudits. *Computer Physics Communications*, 182(10):2285–2294, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002104.

Loke:2013:CQC

[LW13] T. Loke and J. B. Wang. CUGatesDensity — quantum circuit analyser extended to density matrices. *Computer Physics Communications*, 184(12):2834–2839, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300235X.

Lee:2014:BTS

[LW14a] Jungpyo Lee and John C. Wright. A block-tridiagonal solver with two-level parallelization for finite element-spectral codes. *Computer Physics Communications*, 185(10):2598–2608, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002100.

Liu:2014:MAM

[LW14b] Kai Liu and Xinyuan Wu. Multidimensional ARKN methods for general oscillatory second-order initial value problems. *Computer Physics Communications*, 185(7):1999–2007, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001246.

Loke:2016:OVU

[LW16] T. Loke and J. B. Wang. OptQC v1.3: an (updated) optimized parallel quantum compiler. *Computer Physics Communications*, 207(??):531–532, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465516301643.

Loke:2014:OOP

[LWC14] T. Loke, J. B. Wang, and Y. H. Chen. OptQC: an optimized parallel quantum compiler. *Computer Physics Communications*, 185(12):3307–3316, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002653.

Liu:2018:FRF

[LWES18] Xianglin Liu, Yang Wang, Markus Eisenbach, and G. Malcolm Stocks. Fully-relativistic full-potential multiple scattering theory: a pathology-free scheme. *Computer Physics Communications*, 224(??):265–272, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S001046551730351X.

Loppi:2018:HOC

[LWJV18] N. A. Loppi, F. D. Witherden, A. Jameson, and P. E. Vincent. A high-order cross-platform incompressible Navier–Stokes solver via artificial compressibility with application to a turbulent jet. *Computer Physics Communications*, 233(??):193–205, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302248.

Li:2011:MCS

[LWL11] Ying Wai Li, Thomas Wüst, and David P. Landau. Monte Carlo simulations of the HP model (the “Ising model” of protein folding). *Computer Physics Communications*, 182(9):1896–1899, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000051.

Li:2012:HDM

[LWL12] Enying Li, Hu Wang, and Guangyao Li. High dimensional model representation (HDMR) coupled intelligent sampling strategy for nonlinear problems. *Computer Physics Communications*, 183(9):1947–1955, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001567.

Los:2017:IAI

[LWP+17] Marcin M. Loś, Maciej Woźniak, Maciej Paszyński, Andrew Lenharth, Muhamm Amber Hassaan, and Keshav Pingali. IGA–ADS: Isogeometric analysis FEM using ADS solver. *Computer Physics Communications*, 217(??):99–116, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300759.

Luo:2016:GAC

[LWRQ16] Xisheng Luo, Luying Wang, Wei Ran, and Fenghua Qin. GPU accelerated cell-based adaptive mesh refinement on unstructured quadrilateral grid. *Computer Physics Communications*, 207(??):114–122, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301424.

Ling:2010:HTS

[LWW10] Sitao Ling, Minghui Wang, and Musheng Wei. Hermitian tridiagonal solution with the least norm to quaternionic least squares problem. *Computer Physics Communications*, 181(3):481–488, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003403.

Li:2011:TSE

[LWYW11] Jiyong Li, Bin Wang, Xiong You, and Xinyuan Wu. Two-step extended RKN methods for oscillatory systems. *Computer Physics Communications*, 182(12):2486–2507, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002451.

Li:2014:LAB

[LWZ14] Hongwei Li, Xiaonan Wu, and Jiwei Zhang. Local artificial boundary conditions for Schrödinger and heat equations by using high-order azimuth derivatives on circular artificial boundary. *Computer Physics Communications*, 185(6):1606–1615, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000794.

Lang:2012:QBS

[LX12] Feng-Gong Lang and Xiao-Ping Xu. Quintic B-spline collocation method for second order mixed boundary value problem. *Computer Physics Communications*, 183(4):913–921, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100405X.

Li:2014:SCC

[LX14] Chao Li and Hailing Xiong. 3D simulation of the Cluster–Cluster Aggregation model. *Computer Physics Communications*, 185(12):3424–3429, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002951.

Li:2018:CTD

[LXR+18] N. M. Li, X. Q. Xu, T. D. Rognlien, B. Gui, J. Z. Sun, and D. Z. Wang. Calculation of two-dimension radial electric field in boundary plasmas by using BOUT++. *Computer Physics Communications*, 228(??):69–82, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300651.

Lorin:2016:FGA

[LY16] E. Lorin and X. Yang. Frozen Gaussian approximation-based two-level methods for multi-frequency Schrödinger equation. *Computer Physics Communications*, 207(??):145–159, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301473.

Lyakh:2015:ETT

[Lya15] Dmitry I. Lyakh. An efficient tensor transpose algorithm for multicore CPU, Intel Xeon Phi, and NVidia Tesla GPU. *Computer Physics Communications*, 189(??):84–91, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514004330`.

Lee:2019:SNE

[LYJH19] Kyuhyun Lee, Dongsun Yoo, Wonseok Jeong, and Seungwu Han. SIMPLE-NN: an efficient package for training and executing neural-network interatomic potentials. *Computer Physics Communications*, 242(??):95–103, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301298`.

Li:2010:CRN

[LYJY10] Wan-Qing Li, Tang Ying, Wan Jian, and Dong-Jin Yu. Comparison research on the neighbor list algorithms: Verlet table and linked-cell. *Computer Physics Communications*, 181(10):1682–1686, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001827`.

Liu:2017:MSS

[LYL$^+$17] Shaolin Liu, Dinghui Yang, Chao Lang, Wenshuai Wang, and Zhide Pan. Modified symplectic schemes with nearly-analytic discrete operators for acoustic wave simulations. *Computer Physics Communications*, 213(??):52–63, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303678`.

Lani:2014:GEF

[LYP14] Andrea Lani, Mehmet Sarp Yalim, and Stefaan Poedts. A GPU-enabled Finite Volume solver for global magnetospheric simulations on unstructured grids. *Computer Physics Communications*, 185(10):2538–2557, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002057`.

Loncar:2016:OOM

[LYSS+16] Vladimir Loncar, Luis E. Young-S., Srdjan Skrbić, Paulsamy Muruganandam, Sadhan K. Adhikari, and Antun Balaz. OpenMP, OpenMP/MPI, and CUDA/MPI C programs for solving the time-dependent dipolar Gross–Pitaevskii equation. *Computer Physics Communications*, 209(??):190–196, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302272.

Li:2017:CNC

[LYX+17] Fei Li, Peicheng Yu, Xinlu Xu, Frederico Fiuza, Viktor K. Decyk, Thamine Dalichaouch, Asher Davidson, Adam Tableman, Weiming An, Frank S. Tsung, Ricardo A. Fonseca, Wei Lu, and Warren B. Mori. Controlling the numerical Cerenkov instability in PIC simulations using a customized finite difference Maxwell solver and a local FFT based current correction. *Computer Physics Communications*, 214(??):6–17, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300012.

Lu:2013:WGA

[LYZ13] Xiangwen Lu, Jiabin Yuan, and Weiwei Zhang. Workflow of the Grover algorithm simulation incorporating CUDA and GPGPU. *Computer Physics Communications*, 184(9):2035–2041, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001148.

Lonie:2011:XOS

[LZ11a] David C. Lonie and Eva Zurek. XtalOpt: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 182(2):372–387, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003140.

Lonie:2011:XVR

[LZ11b] David C. Lonie and Eva Zurek. XtalOpt version r7: An open-source evolutionary algorithm for crystal structure prediction. *Computer Physics Communications*, 182(10):2305–2306, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100213X.

Lonie:2012:IDC

[LZ12] David C. Lonie and Eva Zurek. Identifying duplicate crystal structures: XtalComp, an open-source solution. *Computer Physics Communications*, 183(3):690–697, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003699.

Li:2017:ESI

[LZ17] Xujing Li and Leonid E. Zakharov. Equilibrium Spline Interface (ESI) for magnetic confinement codes. *Computer Physics Communications*, 221(??):358–382, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302618.

Liu:2018:AAA

[LZ18] Z. R. Liu and R. F. Zhang. AACSD: an atomistic analyzer for crystal structure and defects. *Computer Physics Communications*, 222(??):229–239, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302588.

Li:2011:FPC

[LZL11] Zi Li, Xu Zhang, and Gang Lu. A Fortran program for calculating electron or hole mobility in disordered semiconductors from first-principles. *Computer Physics Communications*, 182(12):2632–2637, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002633.

Levin:2012:FFF

[LZP12] Alan R. Levin, Deyin Zhang, and Eric Polizzi. FEAST fundamental framework for electronic structure calculations: Reformulation and solution of the muffin-tin problem. *Computer Physics Communications*, 183(11):2370–2375, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002056.

Li:2010:SSW

[LZZL10] Xiaofan Li, Tong Zhu, Meigen Zhang, and Guihua Long. Seismic scalar wave equation with variable coefficients modeling by a new convolutional differentiator. *Computer Physics Communications*, 181(11):1850–1858, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002389.

Mohebbi:2011:ENA

[MA11] Akbar Mohebbi and Zohreh Asgari. Efficient numerical algorithms for the solution of "good" Boussinesq equation in water wave propagation. *Computer Physics Communications*, 182(12):2464–2470, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002426.

Magoga:2012:NSF

[MAC12] Michaël Magoga, Fabien Archambault, and Jorge I. Cerdá. Nt_STM: a step forward in Scanning Tunneling Microscopy (STM) simulations. *Computer Physics Communications*, 183(6):1246–1249, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000525.

Magniette:2018:SAP

[Mag18] Frédéric Magniette. Statistical algorithms for particle trajectography. *Computer Physics Communications*, 232(??):59–70, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302066.

Maitre:2012:EHC

[Maî12] Daniel Maître. Extension of HPL to complex arguments. *Computer Physics Communications*, 183(3):846, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003778.

Molero-Armenta:2014:OOI

[MAIVAH14] M. Molero-Armenta, Ursula Iturrarán-Viveros, S. Aparicio, and M. G. Hernández. Optimized OpenCL implementation of the Elastodynamic Finite Integration Technique for viscoelastic media. *Computer Physics Communications*, 185(10):2683–2696, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001702.

Mohammed-Azizi:2014:SPC

[MAM14] B. Mohammed-Azizi and D. E. Medjadi. Single particle calculations for a Woods–Saxon potential with triaxial deformations, and large Cartesian oscillator basis (TRIAXIAL 2014, third version of the code Triaxial). *Computer Physics Communications*, 185(11):3067–3068, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002598.

Marti:2015:CCV

[Mar15] José-María Martí. On the correction of conserved variables for numerical RMHD with staggered constrained transport. *Computer Physics Communications*, 191(??):100–105, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000491.

Marucho:2019:JAC

[Mar19] Marcelo Marucho. A Java application to characterize biomolecules and nanomaterials in electrolyte aqueous solutions. *Computer Physics Communications*, 242(??):104–119, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301249.

Maurer:2016:TVT

[Mau16] Vinzenz Maurer. T3PS v1.0: Tool for parallel processing in parameter scans. *Computer Physics Communications*, 198(??):195–215, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003318.

Madhikar:2018:CGA

[MÅWK18] Pranav Madhikar, Jan Åström, Jan Westerholm, and Mikko Karttunen. CellSim3D: GPU accelerated software for simulations of cellular growth and division in three dimensions. *Computer Physics Communications*, 232(??):206–213, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302091.

Mazzeo:2013:FDG

[Maz13] Marco D. Mazzeo. Fast discontinuous Galerkin lattice-Boltzmann simulations on GPUs via maximal kernel fusion. *Computer Physics Communications*, 184(3):537–549, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003384.

Mazdziarz:2019:CAI

[Maź19] Marcin Maździarz. A comment on the article "Ab initio calculations of pressure-dependence of high-order elastic constants using finite deformations approach" by I. Mosyagin, A. V. Lugovskoy, O. M. Krasilnikov, Yu. Kh. Vekilov, S. I. Simak and I. A. Abrikosov [Computer Physics Communications **220** (2017) 20–30]. *Computer Physics Communications*, 235(??):293–294, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300602. See [MLK+17] and reply [MLK+19].

McIntyre:2012:FJB

[MB12] Timothy J. McIntyre and Alexis I. Bishop. Fringe — a Java-based finite fringe analysis package. *Computer Physics Communications*, 183(9):2014–2018, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001506.

Mosert:2016:PSQ

[MB16] Volker Mosert and Dieter Bauer. Photoelectron spectra with Qprop and t-SURFF. *Computer Physics Communications*, 207(??):452–463, October 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301801.

Mishchenko:2019:PSI

[MBB+19] A. Mishchenko, A. Bottino, A. Biancalani, R. Hatzky, T. Hayward-Schneider, N. Ohana, E. Lanti, S. Brunner, L. Villard, M. Borchardt, R. Kleiber, and A. Könies. Pullback scheme implementation in ORB5. *Computer Physics Communications*, 238(??):194–202, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304181.

Marquardt:2010:PWI

[MBF+10] Oliver Marquardt, Sixten Boeck, Christoph Freysoldt, Tilmann Hickel, and Jörg Neugebauer. Plane-wave implementation of the real-space $k \cdot p$ formalism and continuum elasticity theory. *Computer Physics Communications*, 181(4):765–771, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004019.

Michalicek:2013:ELE

[MBFB13] Gregor Michalicek, Markus Betzinger, Christoph Friedrich, and Stefan Blügel. Elimination of the linearization error and improved basis-set convergence within the FLAPW method. *Computer Physics Communications*, 184(12):2670–2679, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002300.

Moxley:2012:GFD

[MBFD12] Frederick Ira Moxley III, Tim Byrnes, Fumitaka Fujiwara, and Weizhong Dai. A generalized finite-difference time-domain quantum method for the N-body interacting Hamiltonian. *Computer Physics Communications*, 183(11):2434–2440, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200224X.

Mickevicius:2011:FPH

[MBGK11] S. Mickevicius, E. Brazauskas, D. Germanas, and R. K. Kalinauskas. The four-particle harmonic-oscillator brackets: Compact expressions and updated Fortran program. *Computer Physics Communications*, 182(6):1377–1381, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000774`.

Motta:2015:ILM

[MBGV15] M. Motta, G. Bertaina, D. E. Galli, and E. Vitali. Implementation of the linear method for the optimization of Jastrow–Feenberg and backflow correlations. *Computer Physics Communications*, 190(??):62–71, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000338`.

Martin-Bragado:2013:MOK

[MBRV⁺13] Ignacio Martin-Bragado, Antonio Rivera, Gonzalo Valles, Jose Luis Gomez-Selles, and María J. Caturla. MMonCa: an Object Kinetic Monte Carlo simulator for damage irradiation evolution and defect diffusion. *Computer Physics Communications*, 184(12):2703–2710, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002397`.

Melchionna:2010:HAL

[MBS⁺10] Simone Melchionna, Massimo Bernaschi, Sauro Succi, Efthimios Kaxiras, Frank J. Rybicki, Dimitris Mitsouras, Ahmet U. Coskun, and Charles L. Feldman. Hydrokinetic approach to large-scale cardiovascular blood flow. *Computer Physics Communications*, 181(3):462–472, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003385`.

Mohankumar:2010:NAD

[MC10] N. Mohankumar and Tucker Carrington, Jr. A new approach for determining the time step when propagating with the Lanczos algorithm. *Computer Physics Communications*, 181(11):1859–1861, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002523.

Mei:2012:NSR

[MC12] Liquan Mei and Yaping Chen. Numerical solutions of RLW equation using Galerkin method with extrapolation techniques. *Computer Physics Communications*, 183(8):1609–1616, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000914.

Majorosi:2016:FOR

[MC16] Szilárd Majorosi and Attila Czirják. Fourth order real space solver for the time-dependent Schrödinger equation with singular Coulomb potential. *Computer Physics Communications*, 208(??):9–28, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301886.

Myneni:2017:CEE

[MC17] Hemanadhan Myneni and Mark E. Casida. On the calculation of $\Delta(\hat{S}^2)$ for electronic excitations in time-dependent density-functional theory. *Computer Physics Communications*, 213(??):72–91, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303903.

Mani:2017:RPR

[MCA17] B. K. Mani, S. Chattopadhyay, and D. Angom. RCCPAC: a parallel relativistic coupled-cluster program for closed-shell and one-valence atoms and ions in FORTRAN. *Computer Physics Communications*, 213(??):136–154, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303629.

Miqueles:2014:ART

[MCAdF14] Eduardo X. Miqueles, Tiago A. Coimbra, Bruno D. Amaro, and J. J. S. de Figueiredo. Analytical ray tracing system: Introducing art, a C-library designed for seismic applications. *Computer Physics Communications*, 185(1):274–293, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002713.

Mitnik:2011:CMG

[MCGR11] Darío M. Mitnik, Flavio D. Colavecchia, Gustavo Gasaneo, and Juan M. Randazzo. Computational methods for Generalized Sturmians basis. *Computer Physics Communications*, 182(5):1145–1155, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000361.

Mycek:2017:RDD

[MCL+17] Paul Mycek, Andres Contreras, Olivier Le Maître, Khachik Sargsyan, Francesco Rizzi, Karla Morris, Cosmin Safta, Bert Debusschere, and Omar Knio. A resilient domain decomposition polynomial chaos solver for uncertain elliptic PDEs. *Computer Physics Communications*, 216(??):18–34, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730067X.

Melazzi:2012:SFD

[MCM+12] D. Melazzi, D. Curreli, M. Manente, J. Carlsson, and D. Pavarin. SPIREs: a Finite-Difference Frequency-Domain electromagnetic solver for inhomogeneous magnetized plasma cylinders. *Computer Physics Communications*, 183(6):1182–1191, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000355.

McMillan:2017:PMF

[McM17] Ben F. McMillan. A partially mesh-free scheme for representing anisotropic spatial variations along field lines. *Computer Physics Communications*, 212(??):39–46, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303101.

Munoz-Caro:2016:AJJ

[MCNRC16] Camelia Muñoz-Caro, Alfonso Niño, Sebastián Reyes, and Miriam Castillo. APINetworks Java. a Java approach to the efficient treatment of large-scale complex networks. *Computer Physics Communications*, 207(??):549–552, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302004.

Movilla:2010:DPA

[MCP10] J. L. Movilla, J. I. Climente, and J. Planelles. Dielectric polarization in axially-symmetric nanostructures: a computational approach. *Computer Physics Communications*, 181(1):92–98, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002847.

Mellet:2011:CIM

[MCP+11] N. Mellet, W. A. Cooper, P. Popovich, L. Villard, and S. Brunner. Convolution and iterative methods applied to low-frequency waves in 3D warm configurations. *Computer Physics Communications*, 182(3):570–589, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004108.

Madsen:2018:BPI

[MCV18] Georg K. H. Madsen, Jesús Carrete, and Matthieu J. Verstraete. BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. *Computer Physics Communications*, 231(??):140–145, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301632.

Ma:2015:NMM

[MCWJ15] Zu-Hui Ma, Weng Cho Chew, Yu Mao Wu, and Li Jun Jiang. A new multilevel method for electrostatic problems through hierarchical loop basis. *Computer Physics*

Communications, 189(??):99–105, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004354.

Martinez:2016:POS

[MCY+16] Jackelyn A. Martinez, Aleksandr Chernatynskiy, Dundar E. Yilmaz, Tao Liang, Susan B. Sinnott, and Simon R. Phillpot. Potential optimization software for materials (POSMat). *Computer Physics Communications*, 203(??):201–211, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300042.

Macias-Diaz:2010:SET

[MD10a] J. E. Macías-Díaz. On the simulation of the energy transmission in the forbidden band-gap of a spatially discrete double sine–Gordon system. *Computer Physics Communications*, 181(11):1842–1849, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002365.

Mohebbi:2010:HOS

[MD10b] Akbar Mohebbi and Mehdi Dehghan. High-order scheme for determination of a control parameter in an inverse problem from the over-specified data. *Computer Physics Communications*, 181(12):1947–1954, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003541.

Macias-Diaz:2011:SCP

[MD11a] J. E. Macías-Díaz. Sufficient conditions for the preservation of the boundedness in a numerical method for a physical model with transport memory and nonlinear damping. *Computer Physics Communications*, 182(12):2471–2478, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002438.

Miqueles:2011:CLR

[MD11b] Eduardo X. Miqueles and Alvaro R. De Pierro. C-library raft: Reconstruction algorithms for tomography. Applications to X-ray fluorescence tomography. *Computer Physics Communications*, 182(12):2661–2673, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002694.

Mahmoudinobar:2019:GCD

[MD19] Farbod Mahmoudinobar and Cristiano L. Dias. GRADE: a code to determine clathrate hydrate structures. *Computer Physics Communications*, 244(??):385–391, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301833.

Moritz:2011:TRN

[MDF11] B. Moritz, T. P. Devereaux, and J. K. Freericks. Temporal response of nonequilibrium correlated electrons. *Computer Physics Communications*, 182(1):109–111, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001748.

Maniopoulou:2012:IPP

[MDGC+12] Asimina Maniopoulou, Erlend R. M. Davidson, Ricardo Grau-Crespo, Aron Walsh, Ian J. Bush, C. Richard A. Catlow, and Scott M. Woodley. Introducing k-point parallelism into VASP. *Computer Physics Communications*, 183(8):1696–1701, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001142.

Macias-Diaz:2018:PEI

[MDHD18] J. E. Macías-Díaz, A. S. Hendy, and R. H. De Staelen. A pseudo energy-invariant method for relativistic wave equations with Riesz space-fractional derivatives. *Computer Physics Communications*, 224(??):98–107, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303910.

Mai-Duy:2015:IPS

[MDPTK15] N. Mai-Duy, N. Phan-Thien, and B. C. Khoo. Investigation of particles size effects in Dissipative Particle Dynamics (DPD) modelling of colloidal suspensions. *Computer Physics Communications*, 189(??):37–46, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004093.

Mai-Duy:2017:IPP

[MDPTTC17] N. Mai-Duy, N. Phan-Thien, and T. Tran-Cong. Imposition of physical parameters in dissipative particle dynamics. *Computer Physics Communications*, 221(??):290–298, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302874.

Ma:2016:SPC

[MDW16] Pui-Wai Ma, S. L. Dudarev, and C. H. Woo. SPILADY: a parallel CPU and GPU code for spin-lattice magnetic molecular dynamics simulations. *Computer Physics Communications*, 207(??):350–361, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301412.

Martinec:2018:SPS

[ME18] Zdenek Martinec and David Einspigel. SHAVEL: a program for the spherical harmonic analysis of a horizontal vector field sampled in an equiangular grid on a sphere. *Computer Physics Communications*, 233(??):206–214, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302236.

Maintz:2011:SPW

[MED11] Stefan Maintz, Bernhard Eck, and Richard Dronskowski. Speeding up plane-wave electronic-structure calculations using graphics-processing units. *Computer Physics Communications*, 182(7):1421–1427, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000889.

Mercado:2012:WAS

[MEG12] Ydalia Delgado Mercado, Hans Gerd Evertz, and Christof Gattringer. Worm algorithms for the 3-state Potts model with magnetic field and chemical potential. *Computer Physics Communications*, 183(9):1920–1927, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001531.

Meleshko:2019:CSC

[Mel19] Sergey V. Meleshko. Comment on 'Symbolic computation of equivalence transformations and parameter reduction for nonlinear physical models'. *Computer Physics Communications*, 239(??):14–15, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300451. See [Che17].

Mertmann:2011:FSO

[MEM+11] Philipp Mertmann, Denis Eremin, Thomas Mussenbrock, Ralf Peter Brinkmann, and Peter Awakowicz. Fine-sorting one-dimensional particle-in-cell algorithm with Monte–Carlo collisions on a graphics processing unit. *Computer Physics Communications*, 182(10):2161–2167, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001688.

Mendl:2011:FTF

[Men11] Christian B. Mendl. The FermiFab toolbox for fermionic many-particle quantum systems. *Computer Physics Communications*, 182(6):1327–1337, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100066X.

Meyer:2018:ATM

[Mey18] Christoph Meyer. Algorithmic transformation of multi-loop master integrals to a canonical basis with CANONICA. *Computer Physics Communications*, 222(??):295–312, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303016.

Matsuyama:2017:HOI

[MF17] Akinobu Matsuyama and Masaru Furukawa. High-order integration scheme for relativistic charged particle motion in magnetized plasmas with volume preserving properties. *Computer Physics Communications*, 220(??):285–296, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302473`.

Montoliu:2013:IEL

[MFG+13] C. Montoliu, N. Ferrando, M. A. Gosálvez, J. Cerdá, and R. J. Colom. Implementation and evaluation of the Level Set method: Towards efficient and accurate simulation of wet etching for microengineering applications. *Computer Physics Communications*, 184(10):2299–2309, October 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001768`.

Muller:2013:PLA

[MFH+13] Eike H. Müller, Rupert Ford, Matthew C. Hort, Lois Huggett, Graham Riley, and David J. Thomson. Parallelisation of the Lagrangian atmospheric dispersion model NAME. *Computer Physics Communications*, 184(12):2734–2745, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002476`.

Moran:2019:FIT

[MFLY19] J. Morán, A. Fuentes, F. Liu, and J. Yon. FracVAL: an improved tunable algorithm of cluster-cluster aggregation for generation of fractal structures formed by polydisperse primary particles. *Computer Physics Communications*, 239(??):225–237, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300323`.

Mena:2015:GAS

[MFM15] Andres Mena, Jose M. Ferrero, and Jose F. Rodriguez Matas. GPU accelerated solver for nonlinear reaction-diffusion systems. Application to the electrophysiology problem. *Computer Physics Communications*, 196(??):280–289, November

2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002635.

Martins:2010:NSL

[MFS+10a] Samuel F. Martins, Ricardo A. Fonseca, Luís O. Silva, Wei Lu, and Warren B. Mori. Numerical simulations of laser wakefield accelerators in optimal Lorentz frames. *Computer Physics Communications*, 181(5):869–875, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004159.

McConnell:2010:DNV

[MFS10b] Sean McConnell, Stephan Fritzsche, and Andrey Surzhykov. DIRAC: a new version of computer algebra tools for studying the properties and behavior of hydrogen-like ions. *Computer Physics Communications*, 181(3):711–713, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003853.

Muller:2010:GTE

[MG10a] Thomas Müller and Frank Grave. GeodesicViewer — a tool for exploring geodesics in the theory of relativity. *Computer Physics Communications*, 181(2):413–419, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003233.

Muller:2010:UVM

[MG10b] Thomas Müller and Frank Grave. An updated version of the Motion4D-library. *Computer Physics Communications*, 181(3):703, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003427.

Makkonen:2013:SDS

[MGA+13] T. Makkonen, M. Groth, M. I. Airila, R. Dux, A. Janzer, T. Kurki-Suonio, T. Lunt, H. W. Mueller, T. Puetterich, E. Viezzer, and ASDEX Upgrade team. Synthetic Doppler spectroscopy and curvilinear camera diagnostics in the ERO code. *Computer Physics Communications*, 184(8):1842–1847, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001045.

Meena:2018:PPP

[MGB18] Deep Raj Meena, Shridhar R. Gadre, and P. Balanarayan. PAREMD: a parallel program for the evaluation of momentum space properties of atoms and molecules. *Computer Physics Communications*, 224(??):299–310, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304010.

Mostaco-Guidolin:2012:SOS

[MGFRG12] Luiz C. Mostaço-Guidolin, Rafael B. Frigori, Leonid Ruchko, and Ricardo M. O. Galvão. SCTE: an open-source Perl framework for testing equipment control and data acquisition. *Computer Physics Communications*, 183(7):1511–1518, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000665.

Mickevicius:2013:RCF

[MGK13] S. Mickevicius, D. Germanas, and R. K. Kalinauskas. Revised calculation of four-particle harmonic-oscillator transformation brackets matrix. *Computer Physics Communications*, 184(2):409–413, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003074.

Marojevic:2013:EEG

[MGL13] Zelimir Marojević, Ertan Göklü, and Claus Lämmerzahl. Energy eigenfunctions of the 1D Gross–Pitaevskii equation. *Computer Physics Communications*, 184(8):1920–1930, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001318.

Marojevic:2016:APF

[MGL16] Zelimir Marojević, Ertan Göklü, and Claus Lämmerzahl. ATUS–PRO: a FEM-based solver for the time-dependent and stationary Gross–Pitaevskii equation. *Computer Physics Communications*, 202(??):216–232, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004427.

Masala:2013:IMC

[MGO13] G. L. Masala, B. Golosio, and P. Oliva. An improved Marching Cube algorithm for 3D data segmentation. *Computer Physics Communications*, 184(3):777–782, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003281.

Municchi:2016:HES

[MGR16] Federico Municchi, Christoph Goniva, and Stefan Radl. Highly efficient spatial data filtering in parallel using the opensource library CPPPO. *Computer Physics Communications*, 207(??):400–414, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301606.

Malcioglu:2011:TCS

[MGRB11] Osman Bariş Malcioğlu, Ralph Gebauer, Dario Rocca, and Stefano Baroni. turboTDDFT — a code for the simulation of molecular spectra using the Liouville–Lanczos approach to time-dependent density-functional perturbation theory. *Computer Physics Communications*, 182(8):1744–1754, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001512.

Mercado:2013:SWA

[MGS13] Ydalia Delgado Mercado, Christof Gattringer, and Alexander Schmidt. Surface worm algorithm for abelian Gauge–Higgs systems on the lattice. *Computer Physics Communications*, 184(6):1535–1546, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000398.

Melchert:2011:DAC

[MH11] O. Melchert and A. K. Hartmann. A dedicated algorithm for calculating ground states for the triangular random bond Ising model. *Computer Physics Communications*, 182(9):1828–1832, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004315.

Mei:2018:RLC

[MH18] Lijie Mei and Li Huang. Reliability of Lyapunov characteristic exponents computed by the two-particle method. *Computer Physics Communications*, 224(??):108–118, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303909.

Mahmoudi:2012:FHA

[MHA+12] F. Mahmoudi, S. Heinemeyer, A. Arbey, A. Bharucha, T. Goto, T. Hahn, U. Haisch, S. Kraml, M. Muhlleitner, J. Reuter, P. Skands, and P. Slavich. Flavour Les Houches Accord: Interfacing flavour related codes. *Computer Physics Communications*, 183(2):285–298, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003341.

Ma:2011:MCH

[MHHL11] Tianxing Ma, Feiming Hu, Zhongbing Huang, and Hai-Qing Lin. Magnetic correlation in the Hubbard model on a honeycomb lattice. *Computer Physics Communications*, 182(1):52–54, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002298.

Mick:2013:GAG

[MHR+13] Jason Mick, Eyad Hailat, Vincent Russo, Kamel Rushaidat, Loren Schwiebert, and Jeffrey Potoff. GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. *Computer Physics Communications*, 184(12): 2662–2669, December 2013. CODEN CPHCBZ. ISSN 0010-

4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002270.

Maldonis:2017:FHS

[MHV17] Jason J. Maldonis, Jinwoo Hwang, and Paul M. Voyles. FEMSIM + HRMC: Simulation of and structural refinement using fluctuation electron microscopy for amorphous materials. *Computer Physics Communications*, 213(??):217–222, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630385X.

Mei:2019:SAE

[MHWH19] Lijie Mei, Li Huang, Xinyuan Wu, and Shixiang Huang. Semi-analytical exponential RKN integrators for efficiently solving high-dimensional nonlinear wave equations based on FFT techniques. *Computer Physics Communications*, 243(??):68–80, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301341.

Maeshima:2012:PRM

[MiH12] Nobuya Maeshima and Ken ichi Hino. Parallelization of the R-matrix propagation method for the study of intense-laser-driven semiconductor superlattices. *Computer Physics Communications*, 183(1):8–14, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002712.

Militzer:2016:CHT

[Mil16] B. Militzer. Computation of the high temperature Coulomb density matrix in periodic boundary conditions. *Computer Physics Communications*, 204(??):88–96, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300698.

Miszczak:2012:GUT

[Mis12] Jarosław Adam Miszczak. Generating and using truly random quantum states in Mathematica. *Computer Physics Communications*, 183(1):118–124, January 2012. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002748.

Miszczak:2013:EOQ

[Mis13] Jaroslaw Adam Miszczak. Employing online quantum random number generators for generating truly random quantum states in Mathematica. *Computer Physics Communications*, 184(1):257–258, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002780.

Miura:2011:VPI

[Miu11] Shinichi Miura. A variational path integral molecular dynamics study of a solid helium-4. *Computer Physics Communications*, 182(1):274–276, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002596.

Maeyama:2012:HMS

[MIW+12] S. Maeyama, A. Ishizawa, T.-H. Watanabe, N. Nakajima, S. Tsuji-Iio, and H. Tsutsui. A hybrid method of semi-Lagrangian and additive semi-implicit Runge–Kutta schemes for gyrokinetic Vlasov simulations. *Computer Physics Communications*, 183(9):1986–1992, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001683.

Maeyama:2013:NTP

[MIW+13] S. Maeyama, A. Ishizawa, T.-H. Watanabe, N. Nakajima, S. Tsuji-Iio, and H. Tsutsui. Numerical techniques for parallel dynamics in electromagnetic gyrokinetic Vlasov simulations. *Computer Physics Communications*, 184(11):2462–2473, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002087.

Miyatake:2015:DEP

[Miy15] Yuto Miyatake. A derivation of energy-preserving exponentially-fitted integrators for Poisson systems. *Computer Physics Communications*, 187(??):156–161, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003737.

McMillan:2010:RFS

[MJB+10] B. F. McMillan, S. Jolliet, A. Bottino, P. Angelino, T. M. Tran, and L. Villard. Rapid Fourier space solution of linear partial integro-differential equations in toroidal magnetic confinement geometries. *Computer Physics Communications*, 181(4):715–719, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003920.

Moddel:2011:AFP

[MJB11] Monika Möddel, Wolfhard Janke, and Michael Bachmann. Adsorption of finite polymers in different thermodynamic ensembles. *Computer Physics Communications*, 182(9):1961–1965, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004959.

Munoz:2018:NHC

[MJKB18] P. A. Muñoz, N. Jain, P. Kilian, and J. Büchner. A new hybrid code (CHIEF) implementing the inertial electron fluid equation without approximation. *Computer Physics Communications*, 224(??):245–264, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303521.

Mierzwiczak:2010:AMF

[MK10] Magdalena Mierzwiczak and Jan Adam Kolodziej. Application of the method of fundamental solutions and radial basis functions for inverse transient heat source problem. *Computer Physics Communications*, 181(12):2035–2043, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003115.

Morita:2019:CHO

[MK19] Satoshi Morita and Naoki Kawashima. Calculation of higher-order moments by higher-order tensor renormalization group. *Computer Physics Communications*, 236(??):65–71, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830362X.

Morozov:2011:MDS

[MKB+11] I. V. Morozov, A. M. Kazennov, R. G. Bystryi, G. E. Norman, V. V. Pisarev, and V. V. Stegailov. Molecular dynamics simulations of the relaxation processes in the condensed matter on GPUs. *Computer Physics Communications*, 182(9):1974–1978, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005199.

Makwana:2017:TWC

[MKL17] K. D. Makwana, R. Keppens, and G. Lapenta. Two-way coupling of magnetohydrodynamic simulations with embedded particle-in-cell simulations. *Computer Physics Communications*, 221(??):81–94, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302461.

Manka-Krason:2010:CRL

[MKMK10] Anna Mańka-Krasoń, Advera Mwijage, and Krzysztof Kulakowski. Clustering in random line graphs. *Computer Physics Communications*, 181(1):118–121, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003002.

Merz:2012:MDG

[MKR+12] F. Merz, C. Kowitz, E. Romero, J. E. Roman, and F. Jenko. Multi-dimensional gyrokinetic parameter studies based on eigenvalue computations. *Computer Physics Communications*, 183(4):922–930, April 2012. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004061.

Monovasilis:2010:SPR

[MKS10] Th. Monovasilis, Z. Kalogiratou, and T. E. Simos. Symplectic partitioned Runge–Kutta methods with minimal phase-lag. *Computer Physics Communications*, 181(7):1251–1254, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000937.

Matsumoto:2012:ATV

[MKU+12] Masaharu Matsumoto, Yoshihiro Kajimura, Hideyuki Usui, Ikkoh Funaki, and Iku Shinohara. Application of a total variation diminishing scheme to electromagnetic hybrid particle-in-cell plasma simulation. *Computer Physics Communications*, 183(10):2027–2034, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001609.

Moran:2011:DQO

[MKV11] Niall Moran, Graham Kells, and Jiri Vala. Diagonalisation of quantum observables on regular lattices and general graphs. *Computer Physics Communications*, 182(4):1083–1092, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000099.

Melazzi:2014:ASV

[ML14] D. Melazzi and V. Lancellotti. ADAMANT: a surface and volume integral-equation solver for the analysis and design of helicon plasma sources. *Computer Physics Communications*, 185(7):1914–1925, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400099X.

Mortensen:2016:HPP

[ML16] Mikael Mortensen and Hans Petter Langtangen. High performance Python for direct numerical simulations of turbulent flows. *Computer Physics Communications*, 203(??):53–

65, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300200.

Marx:2017:HPX

[ML17] Alain Marx and Hinrich Lütjens. Hybrid parallelization of the XTOR-2F code for the simulation of two-fluid MHD instabilities in tokamaks. *Computer Physics Communications*, 212(??):90–99, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303332.

Mennemann:2019:OCS

[MLEM19] J.-F. Mennemann, T. Langen, L. Exl, and N. J. Mauser. Optimal control of the self-bound dipolar droplet formation process. *Computer Physics Communications*, 244(??):205–216, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301808.

Markosyan:2014:PTF

[MLGVE14] A. H. Markosyan, A. Luque, F. J. Gordillo-Vázquez, and U. Ebert. PumpKin: a tool to find principal pathways in plasma chemical models. *Computer Physics Communications*, 185(10):2697–2702, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001842.

Mosyagin:2017:ICP

[MLK+17] I. Mosyagin, A. V. Lugovskoy, O. M. Krasilnikov, Yu. Kh. Vekilov, S. I. Simak, and I. A. Abrikosov. Ab initio calculations of pressure-dependence of high-order elastic constants using finite deformations approach. *Computer Physics Communications*, 220(??):20–30, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730190X. See comment [Maź19] and reply [MLK+19].

Mosyagin:2019:RCM

[MLK+19] I. Mosyagin, A. V. Lugovskoy, O. M. Krasilnikov, Yu. Kh. Vekilov, S. I. Simak, and I. A. Abrikosov. Reply to the comment by M. Maździarz on the article "Ab initio calculations of pressure-dependence of high-order elastic constants using finite deformations approach" [Computer Physics Communications **220** (2017) 20–30]. *Computer Physics Communications*, 235(??):295–296, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302157`. See [MLK+17, Maź19].

Manuali:2010:GGF

[MLR10] C. Manuali, A. Laganà, and S. Rampino. GriF: a Grid framework for a Web service approach to reactive scattering. *Computer Physics Communications*, 181(7):1179–1185, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000810`.

Meier:2010:SES

[MLS10] E. T. Meier, V. S. Lukin, and U. Shumlak. Spectral element spatial discretization error in solving highly anisotropic heat conduction equation. *Computer Physics Communications*, 181(5):837–841, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046550900410X`.

Marmier:2010:ECP

[MLW+10] Arnaud Marmier, Zoe A. D. Lethbridge, Richard I. Walton, Christopher W. Smith, Stephen C. Parker, and Kenneth E. Evans. ElAM: a computer program for the analysis and representation of anisotropic elastic properties. *Computer Physics Communications*, 181(12):2102–2115, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003401`.

Mokhtari:2010:NSG

[MM10] Reza Mokhtari and Maryam Mohammadi. Numerical solution of GRLW equation using sinc-collocation method.

Computer Physics Communications, 181(7):1266–1274, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000950.

Morhac:2011:ESM

[MM11] Miroslav Morhác and Vladislav Matousek. Event sorting methods of γ-ray spectroscopic data. *Computer Physics Communications*, 182(3):600–610, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004479.

Mokhtari:2012:MMS

[MM12] Reza Mokhtari and Majid Mohseni. A meshless method for solving mKdV equation. *Computer Physics Communications*, 183(6):1259–1268, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000598.

Mangiardi:2017:HAP

[MM17] Chris M. Mangiardi and R. Meyer. A hybrid algorithm for parallel molecular dynamics simulations. *Computer Physics Communications*, 219(??):196–208, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301625.

Minoshima:2015:FVF

[MMA15] Takashi Minoshima, Yosuke Matsumoto, and Takanobu Amano. A finite volume formulation of the multi-moment advection scheme for Vlasov simulations of magnetized plasma. *Computer Physics Communications*, 187(??):137–151, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003695.

Mazzeo:2010:SRT

[MMC10] Marco D. Mazzeo, Steven Manos, and Peter V. Coveney. In situ ray tracing and computational steering for interactive blood flow simulation. *Computer Physics Communications*, 181(2):355–370, February 2010. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003269.

Makarashvili:2017:PAE

[MMO+17] Vakhtang Makarashvili, Elia Merzari, Aleksandr Obabko, Andrew Siegel, and Paul Fischer. A performance analysis of ensemble averaging for high fidelity turbulence simulations at the strong scaling limit. *Computer Physics Communications*, 219(??):236–245, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301650.

Ma:2015:QWQ

[MMSF+15] Changru Ma, Layla Martin-Samos, Stefano Fabris, Alessandro Laio, and Simone Piccinin. QMMMW: a wrapper for QM/MM simulations with Quantum ESPRESSO and LAMMPS. *Computer Physics Communications*, 195(??):191–198, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001678.

Meres:2011:GHP

[MMT+11] Michal Meres, Ivan Melo, Boris Tomásik, Vladimír Balek, and Vladimír Cerný. Generating heavy particles with energy and momentum conservation. *Computer Physics Communications*, 182(12):2561–2566, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002384.

Misawa:2019:MOS

[MMY+19] Takahiro Misawa, Satoshi Morita, Kazuyoshi Yoshimi, Mitsuaki Kawamura, Yuichi Motoyama, Kota Ido, Takahiro Ohgoe, Masatoshi Imada, and Takeo Kato. mVMC-open-source software for many-variable variational Monte Carlo method. *Computer Physics Communications*, 235(??):447–462, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303102.

Mohankumar:2010:IVI

[MN10] N. Mohankumar and A. Natarajan. On an interesting variant of the IMT quadrature. *Computer Physics Communications*, 181(5):842–847, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004111.

Mohankumar:2016:VAN

[MN16] N. Mohankumar and A. Natarajan. On the very accurate numerical evaluation of the Generalized Fermi–Dirac Integrals. *Computer Physics Communications*, 207(??):193–201, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301667.

Mentrelli:2018:APS

[MN18] Andrea Mentrelli and Claudia Negulescu. Asymptotic-preserving scheme for a strongly anisotropic vorticity equation arising in fusion plasma modeling. *Computer Physics Communications*, 229(??):116–128, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301048.

Moreno:2015:CMR

[MNC15] Nicolas Moreno, Suzana P. Nunes, and Victor M. Calo. Consistent model reduction of polymer chains in solution in dissipative particle dynamics: Model description. *Computer Physics Communications*, 196(??):255–266, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500257X.

Mirzoev:2019:MVI

[MNL19] Alexander Mirzoev, Lars Nordenskiöld, and Alexander Lyubartsev. Magic v.3: an integrated software package for systematic structure-based coarse-graining. *Computer Physics Communications*, 237(??):263–273, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304107.

Mushtaq:2011:VHP

[MNOØ11] Asif Mushtaq, Amna Noreen, Kåre Olaussen, and Ingjald Øverbø. Very-high-precision solutions of a class of Schrödinger type equations. *Computer Physics Communications*, 182(9):1810–1813, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000026.

Mirza:2017:TDI

[MNPF17] A. Mirza, P. Nizenkov, M. Pfeiffer, and S. Fasoulas. Three-dimensional implementation of the Low Diffusion method for continuum flow simulations. *Computer Physics Communications*, 220(??):269–278, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302382.

Morris:2014:OTO

[MNPY14] Andrew J. Morris, Rebecca J. Nicholls, Chris J. Pickard, and Jonathan R. Yates. OptaDOS: a tool for obtaining density of states, core-level and optical spectra from electronic structure codes. *Computer Physics Communications*, 185(5):1477–1485, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000460.

McBride:2013:CPE

[MNV13] Carl McBride, Eva G. Noya, and Carlos Vega. A computer program to evaluate the NVM propagator for rigid asymmetric tops for use in path integral simulations of rigid bodies. *Computer Physics Communications*, 184(3):885–890, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003682.

Michielsen:2017:BGB

[MNW+17] Kristel Michielsen, Madita Nocon, Dennis Willsch, Fengping Jin, Thomas Lippert, and Hans De Raedt. Benchmarking gate-based quantum computers. *Computer Physics Communications*, 220(??):44–55, November 2017. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301935.

Mushtaq:2014:ACG

[MO14] Asif Mushtaq and Kåre Olaussen. Automatic code generator for higher order integrators. *Computer Physics Communications*, 185(5):1461–1472, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000253.

Marques:2012:LLE

[MOB12] Miguel A. L. Marques, Micael J. T. Oliveira, and Tobias Burnus. Libxc: a library of exchange and correlation functionals for density functional theory. *Computer Physics Communications*, 183(10):2272–2281, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001750.

Mackay:2013:HFI

[MOD13] F. E. Mackay, S. T. T. Ollila, and C. Denniston. Hydrodynamic forces implemented into LAMMPS through a lattice-Boltzmann fluid. *Computer Physics Communications*, 184(8):2021–2031, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300132X.

Mohammadi:2014:ESS

[Moh14] Reza Mohammadi. An exponential spline solution of nonlinear Schrödinger equations with constant and variable coefficients. *Computer Physics Communications*, 185(3):917–932, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300427X.

Mao:2011:ERM

[MP11] Albert H. Mao and Rohit V. Pappu. Exact recording of Metropolis–Hastings-class Monte Carlo simulations using one bit per sample. *Computer Physics Communications*, 182(7):1452–1454, July 2011. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000919`.

Menz:2010:TIT

[MPB10] William J. Menz, Matthew J. Penna, and Mark J. Biggs. TNAMD: Implementation of TIGER2 in NAMD. *Computer Physics Communications*, 181(12):2082–2085, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003565`.

McClure:2014:NHA

[MPM14] J. E. McClure, J. F. Prins, and C. T. Miller. A novel heterogeneous algorithm to simulate multiphase flow in porous media on multicore CPU–GPU systems. *Computer Physics Communications*, 185(7):1865–1874, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000927`.

Marchand:2013:LPC

[MPS13] R. Marchand, D. Purschke, and J. Samson. LEOrbit: a program to calculate parameters relevant to modeling Low Earth Orbit spacecraft-plasma interaction. *Computer Physics Communications*, 184(3):866–872, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003645`.

Miqueles:2015:GIX

[MPSV15] Eduardo X. Miqueles, Carlos A. Pérez, Vanessa I. Suárez, and Rafael F. C. Vescovi. Grazing-incidence XRF analysis of layered samples: Detailed study of amplitude calculation. *Computer Physics Communications*, 194(??):33–42, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551500140X`.

Mohankumar:2013:SCE

[MR13] N. Mohankumar and Ajay Rawat. Some comments on the evaluation of the Chandrasekhar H function. *Computer*

Physics Communications, 184(3):579–581, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200344X.

Mawson:2014:MTO

[MR14] Mark J. Mawson and Alistair J. Revell. Memory transfer optimization for a lattice Boltzmann solver on Kepler architecture nVidia GPUs. *Computer Physics Communications*, 185(10):2566–2574, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002070.

Malagon-Romero:2018:DDM

[MRL18] A. Malagón-Romero and A. Luque. A domain-decomposition method to implement electrostatic free boundary conditions in the radial direction for electric discharges. *Computer Physics Communications*, 225(??):114–121, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300067.

Mukha:2019:LWM

[MRL19] T. Mukha, S. Rezaeiravesh, and M. Liefvendahl. A library for wall-modelled large-eddy simulation based on OpenFOAM technology. *Computer Physics Communications*, 239(??):204–224, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300335.

Mokos:2015:MPS

[MRSD15] Athanasios Mokos, Benedict D. Rogers, Peter K. Stansby, and José M. Domínguez. Multi-phase SPH modelling of violent hydrodynamics on GPUs. *Computer Physics Communications*, 196(??):304–316, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002659.

Maruhn:2014:TCS

[MRSU14] J. A. Maruhn, P.-G. Reinhard, P. D. Stevenson, and A. S. Umar. The TDHF code Sky3D. *Computer Physics*

Communications, 185(7):2195–2216, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001313.

Mayrhofer:2013:IWB

[MRVF13] Arno Mayrhofer, Benedict D. Rogers, Damien Violeau, and Martin Ferrand. Investigation of wall bounded flows using SPH and the unified semi-analytical wall boundary conditions. *Computer Physics Communications*, 184 (11):2515–2527, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002324.

Mazzeo:2010:LNL

[MRZ10] M. D. Mazzeo, M. Ricci, and C. Zannoni. The Linked Neighbour List (LNL) method for fast off-lattice Monte Carlo simulations of fluids. *Computer Physics Communications*, 181(3):569–581, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003543.

Menshutin:2011:MDD

[MS11] A. Yu. Menshutin and L. N. Shchur. Morphological diagram of diffusion driven aggregate growth in plane: Competition of anisotropy and adhesion. *Computer Physics Communications*, 182(9):1819–1823, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004297.

Matsuoka:2014:AIC

[MS14] Seikichi Matsuoka and Shinsuke Satake. Application of an improved control-variate scheme to local neoclassical transport simulations. *Computer Physics Communications*, 185(9):2313–2321, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001544.

Mohankumar:2015:SRR

[MS15] N. Mohankumar and Soubhadra Sen. Some remarks regarding a modified Gauss–Legendre scheme. *Computer Physics Communications*, 197(??):182–184, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003343.

Munejiri:2011:RSI

[MSH11] Shuji Munejiri, Fuyuki Shimojo, and Kozo Hoshino. Real-space investigation of a transverse wave in a liquid system generated by a molecular-dynamics simulation. *Computer Physics Communications*, 182(1):58–61, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003206.

Munoz-Santiburcio:2017:ACC

[MSHL17] Daniel Muñoz-Santiburcio and Alfonso Hernández-Laguna. AWESoMe 1.1: a code for the calculation of phase and group velocities of acoustic waves in homogeneous solids. *Computer Physics Communications*, 217(??):212–214, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301030.

Munoz-Santiburcio:2015:ACC

[MSHLS15] Daniel Muñoz-Santiburcio, Alfonso Hernández-Laguna, and Juan I. Soto. AWESoMe: a code for the calculation of phase and group velocities of acoustic waves in homogeneous solids. *Computer Physics Communications*, 192(??):272–277, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500082X.

Masuda:2010:SPC

[MSI+10] Nobuyuki Masuda, Takashige Sugie, Tomoyoshi Ito, Shinjiro Tanaka, Yu Hamada, Shin ichi Satake, Tomoaki Kunugi, and Kazuho Sato. Special purpose computer system with highly parallel pipelines for flow visualization using holography technology. *Computer Physics Communications*, 181(12):1986–1989, December 2010. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003474.

Muller:2011:KFA

[MSM+11] Joachim Müller, Sven Simon, Uwe Motschmann, Josef Schüle, Karl-Heinz Glassmeier, and Gavin J. Pringle. A.I.K.E.F.: Adaptive hybrid model for space plasma simulations. *Computer Physics Communications*, 182(4):946–966, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005266.

Molnar:2010:APM

[MSML10] F. Molnár, Jr., T. Szakály, R. Mészáros, and I. Lagzi. Air pollution modelling using a Graphics Processing Unit with CUDA. *Computer Physics Communications*, 181(1): 105–112, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002872.

Milenkovic:2011:CPN

[MSNI11] B. Milenkovic, N. Stevanovic, D. Nikezic, and M. Ivanovic. Computer program Neutron_CR-39 for simulation of neutrons from an Am–Be source and calculation of proton track profiles. *Computer Physics Communications*, 182(7):1536–1542, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001172.

Mayer:2012:NME

[MSPD12] Andreas Mayer, Hanna Salopaasi, Katariina Pussi, and Renee D. Diehl. A novel method for the extraction of intensity-energy spectra from low-energy electron diffraction patterns. *Computer Physics Communications*, 183(7):1443–1447, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000811.

Mohankumar:2010:ECT

[MSR10] N. Mohankumar, S. Sen, and R. Ramar. On the evaluation of correction terms in Gauss–Legendre quadrature. *Computer*

Physics Communications, 181(1):17–20, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002422.

Moreno:2017:SVM

[MSR+17] Javier Moreno, Álvaro Somolinos, Gustavo Romero, Iván González, and Felipe Cátedra. Speed-up of the volumetric method of moments for the approximate RCS of large arbitrary-shaped dielectric targets. *Computer Physics Communications*, 217(??):35–42, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301054.

Mondragon-Shem:2010:ECC

[MSRL10] Ian Mondragon-Shem, Boris A. Rodríguez, and Francisco E. López. Efficient calculation of Coulomb matrix elements for bilayers of confined charge carriers with arbitrary spatial separation. *Computer Physics Communications*, 181(9):1510–1516, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001414.

Murano:2014:FCC

[MSS+14] Koki Murano, Tomoyoshi Shimobaba, Atsushi Sugiyama, Naoki Takada, Takashi Kakue, Minoru Oikawa, and Tomoyoshi Ito. Fast computation of computer-generated hologram using Xeon Phi coprocessor. *Computer Physics Communications*, 185(10):2742–2757, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002148.

Mi:2016:ARS

[MSS+16] Wenhui Mi, Xuecheng Shao, Chuanxun Su, Yuanyuan Zhou, Shoutao Zhang, Quan Li, Hui Wang, Lijun Zhang, Maosheng Miao, Yanchao Wang, and Yanming Ma. ATLAS: a real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, 200(??):87–95, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465515004154.

Matveev:2018:AAM

[MST+18] S. A. Matveev, V. I. Stadnichuk, E. E. Tyrtyshnikov, A. P. Smirnov, N. V. Ampilogova, and N. V. Brilliantov. Anderson acceleration method of finding steady-state particle size distribution for a wide class of aggregation-fragmentation models. *Computer Physics Communications*, 224(??):154–163, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303727.

Meyer:2011:SFD

[MSZW11] H. Meyer, N. Schulmann, J. E. Zabel, and J. P. Wittmer. The structure factor of dense two-dimensional polymer solutions. *Computer Physics Communications*, 182(9):1949–1953, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004741.

Madarassy:2013:NSC

[MT13] Enikö J. M. Madarassy and Viktor T. Toth. Numerical simulation code for self-gravitating Bose–Einstein condensates. *Computer Physics Communications*, 184(4):1339–1343, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004304.

Marcantoni:2017:ROS

[MTE17] L. F. Gutiérrez Marcantoni, J. Tamagno, and S. Elaskar. rhoCentralRfFoam: an OpenFOAM solver for high speed chemically active flows — simulation of planar detonations. *Computer Physics Communications*, 219(??):209–222, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301637.

Miki:2013:HSI

[MTM13] Yohei Miki, Daisuke Takahashi, and Masao Mori. Highly scalable implementation of an N-body code on a GPU cluster. *Computer Physics Communications*, 184(9):2159–2168, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551300146X`.

Marushchenko:2014:RTC

[MTM14] N. B. Marushchenko, Y. Turkin, and H. Maassberg. Ray-tracing code TRAVIS for ECR heating, EC current drive and ECE diagnostic. *Computer Physics Communications*, 185(1):165–176, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003032`.

Moon:2015:ECC

[MTO15] Haksu Moon, Fernando L. Teixeira, and Yuri A. Omelchenko. Exact charge-conserving scatter-gather algorithm for particle-in-cell simulations on unstructured grids: a geometric perspective. *Computer Physics Communications*, 194(??):43–53, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001460`.

Maras:2016:GTP

[MTS+16] E. Maras, O. Trushin, A. Stukowski, T. Ala-Nissila, and H. Jónsson. Global transition path search for dislocation formation in Ge on Si(001). *Computer Physics Communications*, 205(??):13–21, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300893`.

Matsumoto:2011:MDS

[MTSI11] Shigenori Matsumoto, Fumiko Takagi, Takashi Shimada, and Nobuyasu Ito. Molecular dynamics simulation of ribosome jam. *Computer Physics Communications*, 182(9):1958–1960, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004819`.

Muller:2011:GTE

[Mül11a] Thomas Müller. GeodesicViewer — a tool for exploring geodesics in the theory of relativity. *Computer Physics Communications*, 182(6):1382–1383, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465511000683.

Muller:2011:MLE

[Mül11b] Thomas Müller. Motion4D-library extended. *Computer Physics Communications*, 182(6):1386–1388, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000713.

Muller:2014:GRR

[Mül14a] Thomas Müller. GeoViS — relativistic ray tracing in four-dimensional spacetimes. *Computer Physics Communications*, 185(8):2301–2308, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001362.

Muller:2014:MLE

[Mül14b] Thomas Müller. Motion4D-library extended. *Computer Physics Communications*, 185(10):2798–2799, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001568.

Muller:2014:MMP

[Mül14c] Thomas Müller. MPPhys — a many-particle simulation package for computational physics education. *Computer Physics Communications*, 185(3):1100–1108, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004116.

Murakami:2014:SST

[Mur14] Brandon Murakami. SuperLFV: an SLHA tool for lepton flavor violating observables in supersymmetric models. *Computer Physics Communications*, 185(2):622–637, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003287.

Maierhofer:2018:KFI

[MUU18] P. Maierhöfer, J. Usovitsch, and P. Uwer. Kira — a Feynman integral reduction program. *Computer Physics Communications*, 230(??):99–112, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301279.

Morozov:2011:ADW

[MV11] I. V. Morozov and I. A. Valuev. Automatic distributed workflow generation with GridMD library. *Computer Physics Communications*, 182(9):2052–2058, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000257.

Meylan:2016:GDS

[MVI+16] S. Meylan, U. Vimont, S. Incerti, I. Clairand, and C. Villagrasa. Geant4-DNA simulations using complex DNA geometries generated by the DnaFabric tool. *Computer Physics Communications*, 204(??):159–169, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300340.

Mortensen:2015:OHL

[MVS15] Mikael Mortensen and Kristian Valen-Sendstad. Oasis: a high-level/high-performance open source Navier–Stokes solver. *Computer Physics Communications*, 188(??):177–188, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003786.

Magierski:2012:LLI

[MW12] Piotr Magierski and Gabriel Wlazlowski. LINPRO: Linear inverse problem library for data contaminated by statistical noise. *Computer Physics Communications*, 183(10):2264–2271, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001737.

Michel:2014:SBM

[MW14] Kyle Jay Michel and C. Wolverton. Symmetry building Monte Carlo-based crystal structure prediction. *Computer Physics Communications*, 185(5):1389–1393, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000289.

Maynard:2019:MPA

[MW19] C. M. Maynard and D. N. Walters. Mixed-precision arithmetic in the ENDGame dynamical core of the Unified Model, a numerical weather prediction and climate model code. *Computer Physics Communications*, 244(??):69–75, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302127.

Miao:2014:PMP

[MWCY14] Qian Miao, Yunhu Wang, Yong Chen, and Yunqing Yang. PDEBellII: a Maple package for finding bilinear forms, bilinear Bäcklund transformations, Lax pairs and conservation laws of the KdV-type equations. *Computer Physics Communications*, 185(1):357–367, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003068.

Maeyama:2019:IGC

[MWI+19] S. Maeyama, T.-H. Watanabe, Y. Idomura, M. Nakata, and M. Nunami. Implementation of a gyrokinetic collision operator with an implicit time integration scheme and its computational performance. *Computer Physics Communications*, 235(??):9–15, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302728.

Moscicki:2010:LQT

[MWL+10] Jakub T. Mościcki, Maciej Woś, Massimo Lamanna, Philippe de Forcrand, and Owe Philipsen. Lattice QCD thermodynamics on the Grid. *Computer Physics Communications*, 181(10):1715–1726, October 2010. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002043.

Mostofi:2014:UVW

[MYP+14] Arash A. Mostofi, Jonathan R. Yates, Giovanni Pizzi, Young-Su Lee, Ivo Souza, David Vanderbilt, and Nicola Marzari. An updated version of wannier90: a tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, 185(8):2309–2310, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400157X.

Marquard:2014:SMI

[MZ14] Peter Marquard and Nikolai Zerf. SLAM, a Mathematica interface for SUSY spectrum generators. *Computer Physics Communications*, 185(3):1153–1171, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004177.

Mikram:2013:PCP

[MZE13] J. Mikram, F. Zinoun, and A. El Abdllaoui. POINCARÉ CODE: a package of open-source implements for normalization and computer algebra reduction near equilibria of coupled ordinary differential equations. *Computer Physics Communications*, 184(9):2204–2213, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001380.

Zhao:2015:ASE

[mZfXL15] Xiao mei Zhao, Dong fan Xie, and Qi Li. Approaching system equilibrium with accurate or not accurate feedback information in a two-route system. *Computer Physics Communications*, 187(??):106–114, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003543.

Nisar:2016:SSB

[NAQ16] Ubaid Ahmed Nisar, Waqas Ashraf, and Shamsul Qamar. A splitting scheme based on the space–time CE/SE method for solving multi-dimensional hydrodynamical models of semiconductor devices. *Computer Physics Communications*, 205(??):69–86, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301023.

Nath:2009:TVI

[Nat09] S. Nath. TERS v2.0: An improved version of TERS. *Computer Physics Communications*, 180(11):2392–2393, November 2009. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002069. See erratum [Nat10].

Nath:2010:ETV

[Nat10] S. Nath. Erratum to "TERS v2.0: An improved version of TERS" [Comput. Phys. Commun. **180** (2009) 2392]. *Computer Physics Communications*, 181(9):1659, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000202X. See [Nat09].

Nazarov:2012:AMM

[Naz12] Anton Nazarov. `Affine.m` — Mathematica package for computations in representation theory of finite-dimensional and affine Lie algebras. *Computer Physics Communications*, 183(11):2480–2493, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002263.

Neumann:2017:MTM

[NB17] Philipp Neumann and Xin Bian. MaMiCo: Transient multi-instance molecular-continuum flow simulation on supercomputers. *Computer Physics Communications*, 220(??):390–402, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302369.

Niess:2018:BMC

[NBCL18] Valentin Niess, Anne Barnoud, Cristina Cârloganu, and Eve Le Ménédeu. Backward Monte-Carlo applied to muon transport. *Computer Physics Communications*, 229(??):54–67, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300997.

Nakano:2015:FSS

[NBM+15] C. Masato Nakano, Hye Suk Byun, Heng Ma, Tao Wei, and Mohamed Y. El-Naggar. A framework for stochastic simulations and visualization of biological electron-transfer dynamics. *Computer Physics Communications*, 193(??):1–9, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001083.

Nemes:2014:DMR

[NBN+14] Csaba Nemes, Gergely Barcza, Zoltán Nagy, Örs Legeza, and Péter Szolgay. The density matrix renormalization group algorithm on kilo-processor architectures: Implementation and trade-offs. *Computer Physics Communications*, 185(6):1570–1581, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000654.

Needham:2016:EAM

[NBW16] Perri J. Needham, Ashraf Bhuiyan, and Ross C. Walker. Extension of the AMBER molecular dynamics software to Intel's Many Integrated Core (MIC) architecture. *Computer Physics Communications*, 201(??):95–105, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000060.

Nikfarjam:2018:LSI

[NCB18] F. Nikfarjam, Y. Cheny, and O. Botella. The LS-STAG immersed boundary/cut-cell method for non-Newtonian flows in 3D extruded geometries. *Computer Physics Communications*, 226(??):67–80, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300109.

Navarro:2015:PFT

[NCHN15] Cristobal A. Navarro, Fabrizio Canfora, Nancy Hitschfeld, and Gonzalo Navarro. Parallel family trees for transfer matrices in the Potts model. *Computer Physics Communications*, 187(??):55–71, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003464.

Niemeyer:2017:PAJ

[NCS17] Kyle E. Niemeyer, Nicholas J. Curtis, and Chih-Jen Sung. pyJac: Analytical Jacobian generator for chemical kinetics. *Computer Physics Communications*, 215(??):188–203, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300462.

Nellis:2018:FPR

[NDSH18] Chris Nellis, Thomas Danielson, Aditya Savara, and Celine Hin. The F-t-Pj-RG method: an adjacent-rolling-windows based steady-state detection technique for application to kinetic Monte Carlo simulations. *Computer Physics Communications*, 232(??):124–138, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301760.

Nemura:2016:IDE

[Nem16] Hidekatsu Nemura. Instructive discussion of an effective block algorithm for baryon–baryon correlators. *Computer Physics Communications*, 207(??):91–104, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301382.

Nedjalkov:2018:SAS

[NEW+18] Mihail Nedjalkov, Paul Ellinghaus, Josef Weinbub, Toufik Sadi, Asen Asenov, Ivan Dimov, and Siegfried Selberherr. Stochastic analysis of surface roughness models in quantum wires. *Computer Physics Communications*, 228(??):30–37, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300821.

Neumann:2016:MSD

[NFA+16] Philipp Neumann, Hanno Flohr, Rahul Arora, Piet Jarmatz, Nikola Tchipev, and Hans-Joachim Bungartz. MaMiCo: Software design for parallel molecular-continuum flow simulations. *Computer Physics Communications*, 200(??): 324–335, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004129.

Nezamabadi:2019:PIC

[NFD+19] Saeid Nezamabadi, Xavier Frank, Jean-Yves Delenne, Julien Averseng, and Farhang Radjai. Parallel implicit contact algorithm for soft particle systems. *Computer Physics Communications*, 237(??):17–25, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303904.

Nazarov:2017:PSU

[NFI17] Alexey E. Nazarov, Roman G. Fedunov, and Anatoly I. Ivanov. Principals of simulation of ultrafast charge transfer in solution within the multichannel stochastic point-transition model. *Computer Physics Communications*, 210(??):172–180, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302867.

Nishiura:2015:CPS

[NFS15] Daisuke Nishiura, Mikito Furuichi, and Hide Sakaguchi. Computational performance of a smoothed particle hydrodynamics simulation for shared-memory parallel computing. *Computer Physics Communications*, 194(??):18–32, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500137X.

Novaresio:2012:OSL

[NGCI+12] Valerio Novaresio, María García-Camprubí, Salvador Izquierdo, Pietro Asinari, and Norberto Fueyo. An open-source library for the numerical modeling of mass-transfer in solid oxide fuel cells. *Computer Physics Communications*, 183(1):125–146, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100275X.

Naze:2013:RPR

[NGG+13] C. Nazé, E. Gaidamauskas, G. Gaigalas, M. Godefroid, and P. Jönsson. ris 3: a program for relativistic isotope shift calculations. *Computer Physics Communications*, 184(9):2187–2196, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000726.

Noffsinger:2010:EPC

[NGM+10] Jesse Noffsinger, Feliciano Giustino, Brad D. Malone, Cheol-Hwan Park, Steven G. Louie, and Marvin L. Cohen. EPW: a program for calculating the electron-phonon coupling using maximally localized Wannier functions. *Computer Physics Communications*, 181(12):2140–2148, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003218.

Nguyen:2017:GAT

[Ngu17] Trung Dac Nguyen. GPU-accelerated Tersoff potentials for massively parallel molecular dynamics simulations. *Computer Physics Communications*, 212(??):113–122, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303393.

Navarro:2016:AMG

[NHD16] Cristóbal A. Navarro, Wei Huang, and Youjin Deng. Adaptive multi-GPU exchange Monte Carlo for the 3D random field Ising model. *Computer Physics Communications*, 205(??):48–60, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465516300960.

Ng:2014:AAL

[NHS14] K. C. Ng, Y. H. Hwang, and T. W. H. Sheu. On the accuracy assessment of Laplacian models in MPS. *Computer Physics Communications*, 185(10):2412–2426, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001660.

Ng:2015:MPL

[NHSY15] K. C. Ng, Y. H. Hwang, T. W. H. Sheu, and C. H. Yu. Moving Particle Level-Set (MPLS) method for incompressible multiphase flow computation. *Computer Physics Communications*, 196(??):317–334, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002660.

Niehoff:2018:FTC

[Nie18] Benjamin E. Niehoff. Faster tensor canonicalization. *Computer Physics Communications*, 228(??):123–145, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300432.

Nakamura:2012:MBB

[NIK+12a] Y. Nakamura, K.-I. Ishikawa, Y. Kuramashi, T. Sakurai, and H. Tadano. Modified block BiCGSTAB for lattice QCD. *Computer Physics Communications*, 183(1):34–37, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002827.

Nikitin:2012:ECC

[Nik12b] A. V. Nikitin. An efficient code for calculation of the $6C$, $9C$ and $12C$ symbols for C_{3v}, T_d, and O_h point groups. *Computer Physics Communications*, 183(3):733–736, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003742.

Nishimura:2011:PMG

[Nis11] Y. Nishimura. A perturbation method for guiding center orbit following calculations in the presence of Coulomb collisions. *Computer Physics Communications*, 182(1):158–160, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003012.

Naik:2018:CCF

[NJ18] Mit H. Naik and Manish Jain. CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations. *Computer Physics Communications*, 226(??):114–126, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300158.

Naz:2017:DOS

[NJS17] Ehsan Saei Ghareh Naz, Matthew R. Jorgensen, and Oliver G. Schmidt. Density of optical states in rolled-up photonic crystals and quasi crystals. *Computer Physics Communications*, 214(??):117–127, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303897.

Nakamura:2015:PCL

[NKS15] Takenobu Nakamura, Shuhei Kawamoto, and Wataru Shinoda. Precise calculation of the local pressure tensor in Cartesian and spherical coordinates in LAMMPS. *Computer Physics Communications*, 190(??):120–128, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004007.

Nguyen:2019:ISP

[NLB+19] Trung Dac Nguyen, Honghao Li, Debarshee Bagchi, Francisco J. Solis, and Monica Olvera de la Cruz. Incorporating surface polarization effects into large-scale coarse-grained molecular dynamics simulation. *Computer Physics Communications*, 241(??):80–91, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300840.

Noble:2017:DCS

[NLSJ17] J. H. Noble, M. Lubasch, J. Stevens, and U. D. Jentschura. Diagonalization of complex symmetric matrices: Generalized Householder reflections, iterative deflation and implicit shifts. *Computer Physics Communications*, 221(??):304–316, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301960.

Nilmeier:2014:RSU

[NM14] Jerome P. Nilmeier and Jaime Marian. A rigorous sequential update strategy for parallel kinetic Monte Carlo simulation. *Computer Physics Communications*, 185(10):2479–2486, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001982.

Nino:2015:AGA

[NMCR15] Alfonso Niño, Camelia Muñoz-Caro, and Sebastián Reyes. APINetworks: a general API for the treatment of complex networks in arbitrary computational environments. *Computer Physics Communications*, 196(??):446–454, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001976.

Nishiura:2014:PCP

[NMS14] Daisuke Nishiura, Miki Y. Matsuo, and Hide Sakaguchi. ppohDEM: Computational performance for open source code of the discrete element method. *Computer Physics Communications*, 185(5):1486–1495, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000472.

Nakata:2015:ICO

[NNWS15] Motoki Nakata, Masanori Nunami, Tomo-Hiko Watanabe, and Hideo Sugama. Improved collision operator for plasma kinetic simulations with multi-species ions and electrons. *Computer Physics Communications*, 197(??):61–72, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500291X.

Noreen:2012:HPS

[NO12] Amna Noreen and Kåre Olaussen. High precision series solutions of differential equations: Ordinary and regular singular points of second order ODEs. *Computer Physics Communications*, 183(10):2291–2297, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001841.

Narski:2014:APS

[NO14] Jacek Narski and Maurizio Ottaviani. Asymptotic Preserving scheme for strongly anisotropic parabolic equations for arbitrary anisotropy direction. *Computer Physics Communications*, 185(12):3189–3203, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002999.

Nogueira:2017:FRCa

[Nog17a] P. Nogueira. From Feynman rules to conserved quantum numbers, I. *Computer Physics Communications*, 214(??):83–90, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300371.

Nogueira:2017:FRCb

[Nog17b] P. Nogueira. From Feynman rules to conserved quantum numbers, II. *Computer Physics Communications*, 215(??):13–19, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300395.

Nejad:2015:SPV

[NOR15] Bijan Chokoufe Nejad, Thorsten Ohl, and Jürgen Reuter. Simple, parallel virtual machines for extreme computations. *Computer Physics Communications*, 196(??):58–69, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001952.

Novotny:2017:PMG

[Nov17] Filip Novotný. ParticleRecognition, a Mathematica GUI interface for analysis of complex shaped nanoparticles in micrographs. *Computer Physics Communications*, 214(??):98–104, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303137.

Nguyen:2019:APM

[NP19] Trung Dac Nguyen and Steven J. Plimpton. Aspherical particle models for molecular dynamics simulation. *Computer Physics Communications*, 243(??):12–24, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301687.

Nabok:2011:NEI

[NPAD11] Dmitrii Nabok, Peter Puschnig, and Claudia Ambrosch-Draxl. noloco: An efficient implementation of van der Waals density functionals based on a Monte–Carlo integration technique. *Computer Physics Communications*, 182(8):1657–1662, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001469.

Nguyen:2011:RBC

[NPAG11] Trung Dac Nguyen, Carolyn L. Phillips, Joshua A. Anderson, and Sharon C. Glotzer. Rigid body constraints realized in massively-parallel molecular dynamics on graphics processing units. *Computer Physics Communications*, 182(11):2307–2313, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002153.

Nemnes:2016:TBC

[NPM16] G. A. Nemnes, Alexandra Palici, and A. Manolescu. Transparent boundary conditions for time-dependent electron transport in the R-matrix method with applications to nanostructured interfaces. *Computer Physics Communications*, 208(??):109–116, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302375.

Niksic:2014:DRS

[NPVR14] T. Nikšić, N. Paar, D. Vretenar, and P. Ring. DIRHB — a relativistic self-consistent mean-field framework for atomic nuclei. *Computer Physics Communications*, 185(6):1808–1821, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000836`.

Nilles:2012:OTS

[NRSVW12] H. P. Nilles, S. Ramos-Sánchez, P. K. S. Vaudrevange, and A. Wingerter. The orbifolder: a tool to study the low-energy effective theory of heterotic orbifolds. *Computer Physics Communications*, 183(6):1363–1380, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000550`.

Nesterenko:2010:QPP

[NS10] A. V. Nesterenko and C. Simolo. QCDMAPT: Program package for analytic approach to QCD. *Computer Physics Communications*, 181(10):1769–1775, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551000233X`.

Nesterenko:2011:QFV

[NS11a] A. V. Nesterenko and C. Simolo. QCDMAPT_F: Fortran version of QCDMAPT package. *Computer Physics Communications*, 182(10):2303–2304, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002116`.

Nigussa:2011:TII

[NS11b] K. N. Nigussa and J. A. Støvneng. Theoretical investigation of the interaction of oxygen with pure and K-doped NiTi shape memory surface alloys. *Computer Physics Communications*, 182(9):1979–1983, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510005205`.

Ning:2015:HAO

[NS15] Hang Ning and T. E. Simos. High algebraic order Runge–Kutta type two-step method with vanished phase-lag and its first, second, third, fourth, fifth and sixth derivatives. *Computer Physics Communications*, 196(??):226–235, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002544.

Noda:2019:SSI

[NSH+19] Masashi Noda, Shunsuke A. Sato, Yuta Hirokawa, Mitsuharu Uemoto, Takashi Takeuchi, Shunsuke Yamada, Atsushi Yamada, Yasushi Shinohara, Maiku Yamaguchi, Kenji Iida, Isabella Floss, Tomohito Otobe, Kyung-Min Lee, Kazuya Ishimura, Taisuke Boku, George F. Bertsch, Katsuyuki Nobusada, and Kazuhiro Yabana. SALMON: Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience. *Computer Physics Communications*, 235(??):356–365, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303412.

Nguyen:2014:CLM

[NSXZ14] Huy Nguyen, Hao Shi, Jie Xu, and Shiwei Zhang. CPMC-Lab: a Matlab package for Constrained Path Monte Carlo calculations. *Computer Physics Communications*, 185(12):3344–3357, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002707.

Nutma:2014:XFT

[Nut14] Teake Nutma. xTras: a field-theory inspired xAct package for Mathematica. *Computer Physics Communications*, 185(6):1719–1738, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000381.

Nunez-Valdez:2018:ETC

[NVAFO18] Maribel Núñez-Valdez, Zahed Allahyari, Tao Fan, and Artem R. Oganov. Efficient technique for computational design of thermoelectric materials. *Computer Physics Communications*, 222(??):152–157, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303387.

Norris:2013:ALB

[NVW+13] S. Norris, A. Vikartofsky, R. E. Wagner, Q. Su, and R. Grobe. Absorbing-like boundaries for quantum field theoretical grid simulations. *Computer Physics Communications*, 184(11):2412–2418, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001987.

Nie:2014:PNP

[NZQL14] Yufeng Nie, Weiwei Zhang, Nan Qi, and Yiqiang Li. Parallel node placement method by bubble simulation. *Computer Physics Communications*, 185(3):798–808, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004037.

Ozgun:2011:PMB

[OAKS11] Ozlem Ozgun, Gökhan Apaydin, Mustafa Kuzuoglu, and Levent Sevgi. PETOOL: Matlab-based one-way and two-way split-step parabolic equation tool for radiowave propagation over variable terrain. *Computer Physics Communications*, 182(12):2638–2654, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002669.

Oetzel:2010:FSM

[OBH10] Björn Oetzel, Friedhelm Bechstedt, and Karsten Hannewald. Finite-size modelling of electrodes for quantum transport calculations using k-space *ab initio* techniques. *Computer Physics Communications*, 181(4):746–749, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003981.

Olm:2019:SHT

[OBM19] Marc Olm, Santiago Badia, and Alberto F. Martín. Simulation of High Temperature Superconductors and experimental validation. *Computer Physics Communications*, 237(??):154–167, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304132.

Olshevsky:2019:SFP

[OBPL19] V. Olshevsky, F. Bacchini, S. Poedts, and G. Lapenta. Slurm: Fluid particle-in-cell code for plasma modeling. *Computer Physics Communications*, 235(??):16–24, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302224.

Olson:2010:PFL

[OCF10] Spencer E. Olson, Andrew J. Christlieb, and Fredrik K. Fatemi. PID feedback for load-balanced parallel gridless DSMC. *Computer Physics Communications*, 181 (12):2063–2071, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002985.

Ou:2013:EME

[OCL+13] Y. C. Ou, Y. H. Chiu, J. M. Lu, W. P. Su, and M. F. Lin. Electric modulation effect on magneto-optical spectrum of monolayer graphene. *Computer Physics Communications*, 184(8):1821–1826, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000982.

Ortwein:2019:PLA

[OCM+19] Philip Ortwein, Stephen M. Copplestone, Claus-Dieter Munz, Tilman Binder, Wladimir Reschke, and Stefanos Fasoulas. A particle localization algorithm on unstructured curvilinear polynomial meshes. *Computer Physics Communications*, 235(??):63–74, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465518303473.

Odrzywolek:2011:GIR

[Odr11] A. Odrzywolek. Gaussian integration with rescaling of abscissas and weights. *Computer Physics Communications*, 182(12):2533–2539, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002499.

Okuyan:2014:BTP

[OG14] Erhan Okuyan and Ugur Güdükbay. BilKristal 2.0: a tool for pattern information extraction from crystal structures. *Computer Physics Communications*, 185(1):442–443, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003214.

Obrejan:2017:DNZ

[OILK17] Kevin Obrejan, Kenji Imadera, Jiquan Li, and Yasuaki Kishimoto. Development of a new zonal flow equation solver by diagonalisation and its application in non-circular cross-section tokamak plasmas. *Computer Physics Communications*, 216(??):8–17, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300620.

Ohno:2010:RIV

[OK10] Nobuaki Ohno and Akira Kageyama. Region-of-interest visualization by CAVE VR system with automatic control of level-of-detail. *Computer Physics Communications*, 181(4):720–725, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003944.

Odaka:2012:GIS

[OK12] Shigeru Odaka and Yoshimasa Kurihara. GR@PPA 2.8: Initial-state jet matching for weak-boson production processes at hadron collisions. *Computer Physics Communications*, 183(4):1014–1028, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465511004115.

Ozgun:2014:CTA

[OK14] Ozlem Ozgun and Mustafa Kuzuoglu. A coordinate transformation approach for efficient repeated solution of Helmholtz equation pertaining to obstacle scattering by shape deformations. *Computer Physics Communications*, 185(6):1616–1627, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000800.

Odaka:2018:GRM

[OK18] Shigeru Odaka and Yoshimasa Kurihara. GR@PPA 2.9: Radiation matching for simulating photon production processes in hadron collisions. *Computer Physics Communications*, 232(??):214–219, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301814.

Ogren:2011:SSF

[ÖKC11] M. Ögren, K. V. Kheruntsyan, and J. F. Corney. Stochastic simulations of fermionic dynamics with phase-space representations. *Computer Physics Communications*, 182(9):1999–2003, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004273.

Oh:2012:MOO

[OKM12] Kwang Jin Oh, Ji Hoon Kang, and Hun Joo Myung. mm_par2.0: An object-oriented molecular dynamics simulation program parallelized using a hierarchical scheme with MPI and OPENMP. *Computer Physics Communications*, 183(2):440–441, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003407.

Ogoyski:2010:COU

[OKP10] A. I. Ogoyski, S. Kawata, and P. H. Popov. Code OK3 — an upgraded version of OK2 with beam wobbling function.

Computer Physics Communications, 181(7):1332–1333, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000962.

Ogarko:2012:FMA

[OL12] V. Ogarko and S. Luding. A fast multilevel algorithm for contact detection of arbitrarily polydisperse objects. *Computer Physics Communications*, 183(4):931–936, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004073.

Oger:2016:DMM

[OLG+16] G. Oger, D. Le Touzé, D. Guibert, M. de Leffe, J. Biddiscombe, J. Soumagne, and J.-G. Piccinali. On distributed memory MPI-based parallelization of SPH codes in massive HPC context. *Computer Physics Communications*, 200(??):1–14, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003070.

Oquendo:2011:IRC

[OML11] W. F. Oquendo, J. D. Muñoz, and A. Lizcano. Influence of rotations on the critical state of soil mechanics. *Computer Physics Communications*, 182(9):1860–1865, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004649.

Ohzeki:2011:QAJ

[ON11] Masayuki Ohzeki and Hidetoshi Nishimori. Quantum annealing with Jarzynski equality. *Computer Physics Communications*, 182(1):257–259, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002377.

OBroin:2012:OIS

[ÓN12] Cathal Ó Broin and L. A. A. Nikolopoulos. An OpenCL implementation for the solution of the time-dependent Schrödinger equation on GPUs and CPUs. *Computer Physics*

Communications, 183(10):2071–2080, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001774.

OBroin:2014:GBP

[ÓN14] Cathal Ó Broin and L. A. A. Nikolopoulos. A GPGPU based program to solve the TDSE in intense laser fields through the finite difference approach. *Computer Physics Communications*, 185(6):1791–1807, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000630.

Ono:2015:TAE

[ONS+15] Shota Ono, Yoshifumi Noguchi, Ryoji Sahara, Yoshiyuki Kawazoe, and Kaoru Ohno. TOMBO: All-electron mixed-basis approach to condensed matter physics. *Computer Physics Communications*, 189(??):20–30, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003956.

Okuyan:2015:TPI

[OO15a] Erhan Okuyan and Erkan Okuyan. A tool for pattern information extraction and defect quantification from crystal structures. *Computer Physics Communications*, 187(??):266–267, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003233.

Okuyan:2015:BTC

[OO15b] Erkan Okuyan and Ceyda Okuyan. BilKristal 4.0: a tool for crystal parameters extraction and defect quantification. *Computer Physics Communications*, 195(??):214–215, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001459.

Orts:2019:FSE

[OOGP19] F. Orts, G. Ortega, E. M. Garzón, and A. M. Puertas. Finite size effects in active microrheology in colloids. *Computer*

Physics Communications, 236(??):8–14, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303515.

Ohba:2012:LSA

[OOK+12] Nobuko Ohba, Shuji Ogata, Takahisa Kouno, Tomoyuki Tamura, and Ryo Kobayashi. Linear scaling algorithm of real-space density functional theory of electrons with correlated overlapping domains. *Computer Physics Communications*, 183(8):1664–1673, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001099.

Ovaysi:2012:MGA

[OP12] Saeed Ovaysi and Mohammad Piri. Multi-GPU acceleration of direct pore-scale modeling of fluid flow in natural porous media. *Computer Physics Communications*, 183(9):1890–1898, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001464.

Opletal:2011:HHR

[OPO+11] G. Opletal, T. C. Petersen, B. O'Malley, I. K. Snook, D. G. McCulloch, and I. Yarovsky. HRMC_1.1: Hybrid Reverse Monte Carlo method with silicon and carbon potentials. *Computer Physics Communications*, 182(2):542, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004248.

Opletal:2014:HHR

[OPR14] G. Opletal, T. C. Petersen, and S. P. Russo. HRMC_2.1: Hybrid reverse Monte Carlo method with silicon, carbon, germanium and silicon carbide potentials. *Computer Physics Communications*, 185(6):1854–1855, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000782.

Opletal:2013:HHR

[OPSR13] G. Opletal, T. C. Petersen, I. K. Snook, and S. P. Russo. HRMC_2.0: Hybrid Reverse Monte Carlo method with silicon, carbon and germanium potentials. *Computer Physics Communications*, 184(8):1946–1957, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551300101X`.

Ossandon:2017:NNA

[ORCR17] Sebastián Ossandón, Camilo Reyes, Patricio Cumsille, and Carlos M. Reyes. Neural network approach for the calculation of potential coefficients in quantum mechanics. *Computer Physics Communications*, 214(??):31–38, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300061`.

Oredsson:2019:THD

[Ore19] Joel Oredsson. 2HDME: Two-Higgs-Doublet Model Evolver. *Computer Physics Communications*, 244(??):409–426, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S001046551930181X`.

Orgogozo:2015:RNV

[Org15] Laurent Orgogozo. RichardsFoam2: a new version of RichardsFoam devoted to the modelling of the vadose zone. *Computer Physics Communications*, 196(??):619–620, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002787`.

Oskooi:2010:MFF

[ORI+10] Ardavan F. Oskooi, David Roundy, Mihai Ibanescu, Peter Bermel, J. D. Joannopoulos, and Steven G. Johnson. Meep: a flexible free-software package for electromagnetic simulations by the FDTD method. *Computer Physics Communications*, 181(3):687–702, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046550900383X`.

Orgogozo:2014:OSM

[ORS+14] L. Orgogozo, N. Renon, C. Soulaine, F. Hénon, S. K. Tomer, D. Labat, O. S. Pokrovsky, M. Sekhar, R. Ababou, and M. Quintard. An open source massively parallel solver for Richards equation: Mechanistic modelling of water fluxes at the watershed scale. *Computer Physics Communications*, 185(12):3358–3371, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002719.

Osterman:2010:TOT

[Ost10] Natan Osterman. TweezPal — optical tweezers analysis and calibration software. *Computer Physics Communications*, 181(11):1911–1916, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002572.

Ozaki:2011:AFE

[OT11] Taisuke Ozaki and Masayuki Toyoda. Accurate finite element method for atomic calculations based on density functional theory and Hartree–Fock method. *Computer Physics Communications*, 182(6):1245–1252, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000725.

Oxburgh:2014:DTR

[OTC14] Stephen Oxburgh, Tomás Tyc, and Johannes Courtial. Dr TIM: Ray-tracer TIM, with additional specialist scientific capabilities. *Computer Physics Communications*, 185(3):1027–1037, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003767.

Otin:2013:ENB

[Oti13] Ruben Otin. Ermes: a nodal-based finite element code for electromagnetic simulations in frequency domain. *Computer Physics Communications*, 184(11):2588–2595, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300204X.

Otsuka:2011:PTS

[Ots11] Hiromi Otsuka. Phase transitions in square-lattice dimer model with anisotropic interactions. *Computer Physics Communications*, 182(9):1888–1891, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005072.

Otin:2015:FET

[OVSI15] Ruben Otin, Jaco Verpoorte, Harmen Schippers, and Roger Isanta. A finite element tool for the electromagnetic analysis of braided cable shields. *Computer Physics Communications*, 191(??):209–220, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000521.

Ogburn:2014:FDC

[OWS+14] Daniel X. Ogburn, Colin L. Waters, Murray D. Sciffer, Jeff A. Hogan, and Paul C. Abbott. A finite difference construction of the spheroidal wave functions. *Computer Physics Communications*, 185(1):244–253, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002610.

Ozkaynak:2013:SPP

[ÖY13] Fatih Özkaynak and Sirma Yavuz. Security problems for a pseudorandom sequence generator based on the Chen chaotic system. *Computer Physics Communications*, 184(9):2178–2181, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001604.

Ohno:2014:PMD

[OYK+14] Yousuke Ohno, Rio Yokota, Hiroshi Koyama, Gentaro Morimoto, Aki Hasegawa, Gen Masumoto, Noriaki Okimoto, Yoshinori Hirano, Huda Ibeid, Tetsu Narumi, and Makoto Taiji. Petascale molecular dynamics simulation using the fast multipole method on K computer. *Computer Physics Communications*, 185(10):2575–2585, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002082`.

Poursina:2013:CES

[PA13] Mohammad Poursina and Kurt S. Anderson. Canonical ensemble simulation of biopolymers using a coarse-grained articulated generalized divide-and-conquer scheme. *Computer Physics Communications*, 184(3):652–660, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003724`.

Palmai:2012:RMS

[Pál12] T. Pálmai. Regularization of multi-soliton form factors in sine–Gordon model. *Computer Physics Communications*, 183(8):1813–1821, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001166`.

Panzer:2015:ASI

[Pan15] Erik Panzer. Algorithms for the symbolic integration of hyperlogarithms with applications to Feynman integrals. *Computer Physics Communications*, 188(??):148–166, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003658`.

Panopoulos:2011:SES

[PAS11] G. A. Panopoulos, Z. A. Anastassi, and T. E. Simos. A symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrödinger equation and related IVPs with oscillating solutions. *Computer Physics Communications*, 182(8):1626–1637, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001299`.

Paternoster:2012:PSA

[Pat12] Beatrice Paternoster. Present state-of-the-art in exponential fitting. A contribution dedicated to Liviu Ixaru on his 70th birthday. *Computer Physics Communications*, 183(12):2499–2512, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002251.

Patel:2015:PXM

[Pat15] Hiren H. Patel. Package-X: a Mathematica package for the analytic calculation of one-loop integrals. *Computer Physics Communications*, 197(??):276–290, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003033.

Patel:2017:PXM

[Pat17] Hiren H. Patel. Package-X 2.0: a Mathematica package for the analytic calculation of one-loop integrals. *Computer Physics Communications*, 218(??):66–70, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301297.

Pavlyukh:2013:ERI

[PB13] Y. Pavlyukh and J. Berakdar. Electron repulsion integrals for self-energy calculations. *Computer Physics Communications*, 184(2):387–395, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003141.

Puhr:2016:NMC

[PB16] Matthias Puhr and Pavel Buividovich. A numerical method to compute derivatives of functions of large complex matrices and its application to the overlap Dirac operator at finite chemical potential. *Computer Physics Communications*, 208(??):135–148, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302417.

Pepe:2015:USF

[PBD+15] R. Pepe, A. Bonfiglioli, A. D'Angola, G. Colonna, and R. Paciorri. An unstructured shock-fitting solver for hypersonic plasma flows in chemical non-equilibrium. *Computer Physics Communications*, 196(??):179–193, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002507.

Perona:2014:TEM

[PBE14] A. Perona, D. Borgogno, and L.-G. Eriksson. A test electron model for the study of three dimensional magnetic reconnection effects. *Computer Physics Communications*, 185(1):86–95, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002816.

Partl:2016:NMN

[PBF+16] Ondrej Pártl, Michal Benes, Peter Frolkovic, Tissa Illangasekare, and Kathleen Smits. Numerical modeling of non-isothermal gas flow and NAPL vapor transport in soil. *Computer Physics Communications*, 202(??):175–187, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551600031X.

Poli:2018:TPB

[PBL+18] E. Poli, A. Bock, M. Lochbrunner, O. Maj, M. Reich, A. Snicker, A. Stegmeir, F. Volpe, N. Bertelli, R. Bilato, G. D. Conway, D. Farina, F. Felici, L. Figini, R. Fischer, C. Galperti, T. Happel, Y. R. Lin-Liu, N. B. Marushchenko, U. Mszanowski, F. M. Poli, J. Stober, E. Westerhof, R. Zille, A. G. Peeters, and G. V. Pereverzev. TORBEAM 2.0, a paraxial beam tracing code for electron-cyclotron beams in fusion plasmas for extended physics applications. *Computer Physics Communications*, 225(??):36–46, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730423X.

Pardini:2012:FPC

[PBMAD12] Lorenzo Pardini, Valerio Bellini, Franca Manghi, and Claudia Ambrosch-Draxl. First-principles calculation of X-ray dichroic spectra within the full-potential linearized augmented planewave method: An implementation into the Wien2k code. *Computer Physics Communications*, 183(3):628–636, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003985.

Piccinini:2017:GAA

[PBS+17] Enrico Piccinini, Claudia Benedetti, Ilaria Siloi, Matteo G. A. Paris, and Paolo Bordone. GPU-accelerated algorithms for many-particle continuous-time quantum walks. *Computer Physics Communications*, 215(??):235–245, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300668.

Peng:2011:SPF

[PC11] Yu-Cih Peng and Chung-I Chou. Simulation of pedestrian flow through a "T" intersection: a multi-floor field cellular automata approach. *Computer Physics Communications*, 182(1):205–208, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002687.

Piotrowski:2015:SLH

[PCEH15] Lech Wiktor Piotrowski, Marco Casolino, Toshikazu Ebisuzaki, and Kazuhiro Higashide. The simulation of the LANFOS-H food radiation contamination detector using Geant4 package. *Computer Physics Communications*, 187(??):49–54, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003452.

Pfefferle:2014:VLS

[PCGM14] D. Pfefferlé, W. A. Cooper, J. P. Graves, and C. Misev. VENUS–LEVIS and its spline-Fourier interpolation of 3D toroidal magnetic field representation for guiding-centre and full-orbit simulations of charged energetic particles. *Computer Physics Communications*, 185(12):3127–3140, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002744.

Palmer:2017:ACP

[PCR17] Ben Palmer, Brian Connolly, and Mark Read. Activity computer program for calculating ion irradiation activation. *Computer Physics Communications*, 216(??):138–144, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300930.

Pavlov:2011:OFS

[PCVZ11] V. N. Pavlov, M. V. Chukalina, A. A. Veligzhanin, and Y. V. Zubavichus. Optimum filtering and stochastic optimization in EXAFS data analysis. *Computer Physics Communications*, 182(7):1463–1466, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000932.

Plante:2014:CDD

[PDC14] Ianik Plante, Luc Devroye, and Francis A. Cucinotta. Calculations of distance distributions and probabilities of binding by ligands between parallel plane membranes comprising receptors. *Computer Physics Communications*, 185(3):697–707, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003123.

Pueschel:2010:RND

[PDJ10] M. J. Pueschel, T. Dannert, and F. Jenko. On the role of numerical dissipation in gyrokinetic Vlasov simulations of plasma microturbulence. *Computer Physics Communications*, 181(8):1428–1437, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001219.

Peng:2018:CPW

[PDL+18] Xingjie Peng, Pablo Ducru, Shichang Liu, Benoit Forget, Jingang Liang, and Kord Smith. Converting point-wise nuclear cross sections to pole representation using regularized vector fitting. *Computer Physics Communications*, 224(??):52–62, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465517304034`.

Pinho:2019:APA

[PdMML19] S. T. R. Pinho, V. A. G. O. de Meneses, M. S. P. Muniz, and T. C. Petit Lobao. An algorithm for periodicity and almost periodicity of uniform substitution sequences and its implications on aperiodic spin models. *Computer Physics Communications*, 241(??):48–55, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300931`.

Parand:2010:AAS

[PDRG10] K. Parand, Mehdi Dehghan, A. R. Rezaei, and S. M. Ghaderi. An approximation algorithm for the solution of the nonlinear Lane–Emden type equations arising in astrophysics using Hermite functions collocation method. *Computer Physics Communications*, 181(6):1096–1108, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000585`.

Popov:2015:SME

[PE15] Mikhail V. Popov and Tatiana G. Elizarova. Smoothed MHD equations for numerical simulations of ideal quasi-neutral gas dynamic flows. *Computer Physics Communications*, 196(??):348–361, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002726`.

Pei:2017:APS

[PE17] Zongrui Pei and Markus Eisenbach. Acceleration of the Particle Swarm Optimization for Peierls–Nabarro modeling of dislocations in conventional and high-entropy alloys. *Computer Physics Communications*, 215(??):7–12, June 2017.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300346`.

Pei:2018:DDS

[Pei18] Zongrui Pei. DIST: a dislocation-simulation toolkit. *Computer Physics Communications*, 233(??):44–50, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302297`.

Pei:2019:ECC

[PEMS19] Zongrui Pei, Markus Eisenbach, Sai Mu, and G. Malcolm Stocks. Error controlling of the combined cluster-expansion and Wang–Landau Monte-Carlo method and its application to FeCo. *Computer Physics Communications*, 235(??):95–101, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551830331X`.

Peraro:2014:NAI

[Per14] Tiziano Peraro. Ninja: Automated integrand reduction via Laurent expansion for one-loop amplitudes. *Computer Physics Communications*, 185(10):2771–2797, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002227`.

Parcollet:2015:TTR

[PFA+15] Olivier Parcollet, Michel Ferrero, Thomas Ayral, Hartmut Hafermann, Igor Krivenko, Laura Messio, and Priyanka Seth. TRIQS: a toolbox for research on interacting quantum systems. *Computer Physics Communications*, 196(??):398–415, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001666`.

Patriarca:2019:HAQ

[PFFK19] Matteo Patriarca, Patricio Farrell, Jürgen Fuhrmann, and Thomas Koprucki. Highly accurate quadrature-based Scharfetter–Gummel schemes for charge transport in degenerate semiconductors. *Computer Physics Communica-*

tions, 235(??):40–49, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303527.

Peng:2010:AFC

[PG10] Liang-You Peng and Qihuang Gong. An accurate Fortran code for computing hydrogenic continuum wave functions at a wide range of parameters. *Computer Physics Communications*, 181(12):2098–2101, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003413.

Pfeiffer:2017:APC

[PG17] M. Pfeiffer and M. H. Gorji. Adaptive particle-cell algorithm for Fokker–Planck based rarefied gas flow simulations. *Computer Physics Communications*, 213(??):1–8, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303575.

Pinto:2019:GTI

[PG19] M. Pinto and P. Gonçalves. GUIMesh: a tool to import STEP geometries into Geant4 via GDML. *Computer Physics Communications*, 239(??):150–156, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300438.

Pela:2017:LMI

[PGD17] Ronaldo Rodrigues Pela, Andris Gulans, and Claudia Draxl. The LDA-1/2 method implemented in the exciting code. *Computer Physics Communications*, 220(??):263–268, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302345.

Prandini:2019:SCO

[PGMU19] Gianluca Prandini, Mario Galante, Nicola Marzari, and Paolo Umari. SIMPLE code: Optical properties with optimal basis functions. *Computer Physics Communications*, 240(??):106–119, July 2019. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300682.

Poya:2017:HPD

[PGO17] Roman Poya, Antonio J. Gil, and Rogelio Ortigosa. A high performance data parallel tensor contraction framework: Application to coupled electro-mechanics. *Computer Physics Communications*, 216(??):35–52, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300681.

Paul:2011:SGE

[PH11] S. Paul and Y. K. Ho. Solution of the generalized exponential cosine screened Coulomb potential. *Computer Physics Communications*, 182(1):130–133, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001918.

Pall:2013:FAC

[PH13] Szilárd Páll and Berk Hess. A flexible algorithm for calculating pair interactions on SIMD architectures. *Computer Physics Communications*, 184(12):2641–2650, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001975.

Pan:2018:HRM

[PHA18] Shucheng Pan, Xiangyu Y. Hu, and Nikolaus A. Adams. High-resolution method for evolving complex interface networks. *Computer Physics Communications*, 225(??):10–27, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830002X.

Pamela:2019:WAG

[PHT+19] S. Pamela, G. Huijsmans, A. J. Thornton, A. Kirk, S. F. Smith, M. Hoelzl, and T. Eich. A wall-aligned grid generator for non-linear simulations of MHD instabilities in tokamak plasmas. *Computer Physics Communications*, 243(??):41–50, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301560.

Pruett:2011:PIA

[PIH11] C. David Pruett, William H. Ingham, and Ralph D. Herman. Parallel implementation of an adaptive and parameter-free N-body integrator. *Computer Physics Communications*, 182(5):1187–1198, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000348.

Pikelner:2018:FFM

[Pik18] Andrey Pikelner. FMFT: fully massive four-loop tadpoles. *Computer Physics Communications*, 224(??):282–287, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304058.

Pittau:2010:TIN

[Pit10] R. Pittau. Testing and improving the numerical accuracy of the NLO predictions. *Computer Physics Communications*, 181(12):1941–1946, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003589.

Pitzer:2012:ASC

[Pit12] Russell M. Pitzer. Atomic self-consistent-field program by the basis set expansion method: Columbus version. *Computer Physics Communications*, 183(8):1841–1842, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000628.

Pomerantsev:2016:FGB

[PKRS16] V. N. Pomerantsev, V. I. Kukulin, O. A. Rubtsova, and S. K. Sakhiev. Fast GPU-based calculations in few-body quantum scattering. *Computer Physics Communications*, 204(??):121–131, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300765.

Pandit:2015:NSS

[PKT15] Sapna Pandit, Manoj Kumar, and Surabhi Tiwari. Numerical simulation of second-order hyperbolic telegraph type equations with variable coefficients. *Computer Physics Communications*, 187(??):83–90, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003488.

Plante:2016:CST

[Pla16] Ianik Plante. Calculation of the second term of the exact Green's function of the diffusion equation for diffusion-controlled chemical reactions. *Computer Physics Communications*, 198(??):41–46, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003380.

Prusty:2012:SBC

[PLCC12] Manamohan Prusty, Jia Ning Leaw, Shan Shang Chong, and Siew Ann Cheong. Stochastic boundary conditions for grand-canonical-like molecular dynamics simulations of open systems. *Computer Physics Communications*, 183(3):486–496, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003663.

Polyakov:2013:LSF

[PLD+13] A. Yu. Polyakov, T. V. Lyutyy, S. Denisov, V. V. Reva, and P. Hänggi. Large-scale ferrofluid simulations on graphics processing units. *Computer Physics Communications*, 184(6):1483–1489, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000337.

Peralta:2015:GEA

[PLD15] Joaquín Peralta, Claudia Loyola, and Sergio Davis. A GPU enhanced approach to identify atomic vacancies in solid materials. *Computer Physics Communications*, 193(??):66–71, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001216.

Papior:2017:INE

[PLF+17] Nick Papior, Nicolás Lorente, Thomas Frederiksen, Alberto García, and Mads Brandbyge. Improvements on non-equilibrium and transport Green function techniques: the next-generation transiesta. *Computer Physics Communications*, 212(??):8–24, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630306X.

Petran:2014:SC

[PLRT14] M. Petran, J. Letessier, J. Rafelski, and G. Torrieri. SHARE with CHARM. *Computer Physics Communications*, 185(7):2056–2079, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000812.

Plascak:2013:PDF

[PM13] J. A. Plascak and P. H. L. Martins. Probability distribution function of the order parameter: Mixing fields and universality. *Computer Physics Communications*, 184(2):259–269, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003001.

Petrila:2014:MMC

[PM14] Iulian Petrila and Vasile Manta. Metropolis Monte Carlo analysis of all-optical switching. *Computer Physics Communications*, 185(11):2874–2878, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002501.

Patchkovskii:2016:SAE

[PM16] Serguei Patchkovskii and H. G. Muller. Simple, accurate, and efficient implementation of 1-electron atomic time-dependent Schrödinger equation in spherical coordinates. *Computer Physics Communications*, 199(??):153–169, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500394X.

Pfeiffer:2015:TSP

[PMMF15] M. Pfeiffer, A. Mirza, C.-D. Munz, and S. Fasoulas. Two statistical particle split and merge methods for Particle-in-Cell codes. *Computer Physics Communications*, 191(??):9–24, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000302.

Parra-Murillo:2015:ENM

[PMMW15] Carlos A. Parra-Murillo, Javier Madroñero, and Sandro Wimberger. Exact numerical methods for a many-body Wannier–Stark system. *Computer Physics Communications*, 186(??):19–30, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003130.

Poghosyan:2015:AIP

[PMS+15] G. Poghosyan, S. Matta, A. Streit, M. Bejger, and A. Królak. Architecture, implementation and parallelization of the software to search for periodic gravitational wave signals. *Computer Physics Communications*, 188(??):167–176, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003774.

Park:2017:ETS

[PMS+17] J. M. Park, M. Murakami, H. E. St. John, L. L. Lao, M. S. Chu, and R. Prater. An efficient transport solver for tokamak plasmas. *Computer Physics Communications*, 214(??):1–5, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303976.

Ponce:2016:EEP

[PMVG16] S. Poncé, E. R. Margine, C. Verdi, and F. Giustino. EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions. *Computer Physics Communications*, 209(??):116–133, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302260.

Penttinen:2015:FST

[PN15] Olle Penttinen and Håkan Nilsson. A fully synthetic turbulent boundary condition with a homogeneous vortex distribution. *Computer Physics Communications*, 190(??):23–32, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000041.

Pacifici:2013:QRS

[PNL13] Leonardo Pacifici, Danilo Nalli, and Antonio Laganà. Quantum reactive scattering on innovative computing platforms. *Computer Physics Communications*, 184(5):1372–1380, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000076.

Pinto:2014:RCM

[PO14] José Wilson M. Pinto and Luiz N. Oliveira. Recursive computation of matrix elements in the numerical renormalization group. *Computer Physics Communications*, 185(4):1299–1309, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000174.

Poskus:2018:BPC

[Pos18] Andrius Poskus. BREMS: a program for calculating spectra and angular distributions of bremsstrahlung at electron energies less than 3 MeV. *Computer Physics Communications*, 232(??):237–255, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301462.

Poslavsky:2019:REJ

[Pos19] Stanislav Poslavsky. Rings: an efficient Java/Scala library for polynomial rings. *Computer Physics Communications*, 235(??):400–413, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303199.

Park:2013:MFB

[PP13] Won-Kwang Park and Taehoon Park. Multi-frequency based location search algorithm of small electromagnetic inhomogeneities embedded in two-layered medium. *Computer Physics Communications*, 184(7):1649–1659, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000659.

Patelli:2010:GSS

[PPS10] Edoardo Patelli, Helmut J. Pradlwarter, and Gerhart I. Schuëller. Global sensitivity of structural variability by random sampling. *Computer Physics Communications*, 181(12):2072–2081, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002973.

Pankin:2011:SAT

[PPV+11] Alexei Y. Pankin, Alex Pletzer, Srinath Vadlamani, John R. Cary, Ammar Hakim, Scott E. Kruger, Mahmood Miah, Thomas D. Rognlien, Svetlana Shasharina, Glenn Bateman, Arnold H. Kritz, Tariq Rafiq, and FACETS team. Simulation of anomalous transport in tokamaks using the FACETS code. *Computer Physics Communications*, 182(1):180–184, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002717.

Pachucki:2014:EGQ

[PPY14] K. Pachucki, M. Puchalski, and V. A. Yerokhin. Extended Gaussian quadratures for functions with an end-point singularity of logarithmic type. *Computer Physics Communications*, 185(11):2913–2919, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002239.

Piedrahita-Quintero:2017:JGA

[PQTGS17] Pablo Piedrahita-Quintero, Carlos Trujillo, and Jorge Garcia-Sucerquia. JDiffraction: a GPGPU-accelerated JAVA library for numerical propagation of scalar wave fields. *Computer Physics Communications*, 214(??):128–139, May 2017.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303952.

Petersen:2010:ETA

[PR10] T. C. Petersen and S. P. Ringer. An electron tomography algorithm for reconstructing 3D morphology using surface tangents of projected scattering interfaces. *Computer Physics Communications*, 181(3):676–682, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003440.

Petersen:2012:LET

[PR12] T. C. Petersen and S. P. Ringer. Local electron tomography using angular variations of surface tangents: Stomo version 2. *Computer Physics Communications*, 183(3):698–704, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003705.

Parand:2013:KMS

[PR13] K. Parand and J. A. Rad. Kansa method for the solution of a parabolic equation with an unknown spacewise-dependent coefficient subject to an extra measurement. *Computer Physics Communications*, 184(3):582–595, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003451.

Pang:2014:GAO

[PR14] X. Pang and L. Rybarcyk. GPU accelerated online multi-particle beam dynamics simulator for ion linear particle accelerators. *Computer Physics Communications*, 185(3):744–753, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003780.

Pradhan:2011:CWP

[Pra11] Srutarshi Pradhan. Can we predict the failure point of a loaded composite material? *Computer Physics Communications*, 182(9):1984–1988, September 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000397`.

Prausa:2017:ETF

[Pra17] Mario Prausa. `epsilon`: a tool to find a canonical basis of master integrals. *Computer Physics Communications*, 219(??):361–376, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301790`.

Preti:2018:WMP

[Pre18] M. Preti. WiLE: A Mathematica package for weak coupling expansion of Wilson loops in ABJ(M) theory. *Computer Physics Communications*, 227(??):126–147, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517304162`.

Pletzer:2011:EMS

[PS11] Alexander Pletzer and H. R. Strauss. An efficient method for solving elliptic boundary element problems with application to the tokamak vacuum problem. *Computer Physics Communications*, 182(10):2077–2083, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001548`.

Porod:2012:SEI

[PS12] W. Porod and F. Staub. SPheno 3.1: extensions including flavour, CP-phases and models beyond the MSSM. *Computer Physics Communications*, 183(11):2458–2469, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001907`.

Panopoulos:2014:NPF

[PS14] G. A. Panopoulos and T. E. Simos. A new phase-fitted eight-step symmetric embedded predictor-corrector method (EPCM) for orbital problems and related IVPs with oscillating solutions. *Computer Physics Communications*, 185(2):512–523, February 2014. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003330.

Pandey:2011:AAS

[PSB11] Ram K. Pandey, Om. P. Singh, and Vipul K. Baranwal. An analytic algorithm for the space–time fractional advection-dispersion equation. *Computer Physics Communications*, 182(5):1134–1144, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100035X.

Pandey:2012:ASS

[PSBT12] Ram K. Pandey, Om P. Singh, Vipul K. Baranwal, and Manoj P. Tripathi. An analytic solution for the space–time fractional advection-dispersion equation using the optimal homotopy asymptotic method. *Computer Physics Communications*, 183(10):2098–2106, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001816.

Perez:2017:ADS

[PSL+17] R. Navarro Perez, N. Schunck, R.-D. Lasseri, C. Zhang, and J. Sarich. Axially deformed solution of the Skyrme–Hartree–Fock–Bogolyubov equations using the transformed harmonic oscillator basis (III) hfbtho (v3.00): a new version of the program. *Computer Physics Communications*, 220(??):363–375, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302047.

Paissoni:2014:GGT

[PSMS14] C. Paissoni, D. Spiliotopoulos, G. Musco, and A. Spitaleri. GMXPBSA 2.0: a GROMACS tool to perform MM/PBSA and computational alanine scanning. *Computer Physics Communications*, 185(11):2920–2929, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002240.

Paissoni:2015:GGT

[PSMS15] C. Paissoni, D. Spiliotopoulos, G. Musco, and A. Spitaleri. GMXPBSA 2.1: a GROMACS tool to perform MM/PBSA and computational alanine scanning. *Computer Physics Communications*, 186(??):105–107, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003154.

Pratapa:2016:SQM

[PSP16] Phanisri P. Pratapa, Phanish Suryanarayana, and John E. Pask. Spectral Quadrature method for accurate $\mathcal{O}(\mathcal{N})$ electronic structure calculations of metals and insulators. *Computer Physics Communications*, 200(??):96–107, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004166.

Phan-Thien:2014:ETD

[PTMDPK14] N. Phan-Thien, N. Mai-Duy, D. Pan, and B. C. Khoo. Exponential-time differencing schemes for low-mass DPD systems. *Computer Physics Communications*, 185(1):229–235, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003238.

Pekmen:2012:DQS

[PTS12] B. Pekmen and M. Tezer-Sezgin. Differential quadrature solution of nonlinear Klein–Gordon and sine–Gordon equations. *Computer Physics Communications*, 183(8):1702–1713, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001154.

Pigg:2014:ERD

[PUO14] D. A. Pigg, A. S. Umar, and V. E. Oberacker. Eulerian rotations of deformed nuclei for TDDFT calculations. *Computer Physics Communications*, 185(5):1410–1414, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000368.

Payne:2017:ASS

[PVH+17] D. N. R. Payne, C. Vargas, Z. Hameiri, S. R. Wenham, and D. M. Bagnall. An advanced software suite for the processing and analysis of silicon luminescence images. *Computer Physics Communications*, 215(??):223–234, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300644.

Pizzi:2014:BCE

[PVK+14a] Giovanni Pizzi, Dmitri Volja, Boris Kozinsky, Marco Fornari, and Nicola Marzari. BoltzWann: a code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. *Computer Physics Communications*, 185(1):422–429, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003160.

Pizzi:2014:UVB

[PVK+14b] Giovanni Pizzi, Dmitri Volja, Boris Kozinsky, Marco Fornari, and Nicola Marzari. An updated version of BoltzWann: a code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. *Computer Physics Communications*, 185(8):2311–2312, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001581.

Pekkila:2017:MCF

[PVK+17] Johannes Pekkilä, Miikka S. Väisälä, Maarit J. Käpylä, Petri J. Käpylä, and Omer Anjum. Methods for compressible fluid simulation on GPUs using high-order finite differences. *Computer Physics Communications*, 217(??):11–22, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730098X.

Pemmaraju:2018:VGR

[PVK+18] C. D. Pemmaraju, F. D. Vila, J. J. Kas, S. A. Sato, J. J. Rehr, K. Yabana, and David Prendergast. Velocity-gauge real-time TDDFT within a numerical atomic orbital basis set. *Computer Physics Communications*, 226(??):30–38, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300262.

Peng:2014:RCI

[PYW+14] Zhong Peng, Hong Wei Yang, Rui Weng, Yingjie Gao, and Ze Kun Yang. A research on the CN-ICCG-FDTD algorithm of plasma photonic crystals and the transmission coefficient of electromagnetic wave. *Computer Physics Communications*, 185(10):2387–2390, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001623.

Park:2019:PEC

[PZL+19] Jinsu Park, Peng Zhang, Hyunsuk Lee, Sooyoung Choi, Jiankai Yu, and Deokjung Lee. Performance evaluation of CMFD on inter-cycle correlation reduction of Monte Carlo simulation. *Computer Physics Communications*, 235(??):111–119, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830328X.

Pachucki:2016:HFS

[PZY16] K. Pachucki, M. Zientkiewicz, and V. A. Yerokhin. H2SOLV: Fortran solver for diatomic molecules in explicitly correlated exponential basis. *Computer Physics Communications*, 208(??):162–168, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302120.

Pan:2019:TSF

[PZZL19] Dongxin Pan, Chengwen Zhong, Congshan Zhuo, and Sha Liu. A two-stage fourth-order gas-kinetic scheme on unstructured hybrid mesh. *Computer Physics Communications*, 235(??):75–87, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303461.

Qamar:2013:STC

[QA13a] Shamsul Qamar and Sidrah Ahmed. The space–time CE/SE method for solving one-dimensional special relativistic magnetohydrodynamics equations. *Computer Physics Communications*, 184(4):1094–1105, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003967.

Qamar:2013:ACS

[QA13b] Shamsul Qamar and Waqas Ashraf. Application of central schemes for solving radiation hydrodynamical models. *Computer Physics Communications*, 184(5):1349–1363, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004274.

Qian:2013:VCN

[QDZ+13] Guang-Rui Qian, Xiao Dong, Xiang-Feng Zhou, Yongjun Tian, Artem R. Oganov, and Hui-Tian Wang. Variable cell nudged elastic band method for studying solid-solid structural phase transitions. *Computer Physics Communications*, 184(9):2111–2118, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001392.

Quackenbush:2013:PLF

[QGLP13] Seth Quackenbush, Ryan Gavin, Ye Li, and Frank Petriello. W physics at the LHC with FEWZ 2.1. *Computer Physics Communications*, 184(1):209–214, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002913.

Qiu:2010:CSG

[QHC+10] Tian Qiu, Tarik Hadzibeganovic, Guang Chen, Li-Xin Zhong, and Xiao-Run Wu. Cooperation in the snowdrift game on directed small-world networks under self-questioning and noisy conditions. *Computer Physics Communications*, 181(12):2057–2062, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465510003097.

Qiu:2014:RCE

[QHZ+14] Tian Qiu, Teng-Yue Han, Li-Xin Zhong, Zi-Ke Zhang, and Guang Chen. Redundant correlation effect on personalized recommendation. *Computer Physics Communications*, 185(2):489–494, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003263.

Qiang:2010:HOF

[Qia10] Ji Qiang. A high-order fast method for computing convolution integral with smooth kernel. *Computer Physics Communications*, 181(2):313–316, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900318X.

Qiang:2016:ETD

[Qia16] Ji Qiang. Efficient three-dimensional Poisson solvers in open rectangular conducting pipe. *Computer Physics Communications*, 203(??):122–127, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300273.

Qiang:2017:FPP

[Qia17] Ji Qiang. A fast parallel 3D Poisson solver with longitudinal periodic and transverse open boundary conditions for space-charge simulations. *Computer Physics Communications*, 219(??):255–260, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301844.

Qin:2016:IDM

[QJF16] Jingbo Qin, Quanlin Jie, and Zhuo Fan. Implementing the density matrix embedding theory with the hierarchical mean-field approach. *Computer Physics Communications*, 204(??):38–42, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465516300625.

Qiang:2010:PFD

[QL10] Ji Qiang and Xiaoye Li. Particle-field decomposition and domain decomposition in parallel particle-in-cell beam dynamics simulation. *Computer Physics Communications*, 181(12):2024–2034, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003127.

Qiu:2016:PIG

[QLE16] Shi Qiu, Kuang Liu, and Veronica Eliasson. Parallel implementation of geometrical shock dynamics for two dimensional converging shock waves. *Computer Physics Communications*, 207(??):186–192, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301655.

Quinlan:2014:DMF

[QLN14] Nathan J. Quinlan, Libor Lobovský, and Ruairi M. Nestor. Development of the meshless finite volume particle method with exact and efficient calculation of interparticle area. *Computer Physics Communications*, 185(6):1554–1563, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000514.

Qamar:2010:KFV

[QM10] Shamsul Qamar and Sidrah Mudasser. A kinetic flux-vector splitting method for the shallow water magnetohydrodynamics. *Computer Physics Communications*, 181(6):1109–1122, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000597.

Qu:2019:NGT

[QSB19] Feng Qu, Di Sun, and Junqiang Bai. A new genuinely two-dimensional Riemann solver for multidimensional Euler and Navier–Stokes equations. *Computer Physics Communications*, 243(??):1–11, October 2019. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301699.

Qian:2014:SEM

[QSC14] Xu Qian, Songhe Song, and Yaming Chen. A semi-explicit multi-symplectic splitting scheme for a 3-coupled nonlinear Schrödinger equation. *Computer Physics Communications*, 185(4):1255–1264, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004372.

Quan:2015:NOA

[QwWL+15] Ya-Min Quan, Qing wei Wang, Da-Yong Liu, Xiang-Long Yu, and Liang-Jian Zou. Numerical optimization algorithm for rotationally invariant multi-orbital slave-boson method. *Computer Physics Communications*, 191(??):90–99, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000478.

Qi:2018:ADG

[QWZW18] Hongxin Qi, Xianghui Wang, Jie Zhang, and Jianguo Wang. An ADER discontinuous Galerkin method with local time-stepping for transient electromagnetics. *Computer Physics Communications*, 229(??):106–115, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301036.

Qamar:2011:STC

[QYM11] Shamsul Qamar, Muhammad Yousaf, and Sidrah Mudasser. The space–time CE/SE method for solving ultra-relativistic Euler equations. *Computer Physics Communications*, 182(4):994–1004, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005370.

Qiao:2019:ETI

[QZ19] Junfeng Qiao and Weisheng Zhao. Efficient technique for ab-initio calculation of magnetocrystalline anisotropy energy.

Computer Physics Communications, 238(??):203–213, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551830417X`.

Qin:2019:QPP

[QZWU19] Tian Qin, Qi Zhang, Renata M. Wentzcovitch, and Koichiro Umemoto. `qha`: a Python package for quasiharmonic free energy calculation for multi-configuration systems. *Computer Physics Communications*, 237(??):199–207, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303953`.

Raffah:2013:ECW

[RA13] Bahaaudin M. Raffah and Paul C. Abbott. Efficient computation of Wigner–Eisenbud functions. *Computer Physics Communications*, 184(6):1581–1591, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000040`.

Ramadan:2010:AFA

[Ram10] Omar Ramadan. Addendum to: "A FDTD analysis on magnetized plasma of Epstein distribution and reflection calculation" [Computer Physics Communications **180** (1) (2009) 55–60]: a short comment on the equivalence of the shift-operator FDTD method and the bilinear frequency approximation technique for modeling dispersive electromagnetic applications. *Computer Physics Communications*, 181(7):1275–1276, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000822`. See [Yan09].

Ramadan:2012:UME

[Ram12] Omar Ramadan. Unified matrix-exponential FDTD formulations for modeling electrically and magnetically dispersive materials. *Computer Physics Communications*, 183(5):1101–1106, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512000276`.

Ramadan:2014:USS

[Ram14] Omar Ramadan. Unconditionally stable split-step finite difference time domain formulations for double-dispersive electromagnetic materials. *Computer Physics Communications*, 185(12):3094–3098, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400263X.

Ramos:2019:ADE

[Ram19] Alberto Ramos. Automatic differentiation for error analysis of Monte Carlo data. *Computer Physics Communications*, 238(??):19–35, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300013.

Rapaport:2011:EMD

[Rap11] D. C. Rapaport. Enhanced molecular dynamics performance with a programmable graphics processor. *Computer Physics Communications*, 182(4):926–934, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005229.

Rashidi:2009:MDT

[Ras09] M. M. Rashidi. The modified differential transform method for solving MHD boundary-layer equations. *Computer Physics Communications*, 180(11):2210–2217, November 2009. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002094. See corrigendum [Ras17].

Rashidi:2017:CMD

[Ras17] M. M. Rashidi. Corrigendum to “The modified differential transform method for solving MHD boundary-layer equations” [comput. phys. comm. **180** (2009) 2210–2217]. *Computer Physics Communications*, 212(??):285, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303435. See [Ras09].

Rancova:2011:NMS

[RAV11] Olga Rancova, Egidijus Anisimovas, and Tadas Varanavicius. Numerical modeling of structural transitions in few-particle confined 2D systems. *Computer Physics Communications*, 182(9):1914–1918, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000440.

Rawitscher:2015:SPA

[Raw15] George Rawitscher. A spectral phase-amplitude method for propagating a wave function to large distances. *Computer Physics Communications*, 191(??):33–42, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500034X.

Rawitscher:2016:TTB

[Raw16] George Rawitscher. Tunneling through a barrier with the phase-amplitude method. *Computer Physics Communications*, 203(??):138–146, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630042X.

Rayson:2010:RFA

[Ray10] M. J. Rayson. Rapid filtration algorithm to construct a minimal basis on the fly from a primitive Gaussian basis. *Computer Physics Communications*, 181(6):1051–1056, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000512.

Rodriguez:2018:MIC

[RB18] M. Rodriguez and L. Brualla. Many-integrated core (MIC) technology for accelerating Monte Carlo simulation of radiation transport: A study based on the code DPM. *Computer Physics Communications*, 225(??):28–35, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304241.

Rodriguez:2015:OPI

[RBB15] Marcos Rodríguez, Fernando Blesa, and Roberto Barrio. OpenCL parallel integration of ordinary differential equations: Applications in computational dynamics. *Computer Physics Communications*, 192(??):228–236, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000703.

Reinhardt:2019:LMP

[RBG+19] S. Reinhardt, C. Butschkow, S. Geissler, A. Dirnaichner, F. Olbrich, C. E. Lane, D. Schröer, and A. K. Hüttel. Lab::Measurement — a portable and extensible framework for controlling lab equipment and conducting measurements. *Computer Physics Communications*, 234(??):216–222, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302819.

Roudnev:2011:AGC

[RC11] V. Roudnev and Michael Cavagnero. Automatic grid construction for few-body quantum-mechanical calculations. *Computer Physics Communications*, 182(10):2099–2106, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001561.

Reimer:2013:MBF

[RC13] Ashton S. Reimer and Alexei F. Cheviakov. A Matlab-based finite-difference solver for the Poisson problem with mixed Dirichlet–Neumann boundary conditions. *Computer Physics Communications*, 184(3):783–798, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003293. See corrigendum [RC16].

Ramshaw:2015:NSM

[RC15] J. D. Ramshaw and C. H. Chang. Numerical stability in multifluid gas dynamics with implicit drag forces. *Computer Physics Communications*, 195(??):61–67, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001514.

Reimer:2016:CMB

[RC16] Ashton S. Reimer and Alexei F. Cheviakov. Corrigendum to: "A Matlab-based finite difference solver for the Poisson problem with mixed Dirichlet–Neumann boundary conditions" [comput. phys. comm. 184(3) (2013) 783–798]. *Computer Physics Communications*, 209(??):200–201, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302703. See [RC13].

Ridgway:2018:IPF

[RC18] Wesley J. M. Ridgway and Alexei F. Cheviakov. An iterative procedure for finding locally and globally optimal arrangements of particles on the unit sphere. *Computer Physics Communications*, 233(??):84–109, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301292.

Rosiek:2010:SCT

[RCD+10] J. Rosiek, P. H. Chankowski, A. Dedes, S. Jäger, and P. Tanedo. SUSY_FLAVOR: a computational tool for FCNC and CP-violating processes in the MSSM. *Computer Physics Communications*, 181(12):2180–2205, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000295X.

Rangel:2016:WBP

[RCGT16] T. Rangel, D. Caliste, L. Genovese, and M. Torrent. A wavelet-based Projector Augmented-Wave (PAW) method: Reaching frozen-core all-electron precision with a systematic, adaptive and localized wavelet basis set. *Computer Physics Communications*, 208(??):1–8, November 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301771.

Ren:2016:MBD

[RCH16] Chung-Yuan Ren, Yia-Chung Chang, and Chen-Shiung Hsue. A mixed basis density functional approach for one-dimensional systems with B-splines. *Computer Physics*

Communications, 202(??):188–195, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300029.

Ren:2019:AVW

[RCH19] Chung-Yuan Ren, Yia-Chung Chang, and Chen-Shiung Hsue. Application of van der Waals density functionals to two dimensional systems based on a mixed basis approach. *Computer Physics Communications*, 238(??):138–144, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304235.

Rostrup:2010:PHP

[RD10] Scott Rostrup and Hans De Sterck. Parallel hyperbolic PDE simulation on clusters: Cell versus GPU. *Computer Physics Communications*, 181(12):2164–2179, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003152.

Reed:2018:DPR

[RDC+18] Darren S. Reed, Tim Dykes, Rubén Cabezón, Claudio Gheller, and Lucio Mayer. DIAPHANE: A portable radiation transport library for astrophysical applications. *Computer Physics Communications*, 226(??):1–9, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303922.

Russell:2017:ECB

[RDN+17] Francis P. Russell, Peter D. Düben, Xinyu Niu, Wayne Luk, and T. N. Palmer. Exploiting the chaotic behaviour of atmospheric models with reconfigurable architectures. *Computer Physics Communications*, 221(??):160–173, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302564.

Rama:2014:SPI

[RDP14] S. Rama, C. Surendra Dilip, and Rajesh Narayana Perumal. A software program to investigate the nucleation kinetics of solution grown crystals using MATLAB platform. *Computer Physics Communications*, 185(2):661–669, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300338X.

Regnier:2018:FNV

[RDVS18] D. Regnier, N. Dubray, M. Verrière, and N. Schunck. FELIX-2.0: New version of the finite element solver for the time dependent generator coordinate method with the Gaussian overlap approximation. *Computer Physics Communications*, 225(??):180–191, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304125.

Roostaei:2012:EDT

[RE12] B. Roostaei and W. C. Ermler. Electric dipole transition moments and permanent dipole moments for spin-orbit configuration interaction wave functions. *Computer Physics Communications*, 183(3):594–599, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003882.

Raj:2019:PDU

[RE19] Anant Raj and Jacob Eapen. Phonon dispersion using the ratio of zero-time correlations among conjugate variables: Computing full phonon dispersion surface of graphene. *Computer Physics Communications*, 238(??):124–137, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304247.

Roitgrund:2016:IML

[REBS16] Aviad Roitgrund, Gad Eilam, and Shaouly Bar-Shalom. Implementation of the manifest left-right symmetric model in FeynRules. *Computer Physics Communications*, 203(??):18–44, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004476.

Reiter:2010:OCG

[Rei10] T. Reiter. Optimising code generation with haggies. *Computer Physics Communications*, 181(7):1301–1331, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000986`.

Reis:2011:MZD

[Rei11] M. S. Reis. Models for zero-dimensional molecular magnets. *Computer Physics Communications*, 182(5):1169–1177, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000415`.

Reis:2012:MOD

[Rei12] M. S. Reis. Models for one-dimensional molecular magnets. *Computer Physics Communications*, 183(1):99–105, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003055`.

Ramis:2012:MFC

[REtVH12] R. Ramis, K. Eidmann, J. Meyer ter Vehn, and S. Hüller. MULTI-fs — a computer code for laser-plasma interaction in the femtosecond regime. *Computer Physics Communications*, 183(3):637–655, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003481`.

Radtke:2010:SQQ

[RF10] T. Radtke and S. Fritzsche. Simulation of n-qubit quantum systems. V. Quantum measurements. *Computer Physics Communications*, 181(2):440–453, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003282`.

Rahman:2015:ETF

[RF15] Tasmiat Rahman and Kristel Fobelets. Efficient tool flow for 3D photovoltaic modelling. *Computer Physics Communications*, 193(??):124–130, August 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001150.

Rabie:2016:MMC

[RF16] M. Rabie and C. M. Franck. METHES: a Monte Carlo collision code for the simulation of electron transport in low temperature plasmas. *Computer Physics Communications*, 203(??):268–277, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300376.

Rodriguez-Fernandez:2017:GGP

[RFPM+17] Roberto Rodríguez-Fernández, Francisco B. Pereira, Jorge M. C. Marques, Emilio Martínez-Núñez, and Saulo A. Vázquez. GAFit: a general-purpose, user-friendly program for fitting potential energy surfaces. *Computer Physics Communications*, 217(??):89–98, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300607.

Rodrigues:2018:SEW

[RFSF18] Manuel J. Rodrigues, David E. Fernandes, Mário G. Silveirinha, and Gabriel Falcão. Simulating electron wave dynamics in graphene superlattices exploiting parallel processing advantages. *Computer Physics Communications*, 222(??):240–249, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302837.

Rincon:2010:IPT

[RGH10] Julián Rincón, D. J. García, and K. Hallberg. Improved parallelization techniques for the density matrix renormalization group. *Computer Physics Communications*, 181(8):1346–1351, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000998.

Ruokosenmaki:2017:NPI

[RGKR17] Ilkka Ruokosenmäki, Hossein Gholizade, Ilkka Kylänpää, and Tapio T. Rantala. Numerical path integral solution to strong Coulomb correlation in one dimensional Hooke's atom. *Computer Physics Communications*, 210(??):45–53, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302831`.

Rohrer:2011:CSI

[RH11] Jochen Rohrer and Per Hyldgaard. Computational scheme for ab-initio predictions of chemical compositions interfaces realized by deposition growth. *Computer Physics Communications*, 182(9):1814–1818, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000105`.

Rouzbahani:2017:TIS

[RH17] Fardin Rouzbahani and Kazem Hejranfar. A truly incompressible smoothed particle hydrodynamics based on artificial compressibility method. *Computer Physics Communications*, 210(??):10–28, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551630279X`.

Ryssens:2015:CSS

[RHBH15a] W. Ryssens, V. Hellemans, M. Bender, and P.-H. Heenen. Corrigendum to "Solution of the Skyrme-HF+BCS equation on a 3D mesh II. A new version of the Ev8 code" [Comput. Phys. Comm. **187** (2) (2015) 175–194]. *Computer Physics Communications*, 190(??):231, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000314`. See [RHBH15b].

Ryssens:2015:SSH

[RHBH15b] W. Ryssens, V. Hellemans, M. Bender, and P.-H. Heenen. Solution of the Skyrme-HF+BCS equation on a 3D mesh, II: a new version of the Ev8 code. *Computer Physics Communications*, 187(??):175–194, February 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003361. See corrigendum [RHBH15a].

Ren:2015:MBD

[RHC15] Chung-Yuan Ren, Chen-Shiung Hsue, and Yia-Chung Chang. A mixed basis density functional approach for low dimensional systems with B-splines. *Computer Physics Communications*, 188(??):94–102, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003968.

Reuter:2012:SPI

[RHH12] Matthew G. Reuter, Judith C. Hill, and Robert J. Harrison. Solving PDEs in irregular geometries with multiresolution methods I: Embedded Dirichlet boundary conditions. *Computer Physics Communications*, 183(1):1–7, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002396.

Roeller:2012:SSE

[RHHF12] K. Roeller, S. Herminghaus, and A. Hager-Fingerle. Sinusoidal shaking in event-driven simulations. *Computer Physics Communications*, 183(2):251–260, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003110.

Ren:2012:HOU

[RHW+12] Xingang Ren, Zhixiang Huang, Xianliang Wu, Silong Lu, Hui Wang, Lei Wu, and Shen Li. High-order unified symplectic FDTD scheme for the metamaterials. *Computer Physics Communications*, 183(6):1192–1200, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000367.

Rourke:2012:NEH

[RJ12] P. M. C. Rourke and S. R. Julian. Numerical extraction of de Haas–van Alphen frequencies from calculated band energies. *Computer Physics Communications*, 183(2):324–332, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100347X.

Ryu:2016:TES

[RJKC16] Hoon Ryu, Yosang Jeong, Ji-Hoon Kang, and Kyu Nam Cho. Time-efficient simulations of tight-binding electronic structures with Intel Xeon Phi^{TM} many-core processors. *Computer Physics Communications*, 209(??):79–87, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302454.

Ren:2016:IPS

[RJLL16] Jinlian Ren, Tao Jiang, Weigang Lu, and Gang Li. An improved parallel SPH approach to solve 3D transient generalized Newtonian free surface flows. *Computer Physics Communications*, 205(??):87–105, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301035.

Jiang:2011:PIC

[rJmYT11] Zhen ran Jiang, Wei ming Yu, and Ran Tao. Predicting important classes of chemokine family based on kernel method. *Computer Physics Communications*, 182(8):1606–1609, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100124X.

Ren:2019:MMT

[RJW+19] Zhiwei Ren, Lichuan Jin, Tianlong Wen, Yulong Liao, Xiaoli Tang, Huaiwu Zhang, and Zhiyong Zhong. MuFA (Multi-type Fourier Analyzer): a tool for batch generation of MuMax3 input scripts and multi-type Fourier analysis from micromagnetic simulation output data. *Computer Physics Communications*, 244(??):311–318, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302115.

Reith:2011:MWF

[RK11] Dirk Reith and Karl N. Kirschner. A modern workflow for force-field development — bridging quantum mechanics and atomistic computational models. *Computer Physics Communications*, 182(10):2184–2191, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002086.

Reuter:2019:CFP

[RK19] Klaus Reuter and Jürgen Köfinger. CADISHI: Fast parallel calculation of particle-pair distance histograms on CPUs and GPUs. *Computer Physics Communications*, 236(??):274–284, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303667.

Rutkai:2017:IMS

[RKGC+17] Gábor Rutkai, Andreas Köster, Gabriela Guevara-Carrion, Tatjana Janzen, Michael Schappals, Colin W. Glass, Martin Bernreuther, Amer Wafai, Simon Stephan, Maximilian Kohns, Steffen Reiser, Stephan Deublein, Martin Horsch, Hans Hasse, and Jadran Vrabec. ms2: a molecular simulation tool for thermodynamic properties, release 3.0. *Computer Physics Communications*, 221(??):343–351, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302527.

Ragan-Kelley:2014:OPP

[RKVL14] Benjamin Ragan-Kelley, John P. Verboncoeur, and Ming-Chieh Lin. Optimizing physical parameters in 1-D particle-in-cell simulations with Python. *Computer Physics Communications*, 185(10):2487–2494, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001994.

Ramos:2010:REF

[RL10] Higinio Ramos and Cesáreo Lorenzo. Review of explicit Falkner methods and its modifications for solving special second-order I.V.P.s. *Computer Physics Communications*, 181(11):1833–1841, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002341.

Rouet-Leduc:2014:SAS

[RLBC+14] Bertrand Rouet-Leduc, Kipton Barros, Emmanuel Cieren, Venmugil Elango, Christoph Junghans, Turab Lookman, Jamaludin Mohd-Yusof, Robert S. Pavel, Axel Y. Rivera, Dominic Roehm, Allen L. McPherson, and Timothy C. Germann. Spatial adaptive sampling in multiscale simulation. *Computer Physics Communications*, 185(7):1857–1864, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000915.

Rothlisberger:2012:LOL

[RLL12] Beat Röthlisberger, Jörg Lehmann, and Daniel Loss. libCreme: An optimization library for evaluating convex-roof entanglement measures. *Computer Physics Communications*, 183(1):155–165, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002840.

Rewienski:2013:EBI

[RLM13] M. Rewieński, A. Lamecki, and M. Mrozowski. An extended basis inexact shift-invert Lanczos for the efficient solution of large-scale generalized eigenproblems. *Computer Physics Communications*, 184(9):2127–2135, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001410.

Romero-Laorden:2011:FMA

[RLMGM+11] D. Romero-Laorden, O. Martínez-Graullera, C. J. Martín, M. Pérez, and L. G. Ullate. Field modelling acceleration on ultrasonic systems using graphic hardware. *Computer Physics Communications*, 182(3):590–599, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004339.

Regnier:2016:INM

[RLS16] D. Regnier, O. Litaize, and O. Serot. An improved numerical method to compute neutron/gamma deexcitation cascades starting from a high spin state. *Computer Physics Communications*, 201(??):19–28, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515004452`.

Rashidinia:2010:TSA

[RM10a] J. Rashidinia and R. Mohammadi. Tension spline approach for the numerical solution of nonlinear Klein–Gordon equation. *Computer Physics Communications*, 181(1):78–91, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046550900280X`.

Rawat:2010:MRN

[RM10b] Ajay Rawat and N. Mohankumar. Milne, a routine for the numerical solution of Milne's problem. *Computer Physics Communications*, 181(11):1906–1910, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510002560`.

Robinson:2014:NFG

[RM14] M. Robinson and N. A. Marks. NanoCap: a framework for generating capped carbon nanotubes and fullerenes. *Computer Physics Communications*, 185(10):2519–2526, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002033`.

Rocha:2016:UZC

[RMC16] J. C. S. Rocha, L. A. S. Mól, and B. V. Costa. Using zeros of the canonical partition function map to detect signatures of a Berezinskii–Kosterlitz–Thouless transition. *Computer Physics Communications*, 209(??):88–91, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302466`.

Reis:2012:DOP

[RMS+12] Juraci P. Reis, Artur F. Menezes, Edmilson M. Souza, Alessandro Facure, Jose A. C. C. Medeiros, and Ademir X. Silva. Dose optimization in ^{125I} permanent prostate seed implants using the Monte Carlo method. *Computer Physics Communications*, 183(4):847–852, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003900.

Ridgeway:2013:VDA

[RMW13] William K. Ridgeway, David P. Millar, and James R. Williamson. Vectorized data acquisition and fast triple-correlation integrals for Fluorescence Triple Correlation Spectroscopy. *Computer Physics Communications*, 184(4): 1322–1332, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004286.

Rizzo:2019:PPR

[RNdB19] Calogero B. Rizzo, Aiichiro Nakano, and Felipe P. J. de Barros. PAR 2: Parallel random walk particle tracking method for solute transport in porous media. *Computer Physics Communications*, 239(??):265–271, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300190.

Rohe:2016:HPF

[Roh16] Daniel Rohe. Hierarchical parallelisation of functional renormalisation group calculations — hp-fRG. *Computer Physics Communications*, 207(??):160–169, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301485.

Romano:2015:AGR

[Rom15] Paul K. Romano. An algorithm for generating random variates from the Madland–Nix fission energy spectrum. *Computer Physics Communications*, 187(??):152–155, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003713.

Rosiek:2015:SFV

[Ros15] J. Rosiek. SUSY FLAVOR v2.5: a computational tool for FCNC and CP-violating processes in the MSSM. *Computer Physics Communications*, 188(??):208–210, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003385`.

Rosiek:2016:MMP

[Ros16] Janusz Rosiek. MassToMI — a Mathematica package for an automatic Mass Insertion expansion. *Computer Physics Communications*, 201(??):144–158, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551500449X`.

Roehm:2015:DDK

[RPB+15] Dominic Roehm, Robert S. Pavel, Kipton Barros, Bertrand Rouet-Leduc, Allen L. McPherson, Timothy C. Germann, and Christoph Junghans. Distributed Database Kriging for Adaptive Sampling (D^2KAS). *Computer Physics Communications*, 192(??):138–147, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001058`.

Rodrigues:2014:AAC

[RPL+14] Walter Rodrigues, A. Pecchia, M. Lopez, M. Auf der Maur, and A. Di Carlo. Accelerating atomistic calculations of quantum energy eigenstates on graphic cards. *Computer Physics Communications*, 185(10):2510–2518, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002021`.

Ramos:2010:PIM

[RRCSCJ10] E. Ramos, J. E. Roman, S. Cardona-Serra, and J. M. Clemente-Juan. Parallel implementation of the MAGPACK package for the analysis of high-nuclearity spin clusters. *Computer Physics Communications*, 181(12):1929–1940, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003528`.

Ramirez:2012:TIE

[RS12] Hanz Y. Ramírez and Alejandro Santana. Two interacting electrons confined in a 3D parabolic cylindrically symmetric potential, in presence of axial magnetic field: a finite element approach. *Computer Physics Communications*, 183(8):1654–1657, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001075.

Rybczynski:2014:GGI

[RSBB14] Maciej Rybczyński, Grzegorz Stefanek, Wojciech Broniowski, and Piotr Bozek. GLISSANDO 2: GLauber Initial-State Simulation AND mOre…, ver. 2. *Computer Physics Communications*, 185(6):1759–1772, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000502.

Riede:2010:CSD

[RSSH+10] Moritz Riede, Rico Schueppel, Kristian O. Sylvester-Hvid, Martin Kühne, Michael C. Röttger, Klaus Zimmermann, and Andreas W. Liehr. On the communication of scientific data: The Full-Metadata Format. *Computer Physics Communications*, 181(3):651–662, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003890.

Ryan:2010:NMM

[RTA10] Emily M. Ryan, Alexandre M. Tartakovsky, and Cristina Amon. A novel method for modeling Neumann and Robin boundary conditions in smoothed particle hydrodynamics. *Computer Physics Communications*, 181(12):2008–2023, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003139.

Riikila:2015:DEM

[RTÅT15] T. I. Riikilä, T. Tallinen, J. Åström, and J. Timonen. A discrete-element model for viscoelastic deformation and fracture of glacial ice. *Computer Physics*

Communications, 195(??):14–22, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001411.

Roidl:2018:SES

[RTT+18] Benedikt Roidl, Yasushi Todo, Yuichi Takase, Naoto Tsujii, Akira Ejiri, Yusuke Yoshida, Satoru Yajima, and Takahiro Shinya. A simulation environment to simulate lower-hybrid-wave-driven plasmas efficiently. *Computer Physics Communications*, 230(??):38–49, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301346.

Ramis:2016:MIO

[RtV16] R. Ramis and J. Meyer ter Vehn. MULTI–IFE — a one-dimensional computer code for Inertial Fusion Energy (IFE) target simulations. *Computer Physics Communications*, 203(??):226–237, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300297.

Ringl:2012:LIG

[RU12] Christian Ringl and Herbert M. Urbassek. A LAMMPS implementation of granular mechanics: Inclusion of adhesive and microscopic friction forces. *Computer Physics Communications*, 183(4):986–992, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000069.

Ringl:2013:SAC

[RU13] Christian Ringl and Herbert M. Urbassek. A simple algorithm for constructing fractal aggregates with pre-determined fractal dimension. *Computer Physics Communications*, 184(7):1683–1685, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000696.

Ruffoni:2013:FAS

[Ruf13] M. P. Ruffoni. The FTS Atomic Spectrum Tool (FAST) for rapid analysis of line spectra. *Computer Physics Communications*, 184(7):1770–1776, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000386.

Rutter:2018:CTV

[Rut18] M. J. Rutter. C2x: A tool for visualisation and input preparation for castep and other electronic structure codes. *Computer Physics Communications*, 225(??):174–179, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304137.

Reith:2010:IPA

[RV10] Daniel Reith and Peter Virnau. Implementation and performance analysis of bridging Monte Carlo moves for off-lattice single chain polymers in globular states. *Computer Physics Communications*, 181(4):800–805, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004044.

Reith:2011:MCS

[RV11] Daniel Reith and Peter Virnau. Monte Carlo simulations of a single polystyrene chain in spherical confinement. *Computer Physics Communications*, 182(9):1945–1948, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000473X.

Ramos:2014:TFM

[RVA14] Higinio Ramos and J. Vigo-Aguiar. A trigonometrically-fitted method with two frequencies, one for the solution and another one for the derivative. *Computer Physics Communications*, 185(4):1230–1236, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004335.

Regnier:2016:FFE

[RVDS16] D. Regnier, M. Verrière, N. Dubray, and N. Schunck. FELIX-1.0: a finite element solver for the time dependent generator coordinate method with the Gaussian overlap approximation. *Computer Physics Communications*, 200(??):350–363, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500435X.

Rubow:2011:FAC

[RW11] Jürgen Rubow and Ulli Wolff. A factorization algorithm to compute Pfaffians. *Computer Physics Communications*, 182(12):2530–2532, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002487.

Russell:2015:OTD

[RWKS15] Francis P. Russell, Karl A. Wilkinson, Paul H. J. Kelly, and Chris-Kriton Skylaris. Optimised three-dimensional Fourier interpolation: an analysis of techniques and application to a linear-scaling density functional theory code. *Computer Physics Communications*, 187(??):8–19, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551400335X.

Rozanski:2019:ECC

[RZ19] Piotr T. Różański and Michal Zieliński. Efficient computation of Coulomb and exchange integrals for multi-million atom nanostructures. *Computer Physics Communications*, 238(??):254–261, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304272.

Sundararaman:2014:ECD

[SA14] Ravishankar Sundararaman and T. A. Arias. Efficient classical density-functional theories of rigid-molecular fluids and a simplified free energy functional for liquid water. *Computer Physics Communications*, 185(3):818–825, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004062.

Sharma:2015:OHS

[SA15a] Medha Sharma and M. A. H. Ahsan. Organization of the Hilbert space for exact diagonalization of Hubbard model. *Computer Physics Communications*, 193(??):19–29, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001137.

Shokri:2015:HOC

[SA15b] Ali Shokri and Fatemeh Afshari. High-order compact ADI method using predictor-corrector scheme for 2D complex Ginzburg–Landau equation. *Computer Physics Communications*, 197(??):43–50, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002891.

Saltelli:2010:VBS

[SAA+10] Andrea Saltelli, Paola Annoni, Ivano Azzini, Francesca Campolongo, Marco Ratto, and Stefano Tarantola. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. *Computer Physics Communications*, 181(2):259–270, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003087.

Sjostrand:2015:IP

[SAC+15] Torbjörn Sjöstrand, Stefan Ask, Jesper R. Christiansen, Richard Corke, Nishita Desai, Philip Ilten, Stephen Mrenna, Stefan Prestel, Christine O. Rasmussen, and Peter Z. Skands. An introduction to PYTHIA 8.2. *Computer Physics Communications*, 191(??):159–177, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000442.

Staub:2016:HMP

[SAE+16] Florian Staub, Peter Athron, Ulrich Ellwanger, Ramona Gröber, Margarete Mühlleitner, Pietro Slavich, and Alexander Voigt. Higgs mass predictions of public NMSSM spectrum generators. *Computer Physics Communications*, 202(??):113–130, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000242.

Suleimanov:2013:RBC

[SAG13] Yu. V. Suleimanov, J. W. Allen, and W. H. Green. RPMDrate: Bimolecular chemical reaction rates from ring polymer molecular dynamics. *Computer Physics Communications*, 184(3):833–840, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003608.

Solano-Altamirano:2015:DCO

[SAHP15] J. M. Solano-Altamirano and Julio M. Hernández-Pérez. DensToolKit: a comprehensive open-source package for analyzing the electron density and its derivative scalar and vector fields. *Computer Physics Communications*, 196(??):362–371, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500274X.

Sainio:2010:CGA

[Sai10] J. Sainio. CUDAEASY — a GPU accelerated cosmological lattice program. *Computer Physics Communications*, 181(5):906–912, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000159.

SaiToh:2013:ZCL

[Sai13] Akira SaiToh. ZKCM: a C++ library for multiprecision matrix computation with applications in quantum information. *Computer Physics Communications*, 184(8):2005–2020, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001306.

Sala:2012:MPP

[Sal12] Filip A. Sala. Mobile phone as a platform for numerical simulation. *Computer Physics Communications*, 183(1):26–29, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002803.

Salac:2016:GMP

[Sal16] David Salac. A general, mass-preserving Navier–Stokes projection method. *Computer Physics Communications*, 204 (??):97–106, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300704.

Sano:2011:FIW

[San11] Osamu Sano. Flow-induced waterway in a heterogeneous granular material. *Computer Physics Communications*, 182(9):1870–1874, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004728.

Sangwine:2015:CSP

[San15] Stephen J. Sangwine. Comments on 'A structure-preserving method for the quaternion LU decomposition in quaternionic quantum theory' by Minghui Wang and Wenhao Ma. *Computer Physics Communications*, 188(??):128–130, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003993.

Stone:2018:AFR

[SAN18] Christopher P. Stone, Andrew T. Alferman, and Kyle E. Niemeyer. Accelerating finite-rate chemical kinetics with coprocessors: Comparing vectorization methods on GPUs, MICs, and CPUs. *Computer Physics Communications*, 226 (??):18–29, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300286.

Sarkadi:2017:CME

[Sar17a] L. Sarkadi. Calculation of the matrix elements of the Coulomb interaction involving relativistic hydrogenic wave functions. *Computer Physics Communications*, 212(??): 283–284, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303381.

Sarkadi:2017:FPC

[Sar17b] L. Sarkadi. A Fortran program to calculate the matrix elements of the Coulomb interaction involving hydrogenic wave functions. *Computer Physics Communications*, 212(??):280–282, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630337X.

Sokolovski:2011:EMP

[SAS11] D. Sokolovski, E. Akhmatskaya, and S. K. Sen. Extracting S-matrix poles for resonances from numerical scattering data: Type-II Padé reconstruction. *Computer Physics Communications*, 182(2):448–466, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003802.

Savvidy:2015:MRN

[Sav15] Konstantin G. Savvidy. The MIXMAX random number generator. *Computer Physics Communications*, 196(??): 161–165, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002489.

Sanchis-Alepuz:2018:RDB

[SAW18] Hèlios Sanchis-Alepuz and Richard Williams. Recent developments in bound-state calculations using the Dyson–Schwinger and Bethe–Salpeter equations. *Computer Physics Communications*, 232(??):1–21, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301838.

Shao:2018:ANC

[SAY+18] Meiyue Shao, H. Metin Aktulga, Chao Yang, Esmond G. Ng, Pieter Maris, and James P. Vary. Accelerating nuclear configuration interaction calculations through a preconditioned block iterative eigensolver. *Computer Physics Communications*, 222(??):1–13, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302904.

Smadi:2011:CSS

[SB11] Moussa Smadi and Derradji Bahloul. A compact split step Padé scheme for higher-order nonlinear Schrödinger equation (HNLS) with power law nonlinearity and fourth order dispersion. *Computer Physics Communications*, 182(2):366–371, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000411X.

Schram:2013:SPC

[SBB13] Raoul D. Schram, Gerard T. Barkema, and Rob H. Bisseling. SAWdoubler: a program for counting self-avoiding walks. *Computer Physics Communications*, 184(3):891–898, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003694.

Sokolov:2017:FIP

[SBB+17] P. A. Sokolov, M. V. Belousov, S. A. Bondarev, G. A. Zhouravleva, and N. A. Kasyanenko. FibrilJ: ImageJ plugin for fibrils' diameter and persistence length determination. *Computer Physics Communications*, 214(??):199–206, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300231.

Surmin:2016:PCL

[SBE+16] I. A. Surmin, S. I. Bastrakov, E. S. Efimenko, A. A. Gonoskov, A. V. Korzhimanov, and I. B. Meyerov. Particle-in-Cell laser–plasma simulation on Xeon Phi coprocessors. *Computer Physics Communications*, 202(??):204–210, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300194.

Soba:2012:RSD

[SBH+12] Alejandro Soba, Edgar Alejandro Bea, Guillaume Houzeaux, Hadrien Calmet, and José María Cela. Real-space density functional theory and time dependent density functional theory using finite/infinite element methods. *Computer Physics Communications*, 183(12):2581–2588, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002354`.

Schick:2014:UDS

[SBH+14] D. Schick, A. Bojahr, M. Herzog, R. Shayduk, C. von Korff Schmising, and M. Bargheer. UDKM1DSIM — a simulation toolkit for 1D ultrafast dynamics in condensed matter. *Computer Physics Communications*, 185(2):651–660, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003378`.

Sun:2016:PMS

[SBL16] Anbang Sun, Markus M. Becker, and Detlef Loffhagen. PIC/MCC simulation of capacitively coupled discharges: Effect of particle management and integration. *Computer Physics Communications*, 206(??):35–44, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516301199`.

Simona:2019:HOT

[SBPD19] Abele Simona, Luca Bonaventura, Thomas Pugnat, and Barbara Dalena. High order time integrators for the simulation of charged particle motion in magnetic quadrupoles. *Computer Physics Communications*, 239(??):33–52, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300359`.

Scukins:2015:MDI

[SBPN15] Arturs Scukins, Vitaliy Bardik, Evgen Pavlov, and Dmitry Nerukh. Molecular dynamics implementation of BN2D or 'Mercedes Benz' water model. *Computer Physics Communications*, 190(??):129–138, May 2015. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000053.

Squire:2014:VAV

[SBQ14] J. Squire, J. Burby, and H. Qin. VEST: Abstract vector calculus simplification in Mathematica. *Computer Physics Communications*, 185(1):128–135, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002944.

Sprung:2013:FFT

[SBvD13] D. W. L. Sprung, M. I. Betti, and W. van Dijk. Finite Fourier transforms computed by a modified Filon–Euler–Maclaurin method. *Computer Physics Communications*, 184(3):607–616, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003578.

Sarlis:2014:VSR

[SC14] Nicholas V. Sarlis and Stavros-Richard G. Christopoulos. Visualization of the significance of Receiver Operating Characteristics based on confidence ellipses. *Computer Physics Communications*, 185(3):1172–1176, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004219.

Sijoy:2015:TTT

[SC15] C. D. Sijoy and S. Chaturvedi. TRHD: Three-temperature radiation-hydrodynamics code with an implicit non-equilibrium radiation transport using a cell-centered monotonic finite volume scheme on unstructured-grids. *Computer Physics Communications*, 190(??):98–119, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000399.

Sibaev:2016:PFO

[SC16a] Marat Sibaev and Deborah L. Crittenden. PyVCI: a flexible open-source code for calculating accurate molecular infrared spectra. *Computer Physics Communications*, 203(??):290–297, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300418.

Sijoy:2016:CNC

[SC16b] C. D. Sijoy and S. Chaturvedi. Combining node-centered parallel radiation transport and higher-order multi-material cell-centered hydrodynamics methods in three-temperature radiation hydrodynamics code TRHD. *Computer Physics Communications*, 203(??):94–109, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300248.

Samaddar:2017:TPE

[SCB+17a] D. Samaddar, D. P. Coster, X. Bonnin, C. Bergmeister, E. Havlíčková, L. A. Berry, W. R. Elwasif, and D. B. Batchelor. Temporal parallelization of edge plasma simulations using the parareal algorithm and the SOLPS code. *Computer Physics Communications*, 221(??):19–27, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730231X.

Sprengel:2017:CCC

[SCB17b] M. Sprengel, G. Ciaramella, and A. Borzì. A COKOSNUT code for the control of the time-dependent Kohn–Sham model. *Computer Physics Communications*, 214(??):231–238, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300322.

Samaddar:2019:APA

[SCB+19] D. Samaddar, D. P. Coster, X. Bonnin, L. A. Berry, W. R. Elwasif, and D. B. Batchelor. Application of the parareal algorithm to simulations of ELMs in ITER plasma. *Computer Physics Communications*, 235(??):246–257, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303023.

Schmid:2012:AIP

[SCC+12] Nathan Schmid, Clara D. Christ, Markus Christen, Andreas P. Eichenberger, and Wilfred F. van Gunsteren. Architecture, implementation and parallelisation of the GROMOS software for biomolecular simulation. *Computer Physics Communications*, 183(4):890–903, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004024.

Stupovski:2011:ACT

[SCG11] B. M. Stupovski, J. V. Crnjanski, and D. M. Gvozdić. Application of coordinate transformation and finite differences method in numerical modeling of quantum dash band structure. *Computer Physics Communications*, 182(2):289–298, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003590.

Schiller:2014:UOS

[Sch14a] Ulf D. Schiller. A unified operator splitting approach for multi-scale fluid-particle coupling in the lattice Boltzmann method. *Computer Physics Communications*, 185(10):2586–2597, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002094.

Schwenke:2014:CHO

[Sch14b] David W. Schwenke. On the computation of high order Rys quadrature weights and nodes. *Computer Physics Communications*, 185(3):762–763, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003858.

Schmitz:2018:SCL

[Sch18] Holger Schmitz. Schnek: a C++ library for the development of parallel simulation codes on regular grids. *Computer Physics Communications*, 226(??):151–164, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300080.

Searles:2019:MOA

[SCJH19] Robert Searles, Sunita Chandrasekaran, Wayne Joubert, and Oscar Hernandez. MPI + OpenACC: Accelerating radiation transport mini-application, minisweep, on heterogeneous systems. *Computer Physics Communications*, 236(??):176–187, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303552`.

Sheu:2016:DEN

[SCLW16] Tony W. H. Sheu, Y. W. Chung, J. H. Li, and Y. C. Wang. Development of an explicit non-staggered scheme for solving three-dimensional Maxwell's equations. *Computer Physics Communications*, 207(??):258–273, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302053`.

Straatsma:2013:ESC

[SCM13] T. P. Straatsma and Daniel G. Chavarría-Miranda. On eliminating synchronous communication in molecular simulations to improve scalability. *Computer Physics Communications*, 184(12):2634–2640, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551300026X`.

Stella:2014:EEC

[SCM14] Sabrina Stella, Roberto Chignola, and Edoardo Milotti. Efficient and extendible class scheme for the combined reaction-diffusion of multiple molecular species. *Computer Physics Communications*, 185(3):826–835, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004074`.

Stegmeir:2016:FLM

[SCM+16] Andreas Stegmeir, David Coster, Omar Maj, Klaus Hallatschek, and Karl Lackner. The field line map approach for simulations of magnetically confined plasmas. *Computer Physics Communications*, 198(??):139–153, January 2016.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003641.

Sun:2018:MRD

[SCM+18] P. N. Sun, A. Colagrossi, S. Marrone, M. Antuono, and A. M. Zhang. Multi-resolution delta-plus-SPH with tensile instability control: Towards high Reynolds number flows. *Computer Physics Communications*, 224(??):63–80, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303995.

Shirvan:2018:CBC

[SCNJ18] Alireza Javidi Shirvan, Isabelle Choquet, Håkan Nilsson, and Hrvoje Jasak. Coupling boundary condition for high-intensity electric arc attached on a non-homogeneous refractory cathode. *Computer Physics Communications*, 222(??):31–45, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302977.

Scott:2013:ECS

[Sco13] N. S. Scott. Editor's corrigendum to “Phonon dispersion measured directly from molecular dynamics simulations” [Comput. Phys. Comm. **182** (10) (2011) 2201–2207]. *Computer Physics Communications*, 184(4):1348, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003906. See [Kon11].

Scott:2016:E

[Sco16] N. S. Scott. Editorial. *Computer Physics Communications*, 206(??):1, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301187.

Scott:2019:OPG

[Sco19] Stan Scott. Obituary: Philip George Burke 1932–2019. *Computer Physics Communications*, 244(??):1, November 2019.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S001046551930205X.

Shang:2017:LDC

[SCRS17] Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler. Lattice dynamics calculations based on density-functional perturbation theory in real space. *Computer Physics Communications*, 215(??):26–46, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300437.

Schofield:2012:SSM

[SCS12] Grady Schofield, James R. Chelikowsky, and Yousef Saad. A spectrum slicing method for the Kohn–Sham problem. *Computer Physics Communications*, 183(3):497–505, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003675.

Shih:2011:CTC

[SCW+11] Chi-Tin Shih, Yun-Yin Cheng, Stephen A. Wells, Ching-Ling Hsu, and Rudolf A. Römer. Charge transport in cancer-related genes and early carcinogenesis. *Computer Physics Communications*, 182(1):36–38, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002067.

Shizgal:2010:MCC

[SD10a] Bernie D. Shizgal and Raouf Dridi. Maple code for the calculation of the matrix elements of the Boltzmann collision operators for mixtures. *Computer Physics Communications*, 181(9):1633–1640, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001657.

Shokri:2010:KMM

[SD10b] Ali Shokri and Mehdi Dehghan. A Not-a-Knot meshless method using radial basis functions and predictor-corrector scheme to the numerical solution of improved

Boussinesq equation. *Computer Physics Communications*, 181(12):1990–2000, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003425.

Sellier:2014:WBM

[SD14] J. M. Sellier and I. Dimov. The Wigner–Boltzmann Monte Carlo method applied to electron transport in the presence of a single dopant. *Computer Physics Communications*, 185(10):2427–2435, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001672.

Schaich:2015:PSL

[SD15] David Schaich and Thomas DeGrand. Parallel software for lattice $\mathcal{N} = 4$ supersymmetric Yang–Mills theory. *Computer Physics Communications*, 190(??):200–212, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000132.

Sui:2012:SSE

[SDJ+12] Qiao-Hong Sui, Zhong-Jun Ding, Rui Jiang, Wei Huang, Duo Sun, and Bing-Hong Wang. Slow-to-start effect in two-dimensional traffic flow. *Computer Physics Communications*, 183(3):547–551, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003821.

Sturmberg:2016:EOS

[SDL+16] Björn C. P. Sturmberg, Kokou B. Dossou, Felix J. Lawrence, Christopher G. Poulton, Ross C. McPhedran, C. Martijn de Sterke, and Lindsay C. Botten. EMUstack: an open source route to insightful electromagnetic computation via the Bloch mode scattering matrix method. *Computer Physics Communications*, 202(??):276–286, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000035.

Schunck:2012:SSH

[SDM+12] N. Schunck, J. Dobaczewski, J. McDonnell, W. Satula, J. A. Sheikh, A. Staszczak, M. Stoitsov, and P. Toivanen. Solution of the Skyrme–Hartree–Fock–Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis.: (VII) `hfodd` (v2.49t): a new version of the program. *Computer Physics Communications*, 183(1):166–192, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002852`.

Schouten:2015:AME

[SDS15] D. Schouten, A. DeAbreu, and B. Stelzer. Accelerated matrix element method with parallel computing. *Computer Physics Communications*, 192(??):54–59, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000776`.

Schunck:2017:SSH

[SDS+17] N. Schunck, J. Dobaczewski, W. Satula, P. Baczyk, J. Dudek, Y. Gao, M. Konieczka, K. Sato, Y. Shi, X. B. Wang, and T. R. Werner. Solution of the Skyrme–Hartree–Fock–Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis. (VIII) `hfodd` (v2.73y): a new version of the program. *Computer Physics Communications*, 216(??):145–174, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517300942`.

Shcherbakov:2015:FGN

[SEGP15] Dmitry Shcherbakov, Matthias Ehrhardt, Michael Günther, and Michael Peardon. Force-gradient nested multirate methods for Hamiltonian systems. *Computer Physics Communications*, 187(??):91–97, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551400352X`.

Semenov:2016:LPA

[Sem16] A. Semenov. LanHEP — a package for automatic generation of Feynman rules from the Lagrangian. Version 3.2.

Computer Physics Communications, 201(??):167–170, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000199.

Serebrennikov:2010:NSA

[Ser10] Aleksey M. Serebrennikov. A novel semi-analytic method for the analysis of scattering by dielectric objects immersed in uniform media. *Computer Physics Communications*, 181(6):1087–1095, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000573.

Serov:2017:OFS

[Ser17] Vladislav V. Serov. Orthogonal fast spherical Bessel transform on uniform grid. *Computer Physics Communications*, 216(??):63–76, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300772.

Schimeczek:2012:HOC

[SEW12] C. Schimeczek, D. Engel, and G. Wunner. A highly optimized code for calculating atomic data at neutron star magnetic field strengths using a doubly self-consistent Hartree–Fock–Roothaan method. *Computer Physics Communications*, 183(7):1502–1510, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000641.

Schimeczek:2014:HOC

[SEW14] C. Schimeczek, D. Engel, and G. Wunner. A highly optimized code for calculating atomic data at neutron star magnetic field strengths using a doubly self-consistent Hartree–Fock–Roothaan method. *Computer Physics Communications*, 185(5):1498–1499, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000393.

Stamatiadis:2010:ATA

[SF10] S. Stamatiadis and S. C. Farantos. auto_deriv: Tool for automatic differentiation of a Fortran code. *Computer Physics Communications*, 181(10):1818–1819, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002444.

Santos-Filho:2011:MCS

[SFP11] J. B. Santos-Filho and J. A. Plascak. Monte Carlo simulations of the site-diluted three-dimensional XY model. *Computer Physics Communications*, 182(5):1130–1133, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000312.

Salvat:2019:RFS

[SFV19] Francesc Salvat and José M. Fernández-Varea. `radial`: a Fortran subroutine package for the solution of the radial Schrödinger and Dirac wave equations. *Computer Physics Communications*, 240(??):165–177, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300633.

Schlipf:2015:OAG

[SG15] Martin Schlipf and François Gygi. Optimization algorithm for the generation of ONCV pseudopotentials. *Computer Physics Communications*, 196(??):36–44, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001897.

Sargsyan:2018:CCS

[SGAA18] V. V. Sargsyan, S. Yu. Grigoryev, G. G. Adamian, and N. V. Antonenko. Capture cross section with quantum diffusion approach. *Computer Physics Communications*, 233(??):145–155, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302194.

Sant:2016:ITG

[SGDS16] Marco Sant, Andrea Gabrieli, Pierfranco Demontis, and Giuseppe B. Suffritti. InfiniCharges: a tool for generating partial charges via the simultaneous fit of multiframe electrostatic potential (ESP) and total dipole fluctuations (TDF). *Computer Physics Communications*, 200(??):190–198, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003732`.

Sala:2011:EIF

[SGM11a] Jonàs Sala, Elvira Guàrdia, and Marco Masia. Erratum to "Improving the force matching algorithm: Application to a simple point charge flexible model of water" [Comput. Phys. Comm. **182** (9) (2011) 1954–1957]. *Computer Physics Communications*, 182(11):2443, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002359`. See [SGM11b].

Sala:2011:IFM

[SGM11b] Jonàs Sala, Elvira Guàrdia, and Marco Masia. Improving the force matching algorithm: Application to a simple point charge flexible model of water. *Computer Physics Communications*, 182(9):1954–1957, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004753`. See erratum [SGM11a].

Saunders:2018:DSL

[SGM18] William Robert Saunders, James Grant, and Eike Hermann Müller. A domain specific language for performance portable molecular dynamics algorithms. *Computer Physics Communications*, 224(??):119–135, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465517303892`.

Sanchez-Gil:2017:NNG

[SGNL17] Vicente Sánchez-Gil, Eva G. Noya, and Enrique Lomba. NRMC — a GPU code for N-reverse Monte Carlo modeling of fluids in confined media. *Computer Physics*

Communications, 217(??):198–203, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301224.

Starrett:2019:WRE

[SGSG19] C. E. Starrett, N. M. Gill, T. Sjostrom, and C. W. Greeff. Wide ranging equation of state with Tartarus: a hybrid Green's function/orbital based average atom code. *Computer Physics Communications*, 235(??):50–62, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303503.

Shinaoka:2017:CTH

[SGW17] Hiroshi Shinaoka, Emanuel Gull, and Philipp Werner. Continuous-time hybridization expansion quantum impurity solver for multi-orbital systems with complex hybridizations. *Computer Physics Communications*, 215(??):128–136, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300036.

Salib:2012:CRD

[SH12a] Isaac Gabriel Salib and Shimon Haber. Is the cutoff radius in DPD simulations with a fluid of constant density arbitrary? *Computer Physics Communications*, 183(8):1714–1718, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001178.

Siro:2012:EDH

[SH12b] T. Siro and A. Harju. Exact diagonalization of the Hubbard model on graphics processing units. *Computer Physics Communications*, 183(9):1884–1889, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001452.

Siro:2016:EDQ

[SH16] T. Siro and A. Harju. Exact diagonalization of quantum lattice models on coprocessors. *Computer Physics Communications*, 207(??):274–281, October 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302065.

Schmidt:2018:WMP

[SH18] Burkhard Schmidt and Carsten Hartmann. WavePacket: A Matlab package for numerical quantum dynamics. II: Open quantum systems, optimal control, and model reduction. *Computer Physics Communications*, 228(??):229–244, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300614.

Shang:2013:PAL

[Sha13a] Zhi Shang. Performance analysis of large scale parallel CFD computing based on Code_Saturne. *Computer Physics Communications*, 184(2):381–386, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200313X.

Shao:2013:HOA

[Sha13b] Hua-Sheng Shao. HELAC-Onia: an automatic matrix element generator for heavy quarkonium physics. *Computer Physics Communications*, 184(11):2562–2570, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001938.

Shao:2016:HOU

[Sha16] Hua-Sheng Shao. HELAC-Onia 2.0: an upgraded matrix-element and event generator for heavy quarkonium physics. *Computer Physics Communications*, 198(??):238–259, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003495.

Shakirov:2018:CEF

[Sha18] T. Shakirov. Convergence estimation of flat-histogram algorithms based on simulation results. *Computer Physics Communications*, 228(??):38–43, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830081X.

Shizgal:2016:ENQ

[Shi16] Bernie D. Shizgal. An efficient nonclassical quadrature for the calculation of nonresonant nuclear fusion reaction rate coefficients from cross section data. *Computer Physics Communications*, 205(??):61–68, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300972.

Smith:2011:DSI

[SHL+11] Matthew R. Smith, Chieh-Tsan Hung, Kun-Mo Lin, Jong-Shinn Wu, and Jen-Perng Yu. Development of a semi-implicit fluid modeling code using finite-volume method based on Cartesian grids. *Computer Physics Communications*, 182(1):170–172, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001724.

Soin:2011:ESC

[SHNM11] Preetma Soin, A. P. Horsfield, and D. Nguyen-Manh. Efficient self-consistency for magnetic tight binding. *Computer Physics Communications*, 182(6):1350–1360, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000695.

Shtabovenko:2017:FCF

[Sht17] Vladyslav Shtabovenko. FeynHelpers: Connecting FeynCalc to FIRE and Package-X. *Computer Physics Communications*, 218(??):48–65, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301285.

Sarkimaki:2018:ATS

[SHT18] K. Särkimäki, E. Hirvijoki, and J. Terävä. Adaptive time-stepping Monte Carlo integration of Coulomb collisions. *Computer Physics Communications*, 222(??):374–383, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303326.

Sarkar:2018:ECE

[SHW18] Kanchan Sarkar, N. A. W. Holzwarth, and R. M. Wentzcovitch. EPAW-1.0 code for evolutionary optimization of PAW datasets especially for high-pressure applications. *Computer Physics Communications*, 233(??):110–122, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301826.

Senkov:2013:HPF

[SHZ13] R. A. Sen'kov, M. Horoi, and V. G. Zelevinsky. A high-performance Fortran code to calculate spin- and parity-dependent nuclear level densities. *Computer Physics Communications*, 184(1):215–221, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002925.

Saito:2011:PGL

[SI11] Nen Saito and Yukito Iba. Probability of graphs with large spectral gap by multicanonical Monte Carlo. *Computer Physics Communications*, 182(1):223–225, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002328.

Sibidanov:2017:RSB

[Sib17] Alexei Sibidanov. A revision of the subtract-with-borrow random number generators. *Computer Physics Communications*, 221(??):299–303, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302916.

Sierakowski:2016:GCR

[Sie16] Adam J. Sierakowski. GPU-centric resolved-particle disperse two-phase flow simulation using the Physalis method. *Computer Physics Communications*, 207(??):24–34, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301229.

Souto-Iglesias:2013:CM

[SIMGCP13] Antonio Souto-Iglesias, Fabricio Macià, Leo M. González, and Jose L. Cercos-Pita. On the consistency of MPS. *Computer Physics Communications*, 184(3):732–745, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003852. See addendum [SIMGCP14].

Souto-Iglesias:2014:ASC

[SIMGCP14] Antonio Souto-Iglesias, Fabricio Macià, Leo M. González, and Jose L. Cercos-Pita. Addendum to "On the consistency of MPS" [Comput. Phys. Comm. **184** (3) (2013) 732–745]. *Computer Physics Communications*, 185(2):595–598, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003469. See [SIMGCP13].

Sindhikara:2011:MRS

[Sin11] Daniel J. Sindhikara. Modular reweighting software for statistical mechanical analysis of biased equilibrium data. *Computer Physics Communications*, 182(10):2227–2231, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001640.

Sindhikara:2012:MRS

[Sin12a] Daniel J. Sindhikara. Modular reweighting software for statistical mechanical analysis of biased equilibrium data. *Computer Physics Communications*, 183(7):1560–1561, July 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000860.

Sinha:2012:PWL

[Sin12b] Suman Sinha. Performance of Wang–Landau algorithm in lattice model of liquid crystals. *Computer Physics Communications*, 183(12):2616–2621, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465512002536.

Satake:2010:BTD

[SISW10] S. Satake, Y. Idomura, H. Sugama, and T.-H. Watanabe. Benchmark test of drift-kinetic and gyrokinetic codes through neoclassical transport simulations. *Computer Physics Communications*, 181(6):1069–1076, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000536.

Sitnik:2014:DFMa

[Sit14a] I. M. Sitnik. Development of the FUMILI minimization package. *Computer Physics Communications*, 185(2):599–603, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002622.

Sitnik:2014:DFMb

[Sit14b] I. M. Sitnik. Development of the FUMILI minimization package. *Computer Physics Communications*, 185(10):2800, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001696.

Sitnik:2016:NVF

[Sit16] I. M. Sitnik. The new version of the FUMILIM minimization package. *Computer Physics Communications*, 209(??):199, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302338.

Site:2018:GCA

[Sit18] Luigi Delle Site. Grand Canonical adaptive resolution simulation for molecules with electrons: a theoretical framework based on physical consistency. *Computer Physics Communications*, 222(??):94–101, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303259.

Slawinska:2011:MUF

[SJ11] M. Slawinska and S. Jadach. MCdevelop — a universal framework for stochastic simulations. *Computer Physics Communications*, 182(3):748–762, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004236`.

Schnabel:2017:DGA

[SJ17] Stefan Schnabel and Wolfhard Janke. Dynamic greedy algorithms for the Edwards–Anderson model. *Computer Physics Communications*, 220(??):74–80, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302011`.

Sorensen:2019:QCL

[SJHS19] J. J. Sørensen, J. H. M. Jensen, T. Heinzel, and J. F. Sherson. QEngine: a C++ library for quantum optimal control of ultracold atoms. *Computer Physics Communications*, 243(??):135–150, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301377`.

Sun:2010:TTL

[SJW10] Duo Sun, Rui Jiang, and Bing-Hong Wang. Timing of traffic lights and phase separation in two-dimensional traffic flow. *Computer Physics Communications*, 181(2):301–304, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509003142`.

Szidarovszky:2018:LCP

[SJY18] Tamás Szidarovszky, Maho Jono, and Kaoru Yamanouchi. LIMAO: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops. *Computer Physics Communications*, 228(??):219–228, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300626`. See erratum [SJY20].

Szidarovszky:2020:ELC

[SJY20] Tamás Szidarovszky, Maho Jono, and Kaoru Yamanouchi. Erratum to "LIMAO: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops" [Comput. Phys. Comm. **228** (2018) 219–228]. *Computer Physics Communications*, 252(??):Article 107106, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304151`. See [SJY18].

Sobol:2010:NDB

[SK10] I. M. Sobol' and S. Kucherenko. A new derivative based importance criterion for groups of variables and its link with the global sensitivity indices. *Computer Physics Communications*, 181(7):1212–1217, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551000086X`.

Seebacher:2012:TUL

[SK12] J. Seebacher and A. Kendl. Towards a unified linear kinetic transport model with the trace ion module for EIRENE. *Computer Physics Communications*, 183(4):947–959, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511004097`.

Singh:2014:ENT

[SK14] Randhir Singh and Jitendra Kumar. An efficient numerical technique for the solution of nonlinear singular boundary value problems. *Computer Physics Communications*, 185(4):1282–1289, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000034`.

Sen:2015:SBS

[SK15] Shuvam Sen and Jiten C. Kalita. A 4OEC scheme for the biharmonic steady Navier–Stokes equations in non-rectangular domains. *Computer Physics Communications*, 196(??):113–133, November 2015. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002040.

Samana:2010:QNC

[SKB10] A. R. Samana, F. Krmpotić, and C. A. Bertulani. QRAP: a numerical code for projected (Q)uasiparticle (RA)ndom (P)hase approximation. *Computer Physics Communications*, 181(6):1123–1135, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000366.

Seth:2016:TCC

[SKFP16] Priyanka Seth, Igor Krivenko, Michel Ferrero, and Olivier Parcollet. TRIQS/CTHYB: a continuous-time quantum Monte Carlo hybridisation expansion solver for quantum impurity problems. *Computer Physics Communications*, 200(??):274–284, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500404X.

Smith:2010:ROB

[SKH+10] Matthew R. Smith, Fang-An Kuo, Chih-Wei Hsieh, Jen-Perng Yu, Jong-Shinn Wu, and Alex Ferguson. Rapid optimization of blast wave mitigation strategies using Quiet Direct Simulation and Genetic Algorithm. *Computer Physics Communications*, 181(6):1025–1036, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000482.

Sobczak:2011:GAA

[SKK11] Pawel Sobczak, Lukasz Kucharski, and Grzegorz Kamieniarz. Genetic algorithm approach to calculation of geometric configurations of 2D clusters of uniformly charged classical particles. *Computer Physics Communications*, 182(9):1900–1903, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511000075.

Slaby:2017:CEG

[SKK17] Christoph Slaby, Ralf Kleiber, and Axel Könies. Combining electromagnetic gyro-kinetic particle-in-cell simulations with collisions. *Computer Physics Communications*, 218(??):1–9, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551730125X`.

Sato:2019:CSS

[SKK+19] R. Sato, S. Kawata, T. Karino, K. Uchibori, T. Iinuma, H. Katoh, and A. I. Ogoyski. Code O-SUKI: Simulation of direct-drive fuel target implosion in heavy ion inertial fusion. *Computer Physics Communications*, 240(??):83–100, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300815`.

Spiechowicz:2015:GAM

[SKM15] J. Spiechowicz, M. Kostur, and L. Machura. GPU accelerated Monte Carlo simulation of Brownian motors dynamics with CUDA. *Computer Physics Communications*, 191(??):140–149, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000417`.

Simonsen:2011:LSA

[SKML11] Ingve Simonsen, Jacob B. Kryvi, Alexei A. Maradudin, and Tamara A. Leskova. Light scattering from anisotropic, randomly rough, perfectly conducting surfaces. *Computer Physics Communications*, 182(9):1904–1908, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000300`.

Sudheer:2013:DLB

[SKSK13] C. D. Sudheer, S. Krishnan, A. Srinivasan, and P. R. C. Kent. Dynamic load balancing for petascale quantum Monte Carlo applications: the Alias method. *Computer Physics Communications*, 184(2):284–292, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002949`.

Liu:2010:ACD

[sL10] Cheng shi Liu. Applications of complete discrimination system for polynomial for classifications of traveling wave solutions to nonlinear differential equations. *Computer Physics Communications*, 181(2):317–324, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003191.

Sun:2014:CAM

[SL14] Hai-Wei Sun and Leonard Z. Li. A CCD–ADI method for unsteady convection-diffusion equations. *Computer Physics Communications*, 185(3):790–797, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004025.

Santos:2016:OOI

[SL16] Pedro Duarte Santos and Andrea Lani. An object-oriented implementation of a parallel Monte Carlo code for radiation transport. *Computer Physics Communications*, 202(??):233–261, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004555.

Schmidt:2017:WMP

[SL17] Burkhard Schmidt and Ulf Lorenz. WavePacket: a Matlab package for numerical quantum dynamics. I: Closed quantum systems and discrete variable representations. *Computer Physics Communications*, 213(??):223–234, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303861.

Shih:2011:SAM

[SLC11] Chi-Tin Shih, Hsuan-Wen Lin, and Ann-Shyn Chiang. Statistical analysis and modeling of the temperature-dependent sleep behavior of drosophila. *Computer Physics Communications*, 182(1):195–197, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002547.

Stahl:2017:NSR

[SLEF17] A. Stahl, M. Landreman, O. Embréus, and T. Fülöp. NORSE: a solver for the relativistic non-linear Fokker–Planck equation for electrons in a homogeneous plasma. *Computer Physics Communications*, 212(??):269–279, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303459.

Shemyakin:2019:THP

[SLK19] O. P. Shemyakin, P. R. Levashov, and P. A. Krasnova. TFmix: a high-precision implementation of the finite-temperature Thomas–Fermi model for a mixture of atoms. *Computer Physics Communications*, 235(??):378–387, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303229.

Stahl:2017:AAP

[SLLP17] Christian Stahl, Jörg Leske, Marc Lettmann, and Norbert Pietralla. APCAD — analysis program for the continuous-angle DSAM. *Computer Physics Communications*, 214(??):174–198, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300103.

Lu:2013:EUL

[sLqSqL+13] Feng shun Lu, Jun qiang Song, Wang qun Lin, Yu fei Pang, Kai jun Ren, and Pei chang Shi. Efficient utilization of launched threads on GPUs: the spherical harmonic transform as a case study. *Computer Physics Communications*, 184(11):2494–2502, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002269.

Shumlak:2011:APC

[SLR+11] U. Shumlak, R. Lilly, N. Reddell, E. Sousa, and B. Srinivasan. Advanced physics calculations using a multi-fluid plasma model. *Computer Physics Communications*, 182(9):1767–1770, September 2011. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100004X.

Solanpaa:2016:BSP

[SLR16] J. Solanpää, P. J. J. Luukko, and E. Räsänen. Bill2d — a software package for classical two-dimensional Hamiltonian systems. *Computer Physics Communications*, 199(??):133–138, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003744.

Shi:2019:ETD

[SLW19a] Honglong Shi, Minting Luo, and Wenzhong Wang. ElectronDiffraction tools, a DigitalMicrograph package for electron diffraction analysis. *Computer Physics Communications*, 243(??):166–173, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301262.

Shi:2019:ETP

[SLW19b] Honglong Shi, Minting Luo, and Wenzhong Wang. ePDF tools, a processing and analysis package of the atomic pair distribution function for electron diffraction. *Computer Physics Communications*, 238(??):295–301, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304119.

Scheffel:2018:TSA

[SLY18] Jan Scheffel, Kristoffer Lindvall, and Hiu Fai Yik. A time-spectral approach to numerical weather prediction. *Computer Physics Communications*, 226(??):127–135, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300146.

Si:2016:LSM

[SLZ16] Lisha Si, Xiaoyun Liao, and Nengji Zhou. Large-scale Monte Carlo simulations for the depinning transition in Ising-type lattice models. *Computer Physics Communications*, 209(??):34–41, December 2016. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302399.

Silva:2011:STM

[SM11] T. F. Silva and M. N. Martins. Statistical treatment of misalignments in particle accelerators. *Computer Physics Communications*, 182(3):679–682, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004765.

Sauter:2013:TCC

[SM13] O. Sauter and S. Yu. Medvedev. Tokamak coordinate conventions: *COCOS*. *Computer Physics Communications*, 184(2):293–302, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002962.

Sen:2014:MCP

[SM14] Soubhadra Sen and N. Mohankumar. Migpore, a code package for the estimation of migration of radioactive species in a porous medium. *Computer Physics Communications*, 185(1):302–306, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002737.

Schneider:2019:MAM

[SM19] L. Schneider and M. Müller. Multi-architecture Monte-Carlo (MC) simulation of soft coarse-grained polymeric materials: SOft coarse grained Monte-Carlo acceleration (SOMA). *Computer Physics Communications*, 235(??):463–476, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303072.

Stegmeir:2017:AFC

[SMC+17] Andreas Stegmeir, Omar Maj, David Coster, Karl Lackner, Markus Held, and Matthias Wiesenberger. Advances in the flux-coordinate independent approach. *Computer Physics Communications*, 213(??):111–121, April 2017. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303939.

Stankovic:2015:TUM

[SMCB+15] Jelena Stankovic, Predrag Marinkovic, Olivera Ciraj-Bjelac, Jelica Kaljevic, Danijela Arandjic, and Djordje Lazarevic. Toward utilization of MCNP5 particle track output file for simulation problems in photon spectrometry. *Computer Physics Communications*, 195(??):77–83, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001691.

Silva:2014:SSS

[SMdONF14] E. V. Corrêa Silva, G. A. Monerat, G. de Oliveira Neto, and L. G. Ferreira Filho. Spectral: Solving Schroedinger and Wheeler–DeWitt equations in the positive semi-axis by the spectral method. *Computer Physics Communications*, 185(1):380–391, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003081.

Stepsys:2014:HHP

[SMGK14] A. Stepsys, S. Mickevicius, D. Germanas, and R. K. Kalinauskas. HOTB: High precision parallel code for calculation of four-particle harmonic oscillator transformation brackets. *Computer Physics Communications*, 185(11):3062–3064, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002306.

Stepsys:2019:COF

[SMGK19] Augustinas Stepsys, Saulius Mickevicius, Darius Germanas, and Ramutis Kazys Kalinauskas. Calculation of orbital fractional parentage coefficients for five particles in translationally invariant basis. *Computer Physics Communications*, 236(??):26–33, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830359X.

Smirnov:2014:FCP

[Smi14] A. V. Smirnov. FIESTA 3: Cluster-parallelizable multi-loop numerical calculations in physical regions. *Computer Physics Communications*, 185(7):2090–2100, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000952.

Smirnov:2015:FCI

[Smi15] A. V. Smirnov. FIRE5: a C++ implementation of Feynman Integral REduction. *Computer Physics Communications*, 189(??):182–191, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004123.

Smirnov:2016:FOF

[Smi16] A. V. Smirnov. FIESTA4: Optimized Feynman integral calculations with GPU support. *Computer Physics Communications*, 204(??):189–199, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300716.

Schneider:2017:CSA

[SMJ17] Simon Schneider, Marco Mueller, and Wolfhard Janke. Convergence of stochastic approximation Monte Carlo and modified Wang–Landau algorithms: Tests for the Ising model. *Computer Physics Communications*, 216(??):1–7, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300449.

Shtabovenko:2016:NDF

[SMO16a] Vladyslav Shtabovenko, Rolf Mertig, and Frederik Orellana. New developments in FeynCalc 9.0. *Computer Physics Communications*, 207(??):432–444, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301709.

Somogyi:2016:PPT

[SMO16b] Endre Somogyi, Andrew Abi Mansour, and Peter J. Ortoleva. ProtoMD: a prototyping toolkit for multiscale molecular dynamics. *Computer Physics Communications*, 202(??):337–350, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300030`.

Sanna:2019:VNV

[SMOB19] N. Sanna, G. Morelli, S. Orlandini, and I. Baccarelli. VOLSCAT2.0: the new version of the package for electron and positron scattering off molecular targets. *Computer Physics Communications*, 235(??):366–377, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303230`.

Shimizu:2019:TRB

[SMUT19] Noritaka Shimizu, Takahiro Mizusaki, Yutaka Utsuno, and Yusuke Tsunoda. Thick-restart block Lanczos method for large-scale shell-model calculations. *Computer Physics Communications*, 244(??):372–384, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `https://www.sciencedirect.com/science/article/pii/S0010465519301985`.

Sikarudi:2016:NRB

[SN16] M. A. Esmaili Sikarudi and A. H. Nikseresht. Neumann and Robin boundary conditions for heat conduction modeling using smoothed particle hydrodynamics. *Computer Physics Communications*, 198(??):1–11, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002738`.

Schneider:2011:PSM

[SNB11] Kai Schneider, Salah Neffaa, and Wouter J. T. Bos. A pseudo-spectral method with volume penalisation for magnetohydrodynamic turbulence in confined domains. *Computer Physics Communications*, 182(1):2–7, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001736`.

Sebilleau:2011:MMS

[SNG+11] Didier Sébilleau, Calogero Natoli, George M. Gavaza, Haifeng Zhao, Fabiana Da Pieve, and Keisuke Hatada. MsSpec-1.0: a multiple scattering package for electron spectroscopies in material science. *Computer Physics Communications*, 182(12):2567–2579, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002591.

Sho:2019:PDD

[SO19] Shohiro Sho and Shinji Odanaka. Parallel domain decomposition methods for a quantum-corrected drift–diffusion model for MOSFET devices. *Computer Physics Communications*, 237(??):8–16, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303771.

Starinshak:2014:NPA

[SOJ14] D. P. Starinshak, J. M. Owen, and J. N. Johnson. A new parallel algorithm for constructing Voronoi tessellations from distributed input data. *Computer Physics Communications*, 185(12):3204–3214, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003014.

Sokolov:2013:AOI

[Sok13] Igor V. Sokolov. Alternating-order interpolation in a charge-conserving scheme for particle-in-cell simulations. *Computer Physics Communications*, 184(2):320–328, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003013.

Solovyev:2011:RMC

[Sol11] I. V. Solovyev. Realistic modeling of complex oxide materials. *Computer Physics Communications*, 182(1):43–45, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002997.

Shimojo:2013:LNQ

[SOM+13] Fuyuki Shimojo, Satoshi Ohmura, Weiwei Mou, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta. Large nonadiabatic quantum molecular dynamics simulations on parallel computers. *Computer Physics Communications*, 184(1):1–8, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002548`.

Schulz:2011:SDS

[SÓÓN11] Henrik Schulz, Géza Ódor, Gergely Ódor, and Máté Ferenc Nagy. Simulation of 1 + 1 dimensional surface growth and lattices gases using GPUs. *Computer Physics Communications*, 182(7):1467–1476, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001081`.

Staub:2012:TBI

[SOPS12] Florian Staub, Thorsten Ohl, Werner Porod, and Christian Speckner. A tool box for implementing supersymmetric models. *Computer Physics Communications*, 183(10):2165–2206, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551200152X`.

Sorensen:2019:AAS

[Sør19] Kristian Tølbøl Sørensen. `asasim`: Adaptive sampling for electromagnetic simulations. *Computer Physics Communications*, 236(??):268–273, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303655`.

Souvatzis:2014:UVE

[Sou14] Petros Souvatzis. Uquantchem: a versatile and easy to use quantum chemistry computational software. *Computer Physics Communications*, 185(1):415–421, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003159`.

St-Onge:2019:ESS

[SOYHDD19] Guillaume St-Onge, Jean-Gabriel Young, Laurent Hébert-Dufresne, and Louis J. Dubé. Efficient sampling of spreading processes on complex networks using a composition and rejection algorithm. *Computer Physics Communications*, 240(??):30–37, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300608.

Schreilechner:2016:RSF

[SP16] Magdalena Schreilechner and Walter Pötz. Real-space finite difference scheme for the von Neumann equation with the Dirac Hamiltonian. *Computer Physics Communications*, 204(??):43–54, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300637.

Schwendt:2018:TBC

[SP18a] Mathias Schwendt and Walter Pötz. Transparent boundary conditions for the Bogoliubov–de Gennes equation in $(1+1)$D. *Computer Physics Communications*, 229(??):129–147, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830105X.

Shen:2018:PPC

[SP18b] Hua Shen and Matteo Parsani. Positivity-preserving CE/SE schemes for solving the compressible Euler and Navier–Stokes equations on hybrid unstructured meshes. *Computer Physics Communications*, 232(??):165–176, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301747.

Sibalic:2017:AOS

[SPAW17] N. Sibalić, J. D. Pritchard, C. S. Adams, and K. J. Weatherill. ARC: an open-source library for calculating properties of alkali Rydberg atoms. *Computer Physics Communications*, 220(??):319–331, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465517301972.

Shelley:2011:AQC

[SPMM11] Matthew Shelley, Nicolas Poilvert, Arash A. Mostofi, and Nicola Marzari. Automated quantum conductance calculations using maximally-localised Wannier functions. *Computer Physics Communications*, 182(10):2174–2183, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002074.

Suryanarayana:2019:AAR

[SPP19] Phanish Suryanarayana, Phanisri P. Pratapa, and John E. Pask. Alternating Anderson–Richardson method: an efficient alternative to preconditioned Krylov methods for large, sparse linear systems. *Computer Physics Communications*, 234(??):278–285, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830256X.

Singh:2010:SAH

[SPS10] Vineet K. Singh, Rajesh K. Pandey, and Saurabh Singh. A stable algorithm for Hankel transforms using hybrid of block-pulse and Legendre polynomials. *Computer Physics Communications*, 181(1):1–10, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002409.

Solala:2018:TDB

[SPS18] Eelis Solala, Pauli Parkkinen, and Dage Sundholm. Tensor decompositions for the bubbles and cube numerical framework. *Computer Physics Communications*, 232(??):98–103, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301796.

Suryanarayana:2018:SSQ

[SPSP18] Phanish Suryanarayana, Phanisri P. Pratapa, Abhiraj Sharma, and John E. Pask. SQDFT: Spectral quadrature method for large-scale parallel $O(N)$ Kohn–Sham calculations at high temperature. *Computer Physics Communications*, 224(??):288–298, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304022.

Sanchez-Puga:2019:BDP

[SPTPR19] Pablo Sánchez-Puga, Javier Tajuelo, Juan Manuel Pastor, and Miguel A. Rubio. BiconeDrag — a data processing application for the oscillating conical bob interfacial shear rheometer. *Computer Physics Communications*, 239(??):184–196, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300396.

Singh:2011:AZT

[SPY11] Abhishek K. Singh, Evgeni S. Penev, and Boris I. Yakobson. Armchair or zigzag? A tool for characterizing graphene edge. *Computer Physics Communications*, 182(3):804–807, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004820.

Soulaine:2015:PLA

[SQA+15] Cyprien Soulaine, Michel Quintard, Hervé Allain, Bertrand Baudouy, and Rob Van Weelderen. A PISO-like algorithm to simulate superfluid helium flow with the two-fluid model. *Computer Physics Communications*, 187(??):20–28, February 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003415.

Su:2010:FPC

[SQL+10] Wei Su, Ping Qian, Ying Liu, Jiang Shen, and Nan-Xian Chen. First principle calculations of yttrium-doped palladium clusters. *Computer Physics Communications*, 181(4):726–731, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003956.

Shen:2016:IVC

[SQS+16] Chun Shen, Zhi Qiu, Huichao Song, Jonah Bernhard, Steffen Bass, and Ulrich Heinz. The iEBE–VISHNU code package for relativistic heavy-ion collisions. *Computer Physics Communications*, 199(??):61–85, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003392.

Sekhar:2012:EHO

[SR12] T. V. S. Sekhar and B. Hema Sundar Raju. An efficient higher order compact scheme to capture heat transfer solutions in spherical geometry. *Computer Physics Communications*, 183(11):2337–2345, November 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002020.

Schuetrumpf:2018:TCS

[SRS+18] B. Schuetrumpf, P.-G. Reinhard, P. D. Stevenson, A. S. Umar, and J. A. Maruhn. The TDHF code Sky3D version 1.1. *Computer Physics Communications*, 229(??):211–213, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300845.

Sony:2010:GPF

[SS10a] Priya Sony and Alok Shukla. A general purpose Fortran 90 electronic structure program for conjugated systems using Pariser–Parr–Pople model. *Computer Physics Communications*, 181(4):821–830, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046550900407X.

Stavroyiannis:2010:NET

[SS10b] S. Stavroyiannis and T. E. Simos. A nonlinear explicit two-step fourth algebraic order method of order infinity for linear periodic initial value problems. *Computer Physics Communications*, 181(8):1362–1368, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001128.

Shkarofsky:2011:NCC

[SS11a] I. Shkarofsky and M. Shoucri. A numerical code for the calculation of relativistic electron cyclotron damping with an arbitrary distribution function at an arbitrary harmonic. *Computer Physics Communications*, 182(7):1507–1517, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001147`.

Silin:2011:HFV

[SS11b] I. Silin and R. Sydora. Hybrid Fourier–Vlasov simulation in non-inertial reference frames. *Computer Physics Communications*, 182(12):2508–2518, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002463`.

Smiatek:2011:MSE

[SS11c] Jens Smiatek and Friederike Schmid. Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels. *Computer Physics Communications*, 182(9):1941–1944, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004674`.

Schmidt:2012:CCP

[SS12] Barbara Schmidt and Matthias Steinhauser. CRunDec: a C++ package for running and decoupling of the strong coupling and quark masses. *Computer Physics Communications*, 183(9):1845–1848, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001282`.

Sezgin:2013:FBP

[SS13a] Fatin Sezgin and Tevfik Metin Sezgin. Finding the best portable congruential random number generators. *Computer Physics Communications*, 184(8):1889–1897, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001100`.

Shokri:2013:NCI

[SS13b] Ali Shokri and Abbas Ali Shokri. The new class of implicit L-stable hybrid Obrechkoff method for the numerical solution of first order initial value problems. *Computer Physics Communications*, 184(3):529–531, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003360.

Smirnov:2013:FLA

[SS13c] A. V. Smirnov and V. A. Smirnov. FIRE4, LiteRed and accompanying tools to solve integration by parts relations. *Computer Physics Communications*, 184(12):2820–2827, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002105.

Schreiner:2014:WPI

[SS14] Cedric Schreiner and Felix Spanier. Wave-particle-interaction in kinetic plasmas. *Computer Physics Communications*, 185(7):1981–1986, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001088.

Solovjeva:2018:CSE

[SS18] T. M. Solovjeva and A. G. Soloviev. Comparative study of the effectiveness of PROOF with other parallelization methods implemented in the ROOT software package. *Computer Physics Communications*, 233(??):41–43, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302285.

Sataric:2016:HOM

[SSB+16] Bogdan Satarić, Vladimir Slavnić, Aleksandar Belić, Antun Balaz, Paulsamy Muruganandam, and Sadhan K. Adhikari. Hybrid OpenMP/MPI programs for solving the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap. *Computer Physics Communications*, 200(??):411–417, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004440.

Streib:2015:SSI

[SSBS15] Amanda Streib, Noah Streib, Isabel Beichl, and Francis Sullivan. Stratified sampling for the Ising model: a graph-theoretic approach. *Computer Physics Communications*, 191(??):1–8, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000144.

Siegel:2014:ICP

[SSF+14] A. Siegel, K. Smith, K. Felker, P. Romano, B. Forget, and P. Beckman. Improved cache performance in Monte Carlo transport calculations using energy banding. *Computer Physics Communications*, 185(4):1195–1199, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003366.

Schmieschek:2017:LPI

[SSF+17] S. Schmieschek, L. Shamardin, S. Frijters, T. Krüger, U. D. Schiller, J. Harting, and P. V. Coveney. LB3D: a parallel implementation of the Lattice-Boltzmann method for simulation of interacting amphiphilic fluids. *Computer Physics Communications*, 217(??):149–161, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301017.

Schneider:2010:NFP

[SSG+10] Barry I. Schneider, Javier Segura, Amparo Gil, Xiaoxu Guan, and Klaus Bartschat. A new Fortran 90 program to compute regular and irregular associated Legendre functions. *Computer Physics Communications*, 181(12):2091–2097, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003450.

Schneider:2018:NFP

[SSG+18] Barry I. Schneider, Javier Segura, Amparo Gil, Xiaoxu Guan, and Klaus Bartschat. A new Fortran 90 program to compute regular and irregular associated Legendre functions (new version announcement). *Computer Physics*

Communications, 225(??):192–193, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304186.

Shen:2013:HOS

[SSH+13] Jing Shen, Wei E. I. Sha, Zhixiang Huang, Mingsheng Chen, and Xianliang Wu. High-order symplectic FDTD scheme for solving a time-dependent Schrödinger equation. *Computer Physics Communications*, 184(3):480–492, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200330X.

Simon:2016:PIA

[SSH16] Cory M. Simon, Berend Smit, and Maciej Haranczyk. pyIAST: Ideal adsorbed solution theory (IAST) Python package. *Computer Physics Communications*, 200(??):364–380, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004403.

Stoitsov:2013:ADS

[SSK+13] M. V. Stoitsov, N. Schunck, M. Kortelainen, N. Michel, H. Nam, E. Olsen, J. Sarich, and S. Wild. Axially deformed solution of the Skyrme–Hartree–Fock–Bogoliubov equations using the transformed harmonic oscillator basis (II) hfbtho v2.00d: a new version of the program. *Computer Physics Communications*, 184(6):1592–1604, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000301.

Sylwestrzak:2017:MPD

[SSM+17] Marcin Sylwestrzak, Daniel Szlag, Paul J. Marchand, Ashwin S. Kumar, and Theo Lasser. Massively parallel data processing for quantitative total flow imaging with optical coherence microscopy and tomography. *Computer Physics Communications*, 217(??):128–137, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300954.

Sitarek:2016:SRA

[SSP16] S. Sitarek, T. Stacewicz, and M. Posyniak. Software for retrieval of aerosol particle size distribution from multiwavelength lidar signals. *Computer Physics Communications*, 199(??):53–60, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003215`.

Saez:2011:IPC

[SSS+11] Xavier Sáez, Alejandro Soba, Edilberto Sánchez, Ralf Kleiber, Francisco Castejón, and José M. Cela. Improvements of the particle-in-cell code EUTERPE for petascaling machines. *Computer Physics Communications*, 182(9):2047–2051, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551000531X`.

Smirnov:2011:FPM

[SST11] A. V. Smirnov, V. A. Smirnov, and M. Tentyukov. FIESTA 2: Parallelizeable multiloop numerical calculations. *Computer Physics Communications*, 182(3):790–803, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004716`.

Shen:2014:IDB

[SSX14] Chun Shen, Fengxian Sun, and Xinlin Xia. Implementation of density-based solver for all speeds in the framework of OpenFOAM. *Computer Physics Communications*, 185(10):2730–2741, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514002136`.

Schmidt:2019:ESA

[ST19] Oliver T. Schmidt and Aaron Towne. An efficient streaming algorithm for spectral proper orthogonal decomposition. *Computer Physics Communications*, 237(??):98–109, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518304016`.

Staub:2010:SMF

[Sta10] Florian Staub. From superpotential to model files for FeynArts and CalcHep/CompHep. *Computer Physics Communications*, 181(6):1077–1086, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000561.

Staub:2011:ACS

[Sta11] Florian Staub. Automatic calculation of supersymmetric renormalization group equations and loop corrections. *Computer Physics Communications*, 182(3):808–833, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004832.

Staub:2013:SDG

[Sta13] Florian Staub. SARAH 3.2: Dirac gauginos, UFO output, and more. *Computer Physics Communications*, 184(7):1792–1809, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000763.

Staub:2014:STO

[Sta14] Florian Staub. SARAH 4: a tool for (not only SUSY) model builders. *Computer Physics Communications*, 185(6):1773–1790, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000629.

Salinas:2018:WBO

[STA18] Álvaro Salinas, Claudio E. Torres, and Orlando Ayala. Well-balanced open boundary condition in a lattice Boltzmann model for shallow water with arbitrary bathymetry. *Computer Physics Communications*, 230(??):89–98, September 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301371.

Staub:2019:XHA

[Sta19] Florian Staub. xSLHA: an Les Houches Accord reader for Python and Mathematica. *Computer Physics Communications*, 241(??):132–138, August 2019. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300918.

Stein:2017:FPA

[Ste17] Matthew Stein. A fast, parallel algorithm for distant-dependent calculation of crystal properties. *Computer Physics Communications*, 221(??):273–281, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302850.

Sakurai:2010:ABK

[STK10] T. Sakurai, H. Tadano, and Y. Kuramashi. Application of block Krylov subspace algorithms to the Wilson–Dirac equation with multiple right-hand sides in lattice QCD. *Computer Physics Communications*, 181(1):113–117, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002859.

Strater:2015:PDA

[Str15] Hendrik Sträter. PARPLE: Detailed automatized and parallel evaluation of luminescence mappings. *Computer Physics Communications*, 193(??):131–137, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001162.

Sakamoto:2011:SME

[STT11] Shoichi Sakamoto, Hiroyoshi Tsuyuki, and Mitsuyoshi Tomiya. Stochastic mechanics of electron transfer in graphene. *Computer Physics Communications*, 182(1):87–89, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002894.

Studerus:2010:RFI

[Stu10] C. Studerus. Reduze — Feynman integral reduction in C++. *Computer Physics Communications*, 181(7):1293–1300, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000925.

Shabaev:2015:QFP

[STY15] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin. QEDMOD: Fortran program for calculating the model Lamb-shift operator. *Computer Physics Communications*, 189(??):175–181, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004081.

Shabaev:2018:QFP

[STY18] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin. QEDMOD: Fortran program for calculating the model Lamb-shift operator. *Computer Physics Communications*, 223(??):69, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303478.

Sulejmanpasic:2018:APT

[SÜ18] Tin Sulejmanpasic and Mithat Ünsal. Aspects of perturbation theory in quantum mechanics: The BenderWu Mathematica(R) package. *Computer Physics Communications*, 228(??):273–289, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300420.

Stork:2017:DAE

[SUS+17a] C. L. Stork, C. C. Ummel, D. S. Stuart, S. Bodily, and B. L. Goldblum. Dynamic analysis environment for nuclear forensic analyses. *Computer Physics Communications*, 210(??):60–71, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302909.

Sussman:2017:CMP

[Sus17b] Daniel M. Sussman. cellGPU: Massively parallel simulations of dynamic vertex models. *Computer Physics Communications*, 219(??):400–406, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301832.

Stockinger:2012:FMF

[SV12] Dominik Stöckinger and Philipp Varso. FeynArts model file for MSSM transition counterterms from DREG to DRED. *Computer Physics Communications*, 183(2):422–430, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003389.

Schrock:2013:CLM

[SV13] Mario Schröck and Hannes Vogt. Coulomb, Landau and maximally Abelian gauge fixing in lattice QCD with multi-GPUs. *Computer Physics Communications*, 184(8):1907–1919, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300129X.

Sandner:2014:CMI

[SV14] Raimar Sandner and András Vukics. C++QEDv2 Milestone 10: a C++/Python application-programming framework for simulating open quantum dynamics. *Computer Physics Communications*, 185(9):2380–2382, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001349.

Svaneborg:2012:LFD

[Sva12] Carsten Svaneborg. LAMMPS framework for dynamic bonding and an application modeling DNA. *Computer Physics Communications*, 183(8):1793–1802, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001105.

Snytnikov:2010:AMA

[SVG10] A. V. Snytnikov, V. A. Vshivkov, and W. J. Goedheer. Adaptive mass alteration to model ion-ion recombination in a Particle-in-Cell simulation of silane radio-frequency discharges. *Computer Physics Communications*, 181(10):1743–1749, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002225.

Sallam:2018:GMS

[SVGS18] Mai O. Sallam, Guy A. E. Vandenbosch, Georges Gielen, and Ezzeldin A. Soliman. Generalized mode solver for plasmonic transmission lines embedded in layered media based on the Method of Moments. *Computer Physics Communications*, 233(??):1–15, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302078.

Sanchez-Vizuet:2019:HDG

[SVS19] Tonatiuh Sánchez-Vizuet and Manuel E. Solano. A hybridizable discontinuous Galerkin solver for the Grad–Shafranov equation. *Computer Physics Communications*, 235(??):120–132, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303278.

Shapoval:2019:TSP

[SVV19] Olga Shapoval, Jean-Luc Vay, and Henri Vincenti. Two-step perfectly matched layer for arbitrary-order pseudo-spectral analytical time-domain methods. *Computer Physics Communications*, 235(??):102–110, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303291.

Stevenson:2011:PSL

[SW11] Jacob D. Stevenson and Martin Weigel. Percolation and Schramm–Loewner evolution in the 2D random-field Ising model. *Computer Physics Communications*, 182(9):1879–1882, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004790.

Shi:2012:SSA

[SW12a] Wei Shi and Xinyuan Wu. On symplectic and symmetric ARKN methods. *Computer Physics Communications*, 183(6):1250–1258, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465512000586.

Stanislavsky:2012:NSC

[SW12b] Aleksander Stanislavsky and Karina Weron. Numerical scheme for calculating of the fractional two-power relaxation laws in time-domain of measurements. *Computer Physics Communications*, 183(2):320–323, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003468.

Scharoch:2013:EMD

[SW13a] Pawel Scharoch and Maciej Winiarski. An efficient method of DFT/LDA band-gap correction. *Computer Physics Communications*, 184(12):2680–2683, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002361.

Shi:2013:NSS

[SW13b] Wei Shi and Xinyuan Wu. A note on symplectic and symmetric ARKN methods. *Computer Physics Communications*, 184(11):2408–2411, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001951.

Schimeczek:2014:AFE

[SW14a] C. Schimeczek and G. Wunner. Accurate 2 d finite element calculations for hydrogen in magnetic fields of arbitrary strength. *Computer Physics Communications*, 185(2):614–621, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003275.

Schimeczek:2014:MES

[SW14b] C. Schimeczek and G. Wunner. Multi-electron systems in strong magnetic fields I: the 2D Landau–Hartree–Fock–Roothaan method. *Computer Physics Communications*, 185(10):2655–2662, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465514001593.

Shao:2014:NSN

[SW14c] Wenting Shao and Xionghua Wu. The numerical solution of the nonlinear Klein–Gordon and sine-Gordon equations using the Chebyshev tau meshless method. *Computer Physics Communications*, 185(5):1399–1409, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000344.

Su:2011:FPS

[SWL11] W. S. Su, B. R. Wu, and T. C. Leung. A first-principles study on the electromechanical effect of graphene nanoribbon. *Computer Physics Communications*, 182(1):99–102, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002511.

Shao:2015:SOP

[SWL+15] Gui-Fang Shao, Ting-Na Wang, Tun-Dong Liu, Jun-Ren Chen, Ji-Wen Zheng, and Yu-Hua Wen. Structural optimization of Pt–Pd alloy nanoparticles using an improved discrete particle swarm optimization algorithm. *Computer Physics Communications*, 186(??):11–18, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003129.

Shimobaba:2012:CWO

[SWS+12] Tomoyoshi Shimobaba, Jiantong Weng, Takahiro Sakurai, Naohisa Okada, Takashi Nishitsuji, Naoki Takada, Atsushi Shiraki, Nobuyuki Masuda, and Tomoyoshi Ito. Computational wave optics library for C++: CWO++ library. *Computer Physics Communications*, 183(5):1124–1138, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000082.

Xie:2014:PGD

[sX14] Hua sheng Xie. PDRF: a general dispersion relation solver for magnetized multi-fluid plasma. *Computer Physics*

Communications, 185(2):670–675, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003408.

Xie:2019:BUT

[sX19] Hua sheng Xie. BO: a unified tool for plasma waves and instabilities analysis. *Computer Physics Communications*, 244(??):343–371, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302012.

Shao:2018:LSI

[SXW+18] Xuecheng Shao, Qiang Xu, Sheng Wang, Jian Lv, Yanchao Wang, and Yanming Ma. Large-scale ab initio simulations for periodic system. *Computer Physics Communications*, 233(??):78–83, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302595.

Shi:2017:DTP

[SYD17] Huabin Shi, Xiping Yu, and Robert A. Dalrymple. Development of a two-phase SPH model for sediment laden flows. *Computer Physics Communications*, 221(??):259–272, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302849.

Stalter:2018:MDS

[SYE+18] S. Stalter, L. Yelash, N. Emamy, A. Statt, M. Hanke, M. Lukácová-Medvid'ová, and P. Virnau. Molecular dynamics simulations in hybrid particle-continuum schemes: Pitfalls and caveats. *Computer Physics Communications*, 224 (??):198–208, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303569.

Scott:2015:EHS

[SZ15] T. C. Scott and Wenxing Zhang. Efficient hybrid-symbolic methods for quantum mechanical calculations. *Computer*

Physics Communications, 191(??):221–234, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000545`.

Szalmas:2013:ADVb

[Sza13a] Lajos Szalmás. Accelerated discrete velocity method for axial-symmetric flows of gaseous mixtures as defined by the McCormack kinetic model. *Computer Physics Communications*, 184(11):2430–2437, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002014`.

Szalmas:2013:ADVa

[Sza13b] Lajos Szalmás. Accelerated discrete velocity method for axial-symmetric gaseous flows. *Computer Physics Communications*, 184(5):1432–1438, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000283`.

Szalmas:2016:FID

[Sza16] Lajos Szalmás. A fast iterative discrete velocity method for ternary gas mixtures flowing through long tubes. *Computer Physics Communications*, 200(??):44–49, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515004014`.

Sarti:2013:BTE

[SZC+13] E. Sarti, S. Zamuner, P. Cossio, A. Laio, F. Seno, and A. Trovato. BACHSCORE. A tool for evaluating efficiently and reliably the quality of large sets of protein structures. *Computer Physics Communications*, 184(12):2860–2865, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002488`.

Smiljanic:2014:MBP

[SZM+14] J. Smiljanić, M. Zezelj, V. Milanović, J. Radovanović, and I. Stanković. MATLAB-based program for optimization of quantum cascade laser active region parameters and calculation of output characteristics in magnetic field. *Computer Physics Communications*, 185(3):998–1006, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513003706`.

Sa:2012:PUP

[SZY+12] Ben-Hao Sa, Dai-Mei Zhou, Yu-Liang Yan, Xiao-Mei Li, Sheng-Qin Feng, Bao-Guo Dong, and Xu Cai. PACIAE 2.0: An updated parton and hadron cascade model (program) for the relativistic nuclear collisions. *Computer Physics Communications*, 183(2):333–346, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003080`.

Sa:2013:PUI

[SZY+13] Ben-Hao Sa, Dai-Mei Zhou, Yu-Liang Yan, Bao-Guo Dong, and Xu Cai. PACIAE 2.1: an updated issue of the parton and hadron cascade model PACIAE 2.0. *Computer Physics Communications*, 184(5):1476–1479, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000039`.

Tabakin:2016:QQM

[Tab16] Frank Tabakin. QDENSITY/QCWAVE: a Mathematica quantum computer simulation update. *Computer Physics Communications*, 201(??):171–172, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515004531`.

Thierry:2015:IDO

[TACA15] Bertrand Thierry, Xavier Antoine, Chokri Chniti, and Hasan Alzubaidi. μ-diff: an open-source Matlab toolbox for computing multiple scattering problems by disks. *Computer Physics Communications*, 192(??):348–362, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001125`.

Tabriz:2019:STE

[TAFD19] Meisam Farzalipour Tabriz, Bálint Aradi, Thomas Frauenheim, and Peter Deák. SLABCC: Total energy correction code for charged periodic slab models. *Computer Physics Communications*, 240(??):101–105, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300700.

Tanygin:2019:LDS

[Tan19] Bogdan Tanygin. Langevin dynamics simulation with dipole-dipole interactions: Massive performance improvements and advanced analytical integrator. *Computer Physics Communications*, 235(??):169–178, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303205.

Tautz:2010:NSC

[Tau10] Robert C. Tautz. A new simulation code for particle diffusion in anisotropic, large-scale and turbulent magnetic fields. *Computer Physics Communications*, 181(1):71–77, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002811.

Tseung:2014:GPB

[TB14] H. Wan Chan Tseung and C. Beltran. A graphics processor-based intranuclear cascade and evaporation simulation. *Computer Physics Communications*, 185(7):2029–2033, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001301.

Tribello:2014:PNF

[TBB+14] Gareth A. Tribello, Massimiliano Bonomi, Davide Branduardi, Carlo Camilloni, and Giovanni Bussi. PLUMED 2: New feathers for an old bird. *Computer Physics Communications*, 185(2):604–613, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003196.

Tarantola:2012:CTS

[TBZ12] Stefano Tarantola, William Becker, and Dirk Zeitz. A comparison of two sampling methods for global sensitivity analysis. *Computer Physics Communications*, 183(5):1061–1072, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004036.

Tang:2011:ESG

[TC11a] Hui-Chin Tang and Hwapeng Chang. An exhaustive search for good 64-bit linear congruential random number generators with restricted multiplier. *Computer Physics Communications*, 182(11):2326–2330, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002360.

Telnov:2011:TDG

[TC11b] Dmitry A. Telnov and Shih-I Chu. Time-dependent generalized pseudospectral method for accurate treatment of multiphoton processes of diatomic molecules in intense laser fields. *Computer Physics Communications*, 182(1):18–20, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002390.

Tsuchida:2012:IDS

[TC12] Eiji Tsuchida and Yoong-Kee Choe. Iterative diagonalization of symmetric matrices in mixed precision and its application to electronic structure calculations. *Computer Physics Communications*, 183(4):980–985, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000045.

Tran:2018:CSS

[TCCV18] Công Tâm Tran, Benoît Crespin, Manuella Cerbelaud, and Arnaud Videcoq. Colloidal suspension by SRD–MD simulation on GPU. *Computer Physics Communications*, 232(??):35–45, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302121.

Tracey:2015:FMV

[TCK+15] John Tracey, Filippo Federici Canova, Olli Keisanen, David Z. Gao, Peter Spijker, Bernhard Reischl, and Adam S. Foster. Flexible and modular virtual scanning probe microscope. *Computer Physics Communications*, 196(??):429–438, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001939.

Tuttafesta:2013:CUC

[TCP13] Michele Tuttafesta, Gianpiero Colonna, and Giuseppe Pascazio. Computing unsteady compressible flows using Roe's flux-difference splitting scheme on GPUs. *Computer Physics Communications*, 184(6):1497–1510, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000350.

Tapia:2011:PCP

[TD11] José Juan Tapia and Roshan M. D'Souza. Parallelizing the cellular Potts model on graphics processing units. *Computer Physics Communications*, 182(4):857–865, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000490X.

Taleei:2014:TSP

[TD14] Ameneh Taleei and Mehdi Dehghan. Time-splitting pseudo-spectral domain decomposition method for the soliton solutions of the one- and multi-dimensional nonlinear Schrödinger equations. *Computer Physics Communications*, 185(6):1515–1528, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000265.

Tretyakov:2017:IDC

[TD17] Nikita Tretyakov and Burkhard Dünweg. An improved dissipative coupling scheme for a system of molecular dynamics particles interacting with a lattice Boltzmann fluid. *Computer Physics Communications*, 216(??):102–108, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300966.

Torres:2011:AOF

[TdAdSS11] Rodrigo Coura Torres, Andre Rabello dos Anjos, José Manoel de Seixas, and Igor Soloviev. Automatizing the online filter test management for a general-purpose particle detector. *Computer Physics Communications*, 182(3):555–563, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003826.

Tuttafesta:2014:GMC

[TDL+14] M. Tuttafesta, A. D'Angola, A. Laricchiuta, P. Minelli, M. Capitelli, and G. Colonna. GPU and multi-core based Reaction Ensemble Monte Carlo method for non-ideal thermodynamic systems. *Computer Physics Communications*, 185(2):540–549, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003457.

Teunissen:2018:AFQ

[TE18] Jannis Teunissen and Ute Ebert. Afivo: a framework for quadtree/octree AMR with shared-memory parallelization and geometric multigrid methods. *Computer Physics Communications*, 233(??):156–166, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302261.

Terekhov:2017:LFD

[Ter17] Andrew V. Terekhov. The Laguerre finite difference one-way equation solver. *Computer Physics Communications*, 214(??):71–82, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300267.

Tchuen:2014:HNM

[TFBW14] Ghislain Tchuen, Ferdinand Fogang, Yves Burtschell, and Paul Woafo. A hybrid numerical method and its application to inviscid compressible flow problems. *Computer Physics*

Communications, 185(2):479–488, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003251.

Tung:2011:ISM

[TG11] J. C. Tung and G. Y. Guo. An *ab initio* study of the magnetic and electronic properties of Fe, Co, and Ni nanowires on Cu(001) surface. *Computer Physics Communications*, 182(1):84–86, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003371.

Tramm:2016:TBP

[TGH+16] John R. Tramm, Geoffrey Gunow, Tim He, Kord S. Smith, Benoit Forget, and Andrew R. Siegel. A task-based parallelism and vectorized approach to 3D Method of Characteristics (MOC) reactor simulation for high performance computing architectures. *Computer Physics Communications*, 202(??):141–150, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000266.

Tripolt:2019:NAC

[TGUvS19] Ralf-Arno Tripolt, Philipp Gubler, Maksim Ulybyshev, and Lorenz von Smekal. Numerical analytic continuation of Euclidean data. *Computer Physics Communications*, 237(??):129–142, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304041.

Titarenko:2017:HMV

[TH17] Sofya Titarenko and Mark Hildyard. Hybrid multicore/vectorisation technique applied to the elastic wave equation on a staggered grid. *Computer Physics Communications*, 216(??):53–62, July 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300747.

TenBarge:2014:OLA

[THDH14] J. M. TenBarge, G. G. Howes, W. Dorland, and G. W. Hammett. An oscillating Langevin antenna for driving plasma turbulence simulations. *Computer Physics Communications*, 185(2):578–589, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003664.

Teijeiro:2016:EPA

[THDS16] C. Teijeiro, T. Hammerschmidt, R. Drautz, and G. Sutmann. Efficient parallelization of analytic bond-order potentials for large-scale atomistic simulations. *Computer Physics Communications*, 204(??):64–73, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300662.

Torrent:2010:ESP

[THJ+10] Marc Torrent, N. A. W. Holzwarth, François Jollet, David Harris, Nicholas Lepley, and Xiao Xu. Electronic structure packages: Two implementations of the projector augmented wave (PAW) formalism. *Computer Physics Communications*, 181(11):1862–1867, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002699.

Tian:2011:RHO

[Tia11] Zhen F. Tian. A rational high-order compact ADI method for unsteady convection-diffusion equations. *Computer Physics Communications*, 182(3):649–662, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004595.

Tickner:2010:MCS

[Tic10] James Tickner. Monte Carlo simulation of X-ray and gamma-ray photon transport on a graphics-processing unit. *Computer Physics Communications*, 181(11):1821–1832, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002249.

Tickner:2014:APM

[Tic14] James Tickner. Arbitrary perturbations in Monte Carlo neutral-particle transport. *Computer Physics Communications*, 185(6):1628–1638, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000824`.

Tsukahara:2016:ILC

[TIM+16] Hiroshi Tsukahara, Kaoru Iwano, Chiharu Mitsumata, Tadashi Ishikawa, and Kanta Ono. Implementation of low communication frequency 3D FFT algorithm for ultra-large-scale micromagnetics simulation. *Computer Physics Communications*, 207(??):217–220, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516301783`.

Tordella:2013:LES

[TIMM13] D. Tordella, M. Iovieno, S. Massaglia, and A. Mignone. Large-eddy simulation of hypersonic flows. Selective procedure to activate the sub-grid model wherever small scale turbulence is present. *Computer Physics Communications*, 184(12):2651–2661, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513002063`.

Tabakin:2011:QMQ

[TJD11] Frank Tabakin and Bruno Juliá-Díaz. QCWAVE — a Mathematica quantum computer simulation update. *Computer Physics Communications*, 182(8):1693–1707, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001287`.

Tholerus:2017:FMN

[TJH17] Emmi Tholerus, Thomas Johnson, and Torbjörn Hellsten. FOXTAIL: Modeling the nonlinear interaction between Alfvén eigenmodes and energetic particles in tokamaks. *Computer Physics Communications*, 214(??):39–51, May 2017. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300073.

Tang:2014:ADP

[TK14a] Yu-Hang Tang and George Em Karniadakis. Accelerating dissipative particle dynamics simulations on GPUs: Algorithms, numerics and applications. *Computer Physics Communications*, 185(11):2809–2822, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002203.

Tsitouras:2014:BVD

[TK14b] Ch. Tsitouras and V. N. Katsikis. Bounds for variable degree rational L_∞ approximations to the matrix cosine. *Computer Physics Communications*, 185(11):2834–2840, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002422.

Teunissen:2019:GML

[TK19] J. Teunissen and R. Keppens. A geometric multigrid library for quadtree/octree AMR grids coupled to MPI-AMRVAC. *Computer Physics Communications*, 245(??):Article 106866, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930253X.

Teschner:2019:GLD

[TKJ19] Tom-Robin Teschner, László Könözsy, and Karl W. Jenkins. A generalised and low-dissipative multi-directional characteristics-based scheme with inclusion of the local Riemann problem investigating incompressible flows without free-surfaces. *Computer Physics Communications*, 239(??):283–310, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300098.

Tseng:2012:SSV

[TKL+12] K. C. Tseng, T. C. Kuo, S. C. Lin, C. C. Su, and J. S. Wu. Simulations of subsonic vortex-shedding flow past a 2D vertical plate in the near-continuum regime by the parallelized DSMC code. *Computer Physics Communications*, 183(8):1596–1608, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000902.

Timoshenko:2012:RMC

[TKP12] Janis Timoshenko, Alexei Kuzmin, and Juris Purans. Reverse Monte Carlo modeling of thermal disorder in crystalline materials from EXAFS spectra. *Computer Physics Communications*, 183(6):1237–1245, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000513.

Tennyson:2015:MOI

[TKP15] P. Gerald Tennyson, G. M. Karthik, and G. Phanikumar. MPI + OpenCL implementation of a phase-field method incorporating CALPHAD description of Gibbs energies on heterogeneous computing platforms. *Computer Physics Communications*, 186(??):48–64, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003208.

Tang:2013:SIN

[TKR13] Baoming Tang, Ehsan Khatami, and Marcos Rigol. A short introduction to numerical linked-cluster expansions. *Computer Physics Communications*, 184(3):557–564, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003414.

Tadano:2010:APB

[TKS10] H. Tadano, Y. Kuramashi, and T. Sakurai. Application of preconditioned block BiCGGR to the Wilson–Dirac equation with multiple right-hand sides in lattice QCD. *Computer Physics Communications*, 181(5):883–886, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004172.

Tsoulos:2019:DTS

[TKS19] Ioannis G. Tsoulos, O. T. Kosmas, and V. N. Stavrou. DiracSolver: a tool for solving the Dirac equation. *Computer Physics Communications*, 236(??):237–243, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303588.

Trofimov:2018:SPP

[TKZ18] M. Yu. Trofimov, S. B. Kozitskiy, and A. D. Zakharenko. Simulation of the pulse propagation by the interacting mode parabolic equation method. *Computer Physics Communications*, 228(??):54–60, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300791.

Tavakkol:2017:CGA

[TL17] Sasan Tavakkol and Patrick Lynett. Celeris: a GPU-accelerated open source software with a Boussinesq-type wave solver for real-time interactive simulation and visualization. *Computer Physics Communications*, 217(??):117–127, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300784.

Terzani:2019:FAN

[TL19] Davide Terzani and Pasquale Londrillo. A fast and accurate numerical implementation of the envelope model for laser-plasma dynamics. *Computer Physics Communications*, 242(??):49–59, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301195.

Tagliaboschi:2014:PMI

[TM14] Aaron M. Tagliaboschi and Jeremy B. Maddox. POTLIB2Math: a Mathematica interface to the potential energy surface library for chemical systems. *Computer Physics Communications*, 185(1):294–301, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002725.

Tanaka:2019:REM

[TM19] Motohiko Tanaka and Masakatsu Murakami. Relativistic and electromagnetic molecular dynamics simulations for a carbon–gold nanotube accelerator. *Computer Physics Communications*, 241(??):56–63, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300906.

Thirayatorn:2015:FDC

[TMA+15] Ruhan Thirayatorn, Pairot Moontragoon, Vittaya Amornkitbamrung, Santi Meansiri, and Zoran Ikonic. Finite-difference calculation of the electronic structure of artificial graphene, the 2D hexagonal $Al_wGa_{1-w}As/GaAs$ structure with tunable interactions. *Computer Physics Communications*, 191(??):106–118, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000508.

Trieu:2011:EBS

[TMD11] Binh Trieu, Kristel Michielsen, and Hans De Raedt. Event-based simulation of light propagation in lossless dielectric media. *Computer Physics Communications*, 182(3):726–734, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004960.

Todo:2019:PLC

[TMS19] Synge Todo, Haruhiko Matsuo, and Hideyuki Shitara. Parallel loop cluster quantum Monte Carlo simulation of quantum magnets based on global union-find graph algorithm. *Computer Physics Communications*, 239(??):84–93, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300050.

Teodoro:2011:MMS

[TN11] Vítor Duarte Teodoro and Rui Gomes Neves. Mathematical modelling in science and mathematics education. *Computer Physics Communications*, 182(1):8–10, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000175X.

Toyoda:2010:FSB

[TO10a] Masayuki Toyoda and Taisuke Ozaki. Fast spherical Bessel transform via fast Fourier transform and recurrence formula. *Computer Physics Communications*, 181(2):277–282, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003105.

Toyoda:2010:LLN

[TO10b] Masayuki Toyoda and Taisuke Ozaki. LIBERI: Library for numerical evaluation of electron-repulsion integrals. *Computer Physics Communications*, 181(8):1455–1463, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001141.

Tapiador:2014:FBH

[TOB+14] D. Tapiador, W. O'Mullane, A. G. A. Brown, X. Luri, E. Huedo, and P. Osuna. A framework for building hypercubes using MapReduce. *Computer Physics Communications*, 185(5):1429–1438, May 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000423.

Tomasik:2016:DHG

[Tom16] Boris Tomásik. DRoplet and hAdron generator for nuclear collisions: an update. *Computer Physics Communications*, 207(??):545–546, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301758.

Tosiek:2010:FPM

[Tos10] Jaromir Tosiek. The Fedosov $\star$-product in Mathematica. *Computer Physics Communications*, 181(3):704, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003439.

Tuttafesta:2016:MGU

[TPC16] Michele Tuttafesta, Giuseppe Pascazio, and Gianpiero Colonna. Multi-GPU unsteady 2D flow simulation coupled with a state-to-state chemical kinetics. *Computer Physics Communications*, 207(??):243–257, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302041.

Tabik:2012:VRR

[TRM+12] S. Tabik, L. F. Romero, P. Mimica, O. Plata, and E. L. Zapata. VLBI-resolution radio-map algorithms: Performance analysis of different levels of data-sharing on multi-socket, multi-core architectures. *Computer Physics Communications*, 183(9):1937–1946, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001555.

Titus:2016:TRC

[TRN16] L. J. Titus, A. Ross, and F. M. Nunes. Transfer reaction code with nonlocal interactions. *Computer Physics Communications*, 207(??):499–517, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302028.

Troster:2011:WMS

[Trö11] A. Tröster. Wilson's momentum shell renormalization group from Fourier Monte Carlo simulations. *Computer Physics Communications*, 182(9):1837–1841, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004510.

Tueros:2010:TPS

[TS10] Matías Tueros and Sergio Sciutto. TIERRAS: a package to simulate high energy cosmic ray showers underground, underwater and under-ice. *Computer Physics Communications*, 181(2):380–392, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003166.

Tsoulos:2011:ECP

[TS11] Ioannis G. Tsoulos and Athanassios Stavrakoudis. Eucb: a C++ program for molecular dynamics trajectory analysis. *Computer Physics Communications*, 182(3):834–841, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004856.

Tomczak:2019:NGI

[TS19] Tadeusz Tomczak and Roman G. Szafran. A new GPU implementation for lattice-Boltzmann simulations on sparse geometries. *Computer Physics Communications*, 235(??):258–278, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301474.

Takahashi:2016:EBM

[TSIM16] Toru Takahashi, Yuta Shimba, Hiroshi Isakari, and Toshiro Matsumoto. An efficient blocking M2L translation for low-frequency fast multipole method in three dimensions. *Computer Physics Communications*, 202(??):151–164, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000278.

Tegeler:2017:PMF

[TSK+17] Marvin Tegeler, Oleg Shchyglo, Reza Darvishi Kamachali, Alexander Monas, Ingo Steinbach, and Godehard Sutmann. Parallel multiphase field simulations with OpenPhase. *Computer Physics Communications*, 215(??):173–187, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300358.

Teijeiro:2013:PBD

[TSTT13] C. Teijeiro, G. Sutmann, G. L. Taboada, and J. Touriño. Parallel Brownian dynamics simulations with the message-passing and PGAS programming models. *Computer Physics Communications*, 184(4):1191–1202, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004110.

Tong:2011:TDM

[TT11] Xiao-Min Tong and Nobuyuki Toshima. Time-dependent method in the laser-atom interactions. *Computer Physics Communications*, 182(1):21–23, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001992.

Tay:2014:PAD

[TT14] Wei Choon Tay and Eng Leong Tan. Pentadiagonal alternating-direction-implicit finite-difference time-domain method for two-dimensional Schrödinger equation. *Computer Physics Communications*, 185(7):1886–1892, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000940.

Tang:2011:MTM

[TTG11] Chi-Shung Tang, Kristinn Torfason, and Vidar Gudmundsson. Magnetotransport in a time-modulated double quantum point contact system. *Computer Physics Communications*, 182(1):65–67, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002006.

Tomiya:2011:QFD

[TTS11] Mitsuyoshi Tomiya, Hiroyoshi Tsuyuki, and Shoichi Sakamoto. Quantum fidelity and dynamical scar states on chaotic billiard system. *Computer Physics Communications*, 182(1):245–248, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001980.

Tsoulos:2016:PIP

[TTT16] Ioannis G. Tsoulos, Alexandros Tzallas, and Dimitris Tsalikakis. PDoublePop: an implementation of parallel genetic algorithm for function optimization. *Computer Physics Communications*, 209(??):183–189, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302776.

Toll:2014:DMM

[TU14] Tobias Toll and Thomas Ullrich. The dipole model Monte Carlo generator Sar t re 1. *Computer Physics Communications*, 185(6):1835–1853, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000903.

Turemen:2015:GAR

[TUY15] G. Turemen, G. Unel, and B. Yasatekin. A graphical approach to radio frequency quadrupole design. *Computer Physics Communications*, 192(??):108–113, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000879.

Tentyukov:2010:MVF

[TV10] M. Tentyukov and J. A. M. Vermaseren. The multithreaded version of FORM. *Computer Physics Communications*, 181(8):1419–1427, August 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001207.

Timrov:2015:TCS

[TVGB15] Iurii Timrov, Nathalie Vast, Ralph Gebauer, and Stefano Baroni. turboEELS — a code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouville–Lanczos approach to time-dependent density-functional perturbation theory. *Computer Physics Communications*, 196(??):460–469, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002015.

Thierry:2016:GOF

[TVT+16] B. Thierry, A. Vion, S. Tournier, M. El Bouajaji, D. Colignon, N. Marsic, X. Antoine, and C. Geuzaine. GetDDM: an open framework for testing optimized Schwarz methods for time-harmonic wave problems. *Computer Physics Communications*, 203(??):309–330, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465516300455.

Tiana:2015:MIM

[TVZ+15] G. Tiana, F. Villa, Y. Zhan, R. Capelli, C. Paissoni, P. Sormanni, E. Heard, L. Giorgetti, and R. Meloni. MonteGrappa: an iterative Monte Carlo program to optimize biomolecular potentials in simplified models. *Computer Physics Communications*, 186(??):93–104, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003178.

Tsai:2011:EML

[TW11] K. H. Tsai and Ten-Ming Wu. Entropy of a model for liquid Ga: Contribution due to Friedel oscillations. *Computer Physics Communications*, 182(1):62–64, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002468.

Tretiakov:2015:QAE

[TW15] Konstantin V. Tretiakov and Krzysztof W. Wojciechowski. Quick and accurate estimation of the elastic constants using the minimum image method. *Computer Physics Communications*, 189(??):77–83, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004329.

Tu:2015:SFE

[TXZL15] Bin Tu, Yan Xie, Linbo Zhang, and Benzhuo Lu. Stabilized finite element methods to simulate the conductances of ion channels. *Computer Physics Communications*, 188(??):131–139, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004019.

Tian:2010:HOC

[TY10] Zhen F. Tian and P. X. Yu. High-order compact ADI (HOC–ADI) method for solving unsteady 2D Schrödinger equation. *Computer Physics Communications*, 181(5):861–868, May

2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004147.

Tsai:2015:IPC

[TYH+15] T. C. Tsai, H.-S. Yu, M.-S. Hsieh, S. H. Lai, and Y.-H. Yang. Implicit predictor-corrector central finite difference scheme for the equations of magnetohydrodynamic simulations. *Computer Physics Communications*, 196(??):1–12, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001654.

Talamo:2012:MCD

[TZG12] Alberto Talamo, Zhaopeng Zhong, and Yousry Gohar. Monte Carlo and deterministic calculation of the Bell and Glasstone spatial correction factor. *Computer Physics Communications*, 183(9):1904–1910, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001488.

Trofimov:2016:MGB

[TZK16] M. Yu. Trofimov, A. D. Zakharenko, and S. B. Kozitskiy. Mode Gaussian beam tracing. *Computer Physics Communications*, 207(??):179–185, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301631.

Tang:2017:REN

[TZM17] Qinglin Tang, Yong Zhang, and Norbert J. Mauser. A robust and efficient numerical method to compute the dynamics of the rotating two-component dipolar Bose–Einstein condensates. *Computer Physics Communications*, 219(??):223–235, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301649.

Underwood:2017:MPE

[UA17] T. L. Underwood and G. J. Ackland. `monteswitch`: a package for evaluating solid-solid free energy differences via lattice-switch Monte Carlo. *Computer Physics*

Communications, 215(??):204–222, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300632.

Unfer:2010:MSG

[UBRT10] Thomas Unfer, Jean-Pierre Boeuf, François Rogier, and Frédéric Thivet. Multi-scale gas discharge simulations using asynchronous adaptive mesh refinement. *Computer Physics Communications*, 181(2):247–258, February 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003075.

Utamuratov:2019:CSM

[UFKB19] R. Utamuratov, D. V. Fursa, A. S. Kadyrov, and I. Bray. Configuration space method to calculate rearrangement matrix elements. *Computer Physics Communications*, 239(??):64–71, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300165.

Urakami:2011:SCL

[UIY11] Naohito Urakami, Junko Imada, and Takashi Yamamoto. Simulation of chain length recognition observed in formation of inclusion complex. *Computer Physics Communications*, 182(1):240–242, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001694.

Ulybyshev:2019:SCS

[UKKB19] Maksim Ulybyshev, Nils Kintscher, Karsten Kahl, and Pavel Buividovich. Schur complement solver for quantum Monte-Carlo simulations of strongly interacting fermions. *Computer Physics Communications*, 236(??):118–127, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303710.

Umeda:2018:TSB

[Ume18] Takayuki Umeda. A three-step Boris integrator for Lorentz force equation of charged particles. *Computer Physics Com-*

munications, 228(??):1–4, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300912.

Umeda:2019:MSB

[Ume19] Takayuki Umeda. Multi-step Boris rotation schemes for Lorentz force equation of charged particles. *Computer Physics Communications*, 237(??):37–41, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830393X.

Umeda:2012:NOC

[UNK12] Takayuki Umeda, Yasuhiro Nariyuki, and Daichi Kariya. A non-oscillatory and conservative semi-Lagrangian scheme with fourth-degree polynomial interpolation for solving the Vlasov equation. *Computer Physics Communications*, 183(5):1094–1100, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000264.

Urano:2015:DWR

[UO15a] Ryo Urano and Yuko Okamoto. Designed-walk replica-exchange method for simulations of complex systems. *Computer Physics Communications*, 196(??):380–383, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002763.

Urano:2015:DRE

[UO15b] Ryo Urano and Yuko Okamoto. Deterministic replica-exchange method without pseudo random numbers for simulations of complex systems. *Computer Physics Communications*, 197(??):128–135, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003069.

Urbach:2018:RVH

[Urb18] Carsten Urbach. Reversibility violation in the Hybrid Monte Carlo algorithm. *Computer Physics Communications*, 224

(??):44–51, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517304046.

Urbanek:2016:PIT

[US16] Miroslav Urbanek and Pavel Soldán. Parallel implementation of the time-evolving block decimation algorithm for the Bose–Hubbard model. *Computer Physics Communications*, 199(??):170–177, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003963.

Unel:2018:CPP

[ÜS18] Gökhan Ünel and Sezen Sekmen. CutLang: a particle physics analysis description language and runtime interpreter. *Computer Physics Communications*, 233(??):215–236, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302315.

Utsuno:2013:ECH

[USOA13] Yutaka Utsuno, Noritaka Shimizu, Takaharu Otsuka, and Takashi Abe. Efficient computation of Hamiltonian matrix elements between non-orthogonal Slater determinants. *Computer Physics Communications*, 184(1):102–108, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002883.

Utyuzhnikov:2014:TDU

[Uty14] S. V. Utyuzhnikov. Towards development of unsteady near-wall interface boundary conditions for turbulence modeling. *Computer Physics Communications*, 185(11):2879–2884, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002513.

Umansky:2012:NAM

[UW12] Moti Umansky and Daphne Weihs. Novel algorithm and MATLAB-based program for automated power law analysis of single particle, time-dependent mean-square displacement.

Computer Physics Communications, 183(8):1783–1792, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001063.

Vanni:2015:AMF

[Van15] Marco Vanni. Accurate modelling of flow induced stresses in rigid colloidal aggregates. *Computer Physics Communications*, 192(??):70–90, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000806.

Varley:2016:EPP

[Var16] Ryan Varley. ExoData: a Python package to handle large exoplanet catalogue data. *Computer Physics Communications*, 207(??):298–309, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301254.

Vogel:2011:APN

[VB11] Thomas Vogel and Michael Bachmann. Adsorption of polymers at nanowires. *Computer Physics Communications*, 182(9):1928–1931, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004534.

Voyiatzis:2019:OSI

[VB19] Evangelos Voyiatzis and Michael C. Böhm. An open-source implementation of a quasi harmonic approach to compute the intramolecular entropy of particle systems. *Computer Physics Communications*, 234(??):286–293, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302558.

Velasco:2012:IIS

[VBC+12] J. L. Velasco, A. Bustos, F. Castejón, L. A. Fernández, V. Martin-Mayor, and A. Tarancón. ISDEP: Integrator of stochastic differential equations for plasmas. *Computer Physics Communications*, 183(9):1877–1883, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200135X.

Valiev:2010:NCS

[VBG+10] M. Valiev, E. J. Bylaska, N. Govind, K. Kowalski, T. P. Straatsma, H. J. J. Van Dam, D. Wang, J. Nieplocha, E. Apra, T. L. Windus, and W. A. de Jong. NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations. *Computer Physics Communications*, 181(9):1477–1489, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001438.

Voyiatzis:2015:GAI

[VBMP15] Evangelos Voyiatzis, Michael C. Böhm, and Florian Müller-Plathe. A geometric approach to identify cavities in particle systems. *Computer Physics Communications*, 196(??):247–254, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002568.

Voronych:2017:NME

[VBMS17] Oksana Voronych, Adam Buraczewski, Michal Matuszewski, and Magdalena Stobińska. Numerical modeling of exciton-polariton Bose–Einstein condensate in a microcavity. *Computer Physics Communications*, 215(??):246–258, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300735.

Vecharynski:2017:EBP

[VBS+17] Eugene Vecharynski, Jiri Brabec, Meiyue Shao, Niranjan Govind, and Chao Yang. Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory. *Computer Physics Communications*, 221(??):42–52, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302370.

Viehland:2010:TCS

[VC10] Larry A. Viehland and Yongbin Chang. Transport cross sections for collisions between particles. *Computer Physics Communications*, 181(10):1687–1696, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001852.

Vorwerk:2016:LMM

[VCD16] Christian Vorwerk, Caterina Cocchi, and Claudia Draxl. LayerOptics: Microscopic modeling of optical coefficients in layered materials. *Computer Physics Communications*, 201(??):119–125, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000205.

Varini:2013:EDC

[VCMS+13] Nicola Varini, Davide Ceresoli, Layla Martin-Samos, Ivan Girotto, and Carlo Cavazzoni. Enhancement of DFT-calculations at petascale: Nuclear magnetic resonance, hybrid density functional theory and Car–Parrinello calculations. *Computer Physics Communications*, 184(8):1827–1833, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001008.

Verbrugghe:2019:NLW

[VDA+19] Tim Verbrugghe, J. M. Domínguez, Corrado Altomare, Angelantonio Tafuni, Renato Vacondio, Peter Troch, and Andreas Kortenhaus. Non-linear wave generation and absorption using open boundaries within DualSPHysics. *Computer Physics Communications*, 240(??):46–59, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300463.

Vergez:2016:FET

[VDAH16] Guillaume Vergez, Ionut Danaila, Sylvain Auliac, and Frédéric Hecht. A finite-element toolbox for the stationary Gross–Pitaevskii equation with rotation. *Computer Physics Communications*, 209(??):144–162, December 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516302508`.

Valuev:2014:IIF

[VDB14] Ilya Valuev, Alexei Deinega, and Sergey Belousov. Implementation of the iterative finite-difference time-domain technique for simulation of periodic structures at oblique incidence. *Computer Physics Communications*, 185(4): 1273–1281, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514000022`.

Valentim:2015:EST

[VDF15] A. Valentim, Claudio J. DaSilva, and Carlos E. Fiore. Efficient simulated tempering with approximated weights: Applications to first-order phase transitions. *Computer Physics Communications*, 196(??):212–220, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002520`.

Vladimirov:2011:GWI

[VDJ+11] A. E. Vladimirov, S. W. Digel, G. Jóhannesson, P. F. Michelson, I. V. Moskalenko, P. L. Nolan, E. Orlando, T. A. Porter, and A. W. Strong. GALPROP WebRun: An Internet-based service for calculating galactic cosmic ray propagation and associated photon emissions. *Computer Physics Communications*, 182(5):1156–1161, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000373`.

Valentim:2014:DET

[VdLF14] A. Valentim, M. G. E. da Luz, and Carlos E. Fiore. Determining efficient temperature sets for the simulated tempering method. *Computer Physics Communications*, 185(7):2046–2055, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001337`.

vanderSman:2010:MLB

[vdS10] R. G. M. van der Sman. MRT lattice Boltzmann schemes for confined suspension flows. *Computer Physics Communications*, 181(9):1562–1569, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000161X.

vanderSman:2013:ILB

[vdS13] R. G. M. van der Sman. Investigation of Lattice Boltzmann wetting boundary conditions for capillaries with irregular polygonal cross-section. *Computer Physics Communications*, 184(12):2751–2760, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002506.

vanderSman:2016:AIL

[vdSM16] R. G. M. van der Sman and M. B. J. Meinders. Analysis of improved Lattice Boltzmann phase field method for soluble surfactants. *Computer Physics Communications*, 199(??):12–21, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003677.

Veberic:2012:LFA

[Veb12] Darko Veberič. Lambert W function for applications in physics. *Computer Physics Communications*, 183(12):2622–2628, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002366.

Varin:2018:EFS

[VEB+18] Charles Varin, Rhys Emms, Graeme Bart, Thomas Fennel, and Thomas Brabec. Explicit formulation of second and third order optical nonlinearity in the FDTD framework. *Computer Physics Communications*, 222(??):70–83, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303053.

Voitcu:2012:CSF

[VEM12] Gabriel Voitcu, Marius Echim, and Richard Marchand. Comparative study of forward and backward test-kinetic simulation approaches. *Computer Physics Communications*, 183(12):2561–2569, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002330.

Verheyen:2016:RCP

[Ver16] Rob Verheyen. RGIsearch: a C++ program for the determination of renormalization group invariants. *Computer Physics Communications*, 202(??):351–355, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300170.

dePut:2019:SAS

[VFV19] Maarten L. Van de Put, Massimo V. Fischetti, and William G. Vandenberghe. Scalable atomistic simulations of quantum electron transport using empirical pseudopotentials. *Computer Physics Communications*, 244(??):156–169, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301961.

Vranic:2015:PMA

[VGM+15] M. Vranic, T. Grismayer, J. L. Martins, R. A. Fonseca, and L. O. Silva. Particle merging algorithm for PIC codes. *Computer Physics Communications*, 191(??):65–73, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000405.

vonHippel:2010:TMA

[vH10] G. M. von Hippel. TaylUR 3, a multivariate arbitrary-order automatic differentiation package for Fortran 95. *Computer Physics Communications*, 181(3):705–706, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003464.

vanHameren:2011:OEO

[vH11] A. van Hameren. OneLOop: For the evaluation of one-loop scalar functions. *Computer Physics Communications*, 182(11):2427–2438, November 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002219.

vanHameren:2018:KPL

[vH18] A. van Hameren. KaTie: For parton-level event generation with k_T-dependent initial states. *Computer Physics Communications*, 224(??):371–380, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303880.

Voglis:2015:PMP

[VHP+15] C. Voglis, P. E. Hadjidoukas, K. E. Parsopoulos, D. G. Papageorgiou, I. E. Lagaris, and M. N. Vrahatis. p-MEMPSODE: Parallel and irregular memetic global optimization. *Computer Physics Communications*, 197(??):190–211, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002805.

Vitolo:2019:CHO

[Vit19] R. Vitolo. Computing with Hamiltonian operators. *Computer Physics Communications*, 244(??):228–245, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301705.

Vu:2012:FHS

[VJC12] K. T. Vu, G. F. Jefferson, and J. Carminati. Finding higher symmetries of differential equations using the Maple package DESOLVII. *Computer Physics Communications*, 183(4):1044–1054, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000070.

Vitek:2014:TDM

[VK14] Ales Vítek and René Kalus. Two-dimensional multiple-histogram method applied to isothermal-isobaric Monte Carlo simulations of molecular clusters. *Computer Physics Communications*, 185(6):1595–1605, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000770.

Vuorinen:2016:DGT

[VK16] V. Vuorinen and K. Keskinen. DNSLab: a gateway to turbulent flow simulation in Matlab. *Computer Physics Communications*, 203(??):278–289, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300388.

Villalobos:2011:SDW

[VKLM11] Gabriel Villalobos, Ferenc Kun, Dorian L. Linero, and José D. Muñoz. Size distribution and waiting times for the avalanches of the Cell Network Model of Fracture. *Computer Physics Communications*, 182(9):1824–1827, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004303.

Vanaverbeke:2014:GPM

[VKP14] S. Vanaverbeke, R. Keppens, and S. Poedts. GRADSPMHD: a parallel MHD code based on the SPH formalism. *Computer Physics Communications*, 185(3):1053–1073, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003998.

Vlasenko:2016:EGA

[VKS16] A. V. Vlasenko, A. Köhl, and D. Stammer. The efficiency of geophysical adjoint codes generated by automatic differentiation tools. *Computer Physics Communications*, 199(??):22–28, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003884.

Vandenhoeck:2019:IHO

[VL19] Ray Vandenhoeck and Andrea Lani. Implicit high-order flux reconstruction solver for high-speed compressible flows. *Computer Physics Communications*, 242(??):1–24, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301328.

Varet:2012:EDN

[VLD+12] Suzanne Varet, Sidonie Lefebvre, Gérard Durand, Antoine Roblin, and Serge Cohen. Effective discrepancy and numerical experiments. *Computer Physics Communications*, 183(12):2535–2541, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002305.

Vincenti:2017:EPS

[VLL+17] H. Vincenti, M. Lobet, R. Lehe, R. Sasanka, and J.-L. Vay. An efficient and portable SIMD algorithm for charge/current deposition in Particle-In-Cell codes. *Computer Physics Communications*, 210(??):145–154, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302764.

Villalobos:2011:SMF

[VLM11] Gabriel Villalobos, Dorian L. Linero, and José D. Muñoz. A statistical model of fracture for a 2D hexagonal mesh: The Cell Network Model of Fracture for the bamboo *Guadua angustifolia*. *Computer Physics Communications*, 182(1):188–191, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000192X.

Valero-Lara:2014:FFD

[VLPPM14] Pedro Valero-Lara, Alfredo Pinelli, and Manuel Prieto-Matias. Fast finite difference Poisson solvers on heterogeneous architectures. *Computer Physics Communications*, 185(4):1265–1272, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL

http://www.sciencedirect.com/science/article/pii/S0010465513004384.

Volpe:2017:HFW

[VLZ17] F. A. Volpe, P.-D. Létourneau, and A. Zhao. Huygens–Fresnel wavefront tracing. *Computer Physics Communications*, 212(??):123–131, March 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630340X.

vanMilligen:2014:SNM

[vMB14] B. Ph. van Milligen and P. D. Bons. Simplified numerical model for clarifying scaling behavior in the intermediate dispersion regime in homogeneous porous media. *Computer Physics Communications*, 185(12):3291–3301, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003117.

Vranic:2016:CRR

[VMFS16] M. Vranic, J. L. Martins, R. A. Fonseca, and L. O. Silva. Classical radiation reaction in particle-in-cell simulations. *Computer Physics Communications*, 204(??):141–151, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630090X.

Vigano:2019:SBH

[VMGP+19] Daniele Viganò, David Martínez-Gómez, José A. Pons, Carlos Palenzuela, Federico Carrasco, Borja Miñano, Antoni Arbona, Carles Bona, and Joan Massó. A Simflowny-based high-performance 3D code for the generalized induction equation. *Computer Physics Communications*, 237(??):168–183, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304144.

Voyiatzis:2013:MPE

[Voy13] E. Voyiatzis. Mechanical properties and elastic constants of atomistic systems through the stress-fluctuation formalism. *Computer Physics Communications*, 184(1):27–33, January

2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002573.

Vigano:2012:NCH

[VPM12] D. Viganò, J. A. Pons, and J. A. Miralles. A new code for the Hall-driven magnetic evolution of neutron stars. *Computer Physics Communications*, 183(10):2042–2053, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001713.

Vergara-Perez:2016:MMP

[VPM16] Sandra Vergara-Perez and Marcelo Marucho. MPBEC, a Matlab Program for Biomolecular Electrostatic Calculations. *Computer Physics Communications*, 198(??):179–194, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003288.

Vazquez-Poletti:2017:SEA

[VPMVH+17] J. L. Vázquez-Poletti, R. Moreno-Vozmediano, R. Han, W. Wang, and I. M. Llorente. SaaS enabled admission control for MCMC simulation in cloud computing infrastructures. *Computer Physics Communications*, 211(??):88–97, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301862.

Voglis:2012:MGO

[VPP+12] C. Voglis, K. E. Parsopoulos, D. G. Papageorgiou, I. E. Lagaris, and M. N. Vrahatis. MEMPSODE: a global optimization software based on hybridization of population-based algorithms and local searches. *Computer Physics Communications*, 183(5):1139–1154, May 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000136.

Verbeke:2015:FRE

[VRV15] J. M. Verbeke, J. Randrup, and R. Vogt. Fission Reaction Event Yield Algorithm, FREYA — for event-by-event simulation of fission. *Computer Physics Communi-*

cations, 191(??):178–202, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000466.

Verbeke:2018:FRE

[VRV18] J. M. Verbeke, J. Randrup, and R. Vogt. Fission reaction event yield algorithm FREYA 2.0.2. *Computer Physics Communications*, 222(??):263–266, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730293X.

vonRudorff:2014:EIA

[vRWS14] Guido Falk von Rudorff, Christoph Wehmeyer, and Daniel Sebastiani. Efficient implementation and application of the artificial bee colony algorithm to low-dimensional optimization problems. *Computer Physics Communications*, 185(6):1639–1646, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000861.

Vetter:2019:FOR

[VS19a] Roman Vetter and Jürgen O. Schumacher. Free open reference implementation of a two-phase PEM fuel cell model. *Computer Physics Communications*, 234(??):223–234, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518302807.

Vovchenko:2019:TFP

[VS19b] Volodymyr Vovchenko and Horst Stoecker. Thermal-FIST: a package for heavy-ion collisions and hadronic equation of state. *Computer Physics Communications*, 244(??):295–310, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302139.

Varier:2017:TNJ

[VSG17] K. Muraleedhara Varier, V. Sankar, and M. P. Gangadathan. TrackEtching — a Java based code for etched track profile calculations in SSNTDs. *Computer Physics*

Communications, 218(??):43–47, September 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301273.

Vela:2018:AAC

[VSG18] Luis Vela Vela, Raul Sanchez, and Joachim Geiger. ALARIC: an algorithm for constructing arbitrarily complex initial density distributions with low particle noise for SPH/SPMHD applications. *Computer Physics Communications*, 224(??):186–197, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303570.

vanSetten:2018:PTG

[vSGB+18] M. J. van Setten, M. Giantomassi, E. Bousquet, M. J. Verstraete, D. R. Hamann, X. Gonze, and G.-M. Rignanese. The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. *Computer Physics Communications*, 226(??):39–54, May 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465518300250.

VanLiedekerke:2013:SMF

[VSO+13] P. Van Liedekerke, B. Smeets, T. Odenthal, E. Tijskens, and H. Ramon. Solving microscopic flow problems using Stokes equations in SPH. *Computer Physics Communications*, 184(7):1686–1696, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000702.

Vukics:2012:CMA

[Vuk12] András Vukics. C++QEDv2: The multi-array concept and compile-time algorithms in the definition of composite quantum systems. *Computer Physics Communications*, 183(6):1381–1396, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000562.

Vincenti:2016:DAE

[VV16] H. Vincenti and J.-L. Vay. Detailed analysis of the effects of stencil spatial variations with arbitrary high-order finite-difference Maxwell solver. *Computer Physics Communications*, 200(??):147–167, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515004208`.

Vincenti:2018:UOM

[VV18] Henri Vincenti and Jean-Luc Vay. Ultrahigh-order Maxwell solver with extreme scalability for electromagnetic PIC simulations of plasmas. *Computer Physics Communications*, 228(??):22–29, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300900`.

Verstichel:2011:VDM

[VvAV+11a] Brecht Verstichel, Helen van Aggelen, Dimitri Van Neck, Paul W. Ayers, and Patrick Bultinck. Variational density matrix optimization using semidefinite programming. *Computer Physics Communications*, 182(9):2025–2028, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510005278`.

Verstichel:2011:PDS

[VvAV+11b] Brecht Verstichel, Helen van Aggelen, Dimitri Van Neck, Patrick Bultinck, and Stijn De Baerdemacker. A primal-dual semidefinite programming algorithm tailored to the variational determination of the two-body density matrix. *Computer Physics Communications*, 182(6):1235–1244, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000646`.

Vudragovic:2012:CPS

[VVB+12] Dusan Vudragović, Ivana Vidanović, Antun Balaz, Paulsamy Muruganandam, and Sadhan K. Adhikari. C programs for solving the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap. *Computer Physics Communications*, 183(9):2021–2025, September 2012. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001270.

vonWinckel:2010:QFK

[vWB10] G. von Winckel and A. Borzi‘. QUCON: a fast Krylov–Newton code for dipole quantum control problems. *Computer Physics Communications*, 181(12):2158–2163, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003164.

Windisch:2013:EAS

[WAHL13] Andreas Windisch, Reinhard Alkofer, Gundolf Haase, and Manfred Liebmann. Examining the analytic structure of Green's functions: Massive parallel complex integration using GPUs. *Computer Physics Communications*, 184(1):109–116, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002895.

Wainwright:2012:CCC

[Wai12] Carroll L. Wainwright. CosmoTransitions: Computing cosmological phase transition temperatures and bubble profiles with multiple fields. *Computer Physics Communications*, 183(9):2006–2013, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001348.

Walters:2011:EWP

[Wal11] Zachary B. Walters. Efficient wavefunction propagation by minimizing accumulated action. *Computer Physics Communications*, 182(4):935–939, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005230.

Wang:2010:ECT

[Wan10a] Hanquan Wang. An efficient Chebyshev–Tau spectral method for Ginzburg–Landau–Schrödinger equations. *Computer Physics Communications*, 181(2):325–340, February

2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003208.

Wang:2010:AQL

[Wan10b] Minghui Wang. Algorithm Q–LSQR for the least squares problem in quaternionic quantum theory. *Computer Physics Communications*, 181(6):1047–1050, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000500.

Wang:2016:STB

[Wan16] Wenlong Wang. Simulating thermal boundary conditions of spin-lattice models with weighted averages. *Computer Physics Communications*, 204(??):82–87, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300686.

Ward:2016:IID

[War16] B. F. L. Ward. IR-improved DGLAP-CS QCD parton showers in Pythia8. *Computer Physics Communications*, 201(??):29–32, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004464.

Wong:2014:EMS

[WAW14] Un-Hong Wong, Takayuki Aoki, and Hon-Cheng Wong. Efficient magnetohydrodynamic simulations on distributed multi-GPU systems using a novel GPU Direct-MPI hybrid approach. *Computer Physics Communications*, 185(7):1901–1913, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000988.

White:2018:DOB

[WBS+18] C. White, M. K. Borg, T. J. Scanlon, S. M. Longshaw, B. John, D. R. Emerson, and J. M. Reese. dsmcFoam+: an OpenFOAM based direct simulation Monte Carlo solver. *Computer Physics Communications*, 224(??):22–43, March

2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303375.

Wen:2011:CAC

[WBY11] M. Wen, A. Barnoush, and K. Yokogawa. Calculation of all cubic single-crystal elastic constants from single atomistic simulation: Hydrogen effect and elastic constants of nickel. *Computer Physics Communications*, 182(8):1621–1625, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001275.

Wang:2010:PMH

[WC10] Xiao-Gang Wang and Tucker Carrington, Jr. Parallel methods for high-dimensional quantum dynamics. *Computer Physics Communications*, 181(3):455–461, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003373.

Wittek:2013:SOD

[WC13] Peter Wittek and Fernando M. Cucchietti. A second-order distributed Trotter–Suzuki solver with a hybrid CPU–GPU kernel. *Computer Physics Communications*, 184(4):1165–1171, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004043.

Wittek:2015:ECK

[WC15] Peter Wittek and Luca Calderaro. Extended computational kernels in a massively parallel implementation of the Trotter–Suzuki approximation. *Computer Physics Communications*, 197(??):339–340, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002957.

Wang:2014:YPC

[WCL14] Yi Wang, Long-Qing Chen, and Zi-Kui Liu. YPHON: a package for calculating phonons of polar materials. *Computer Physics Communications*, 185(11):2950–2968, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002288.

Wu:2011:SMM

[WCT11] Hao-Yun Wu, Chung-I Chou, and Jie-Jun Tseng. A simple marriage model for the power-law behaviour in the frequency distributions of family names. *Computer Physics Communications*, 182(1):201–204, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003383.

Wendt:2011:TLS

[WDL11] Kyle A. Wendt, Joaquín E. Drut, and Timo A. Lähde. Toward large-scale hybrid Monte Carlo simulations of the Hubbard model on graphics processing units. *Computer Physics Communications*, 182(8):1651–1656, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001457.

Winczewski:2016:HET

[WDR16] Szymon Winczewski, Jacek Dziedzic, and Jaroslaw Rybicki. A highly-efficient technique for evaluating bond-orientational order parameters. *Computer Physics Communications*, 198(??):128–138, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003471.

Wiesenberger:2019:RAP

[WEH+19] Matthias Wiesenberger, Lukas Einkemmer, Markus Held, Albert Gutierrez-Milla, Xavier Sáez, and Roman Iakymchuk. Reproducibility, accuracy and performance of the Feltor code and library on parallel computer architectures. *Computer Physics Communications*, 238(??):145–156, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304223.

Wei:1999:UAE

[Wei99] Liqiang Wei. Unified approach for exact calculation of angular momentum coupling and recoupling coefficients. *Com-*

puter Physics Communications, 120(2–3):222–230, August 1999. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465599002325`. See erratum [Wei11a].

Wei:2011:DEC

[Wei11a] Liqiang Wei. Direct and exact compute and table of entire $3j$, $6j$, and $9j$ symbols: Erratum to CPC **120** (1999) 222–230. *Computer Physics Communications*, 182(5):1199, May 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000282`. See [Wei99].

Weigel:2011:SSM

[Wei11b] Martin Weigel. Simulating spin models on GPU. *Computer Physics Communications*, 182(9):1833–1836, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004327`.

Weinzierl:2012:SJA

[Wei12] Stefan Weinzierl. The SISCone jet algorithm optimised for low particle multiplicities. *Computer Physics Communications*, 183(3):813–820, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551100395X`.

Wang:2019:EOS

[WFDK19] Y. L. Wang, G. Fabbris, M. P. M. Dean, and G. Kotliar. EDRIXS: an open source toolkit for simulating spectra of resonant inelastic X-ray scattering. *Computer Physics Communications*, 243(??):151–165, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301353`.

Walewski:2014:RPI

[WFM14] Lukasz Walewski, Harald Forbert, and Dominik Marx. Reactive path integral quantum simulations of molecules solvated in superfluid helium. *Computer Physics Communications*, 185(3):884–899, March 2014. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004232.

Witherden:2014:POS

[WFV14] F. D. Witherden, A. M. Farrington, and P. E. Vincent. PyFR: an open source framework for solving advection-diffusion type problems on streaming architectures using the flux reconstruction approach. *Computer Physics Communications*, 185(11):3028–3040, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002549.

Wang:2019:MGF

[WFZG19] Yuan Wang, Xueshang Feng, Yufen Zhou, and Xinbiao Gan. A multi-GPU finite volume solver for magnetohydrodynamics-based solar wind simulations. *Computer Physics Communications*, 238(??):181–193, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304193.

Welling:2011:ELC

[WG11] Ulrich Welling and Guido Germano. Efficiency of linked cell algorithms. *Computer Physics Communications*, 182(3):611–615, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004480.

Waltz:2012:CMM

[WG12] J. Waltz and T. A. Gianakon. A comparison of mix models for the Rayleigh–Taylor instability. *Computer Physics Communications*, 183(1):70–79, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551100302X.

Walczak:2016:BBA

[WG16a] Michal Walczak and Helmut Grubmüller. BASDet: Bayesian approach(es) for structure determination from single molecule X-ray diffraction images. *Computer Physics Communications*, 201(??):159–166, April 2016. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551500452X.

Wang:2016:SIG

[WG16b] Peng Wang and Zhaoli Guo. A semi-implicit gas-kinetic scheme for smooth flows. *Computer Physics Communications*, 205(??):22–31, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300947.

Warren:2016:GOS

[WGG16] Craig Warren, Antonios Giannopoulos, and Iraklis Giannakis. gprMax: Open source software to simulate electromagnetic wave propagation for Ground Penetrating Radar. *Computer Physics Communications*, 209(??):163–170, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302533.

Warren:2019:CBG

[WGG+19] Craig Warren, Antonios Giannopoulos, Alan Gray, Iraklis Giannakis, Alan Patterson, Laura Wetter, and Andre Hamrah. A CUDA-based GPU engine for gprMax: Open source FDTD electromagnetic simulation software. *Computer Physics Communications*, 237(??):208–218, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303990.

Wang:2017:HPC

[WGVPL17] Jue Wang, Fei Gao, Jose Luis Vazquez-Poletti, and Jianjiang Li. High performance computing for advanced modeling and simulation of materials. *Computer Physics Communications*, 211(??):1, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302478.

Huang:2015:MGR

[wH15] Ding wei Huang. Modeling gridlock at roundabout. *Computer Physics Communications*, 189(??):72–76, April 2015.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004317.

Wagner:2016:CAT

[WHB16] Michael Wagner, Uwe Hampel, and Martina Bieberle. Correct averaging in transmission radiography: Analysis of the inverse problem. *Computer Physics Communications*, 202(??):196–203, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300169.

Wallerberger:2019:WLO

[WHG+19] Markus Wallerberger, Andreas Hausoel, Patrik Gunacker, Alexander Kowalski, Nicolaus Parragh, Florian Goth, Karsten Held, and Giorgio Sangiovanni. w2dynamics: Local one- and two-particle quantities from dynamical mean field theory. *Computer Physics Communications*, 235(??):388–399, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303217.

Hsu:2011:DCD

[wHwH11] Jiann wien Hsu and Ding wei Huang. Dynamics of citation distribution. *Computer Physics Communications*, 182(1):185–187, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000264X.

Wiebusch:2013:NCV

[Wie13] M. Wiebusch. Numerical computation of p-values with myFitter. *Computer Physics Communications*, 184(11):2438–2445, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002026.

Wiebusch:2015:HMP

[Wie15] Martin Wiebusch. HEPMath 1.4: a Mathematica package for semi-automatic computations in high energy physics.

Computer Physics Communications, 195(??):172–190, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001642.

Wiecha:2018:PPP

[Wie18] Peter R. Wiecha. pyGDM — a Python toolkit for full-field electro-dynamical simulations and evolutionary optimization of nanostructures. *Computer Physics Communications*, 233(??):167–192, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830225X.

Wilson:2015:EIF

[Wil15] Hugh F. Wilson. Efficient ab initio free energy calculations by classically assisted trajectory sampling. *Computer Physics Communications*, 197(??):1–6, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002775.

Wilson:2019:GFD

[Wil19] Joshua P. Wilson. Generalized Finite-Difference Time-Domain method with absorbing boundary conditions for solving the nonlinear Schrödinger equation on a GPU. *Computer Physics Communications*, 235(??):279–292, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300419.

Wallerberger:2011:FCC

[WISA11] Markus Wallerberger, Katharina Igenbergs, Josef Schweinzer, and Friedrich Aumayr. Fast computation of close-coupling exchange integrals using polynomials in a tree representation. *Computer Physics Communications*, 182(3):775–778, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004285.

Witzens:2014:ICD

[Wit14] Jeremy Witzens. Ab initio calculation of the deformation potential and photoelastic coefficients of silicon with a non-uniform finite-difference solver based on the local density approximation. *Computer Physics Communications*, 185(8):2221–2231, August 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000964.

Walter:2018:LCT

[WJCZ18] Nathan P. Walter, Abhishek Jaiswal, Zhikun Cai, and Yang Zhang. LiquidLib: A comprehensive toolbox for analyzing classical and ab initio molecular dynamics simulations of liquids and liquid-like matter with applications to neutron scattering experiments. *Computer Physics Communications*, 228(??):209–218, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300778.

Wang:2014:PTM

[WJHW14] Yu-Qing Wang, Rui Jiang, Mao-Bin Hu, and Qing-Song Wu. Phase transition in a mesoscopic ring with multiple diffusive channels. *Computer Physics Communications*, 185(11):2823–2828, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002252.

Wang:2011:MMP

[WL11a] Lai Wang and Frank X. Lee. MathQCDSR: a Mathematica package for QCD sum rules calculations. *Computer Physics Communications*, 182(8):1721–1731, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001482.

Wu:2011:NPT

[WL11b] M.-C. Wu and W.-C. Liu. Non-perturbative time-dependent numerical simulation for electromagnetically induced transparency and slow light in three-level Λ-type atoms. *Computer Physics Communications*, 182(1):143–145, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002286.

Wang:2013:UVM

[WLG+13] Zhijun Wang, Junjie Li, Yaolin Guo, Sai Tang, and Jincheng Wang. Unique visualization of multiply oriented lattice structures using a continuous wavelet transform. *Computer Physics Communications*, 184(11):2489–2493, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002129.

Wang:2018:EMH

[WLGY18] Maoyuan Wang, Gui-Bin Liu, Hong Guo, and Yugui Yao. An efficient method for hybrid density functional calculation with spin-orbit coupling. *Computer Physics Communications*, 224(??):90–97, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303934.

Wei:2012:ESM

[WLH+12] Pengfei Wei, Zhenzhou Lu, Wenrui Hao, Jun Feng, and Bintuan Wang. Efficient sampling methods for global reliability sensitivity analysis. *Computer Physics Communications*, 183(8):1728–1743, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001191.

Wickersham:2014:CFP

[WLM14] Andrew J. Wickersham, Xuesong Li, and Lin Ma. Comparison of Fourier, principal component and wavelet analyses for high speed flame measurements. *Computer Physics Communications*, 185(4):1237–1245, April 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004347.

Wang:2017:APT

[WLQ+17] Yulei Wang, Jian Liu, Hong Qin, Zhi Yu, and Yicun Yao. The accurate particle tracer code. *Computer Physics Communications*, 220(??):212–229, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302163.

Wei:2013:NVB

[WLS13] Pengfei Wei, Zhenzhou Lu, and Jingwen Song. A new variance-based global sensitivity analysis technique. *Computer Physics Communications*, 184(11):2540–2551, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002348.

Wiklund:2011:BCC

[WLU11] H. S. Wiklund, S. B. Lindström, and T. Uesaka. Boundary condition considerations in lattice Boltzmann formulations of wetting binary fluids. *Computer Physics Communications*, 182(10):2192–2200, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002098.

Wang:2012:CMC

[WLZM12] Yanchao Wang, Jian Lv, Li Zhu, and Yanming Ma. CALYPSO: a method for crystal structure prediction. *Computer Physics Communications*, 183(10):2063–2070, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001762.

Wu:2017:HOS

[WLZN17] Baodong Wu, Shigang Li, Yunquan Zhang, and Ningming Nie. Hybrid-optimization strategy for the communication of large-scale Kinetic Monte Carlo simulation. *Computer Physics Communications*, 211(??):113–123, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301904.

Wang:2013:SPM

[WM13] Minghui Wang and Wenhao Ma. A structure-preserving method for the quaternion LU decomposition in quaternionic quantum theory. *Computer Physics Communications*, 184(9):2182–2186, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001616.

Wu:2019:ETS

[WMI19] Hao Wu, Peter C. Ma, and Matthias Ihme. Efficient time-stepping techniques for simulating turbulent reactive flows with stiff chemistry. *Computer Physics Communications*, 243(??):81–96, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930133X.

Wang:2011:IVP

[WMK11] Manhui Wang, Andrew J. May, and Peter J. Knowles. Improved version of parallel programming interface for distributed data with multiple helper servers. *Computer Physics Communications*, 182(7):1502–1506, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001135.

Winkler:2017:GSM

[WMRR17] Daniel Winkler, Michael Meister, Massoud Rezavand, and Wolfgang Rauch. gpuSPHASE — a shared memory caching implementation for 2D SPH using CUDA. *Computer Physics Communications*, 213(??):165–180, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516303666.

Watson:2010:MIK

[WN10] Michael Watson and Ken-Ichi Nishikawa. A method for incorporating the Kerr–Schild metric in electromagnetic particle-in-cell code. *Computer Physics Communications*, 181(10):1750–1757, October 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002237.

Watanabe:2019:SVL

[WN19] Hiroshi Watanabe and Koh M. Nakagawa. SIMD vectorization for the Lennard-Jones potential with AVX2 and AVX-512 instructions. *Computer Physics Communications*, 237(??):1–7, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830376X.

Wang:2017:CHS

[WNYP17] Chao Wang, Håkan Nilsson, Jiandong Yang, and Olivier Petit. 1D–3D coupling for hydraulic system transient simulations. *Computer Physics Communications*, 210(??):1–9, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302788.

Wegner:2010:ISE

[WP10a] Tadeusz Wegner and Andrzej Peczak. Implementation of a strain energy-based nonlinear finite element in the object-oriented environment. *Computer Physics Communications*, 181(3):520–531, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003488.

Wolkov:2010:HOD

[WP10b] A. V. Wolkov and N. B. Petrovskaya. Higher order discontinuous Galerkin method for acoustic pulse problem. *Computer Physics Communications*, 181(7):1186–1194, July 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000834.

Walizer:2011:BBS

[WP11] Laura E. Walizer and John F. Peters. A bounding box search algorithm for DEM simulation. *Computer Physics Communications*, 182(2):281–288, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000353X.

Wouters:2014:CFO

[WPAV14] Sebastian Wouters, Ward Poelmans, Paul W. Ayers, and Dimitri Van Neck. CheMPS2: a free open-source spin-adapted implementation of the density matrix renormalization group for ab initio quantum chemistry. *Computer Physics Communications*, 185(6):1501–1514, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000496.

Wouters:2015:CID

[WPD+15] Sebastian Wouters, Ward Poelmans, Stijn De Baerdemacker, Paul W. Ayers, and Dimitri Van Neck. CheMPS2: Improved DMRG–SCF routine and correlation functions. *Computer Physics Communications*, 191(??):235–237, June 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000168.

Warmbier:2018:BZG

[WQ18] Robert Warmbier and Alexander Quandt. Brillouin zone grid refinement for highly resolved ab initio THz optical properties of graphene. *Computer Physics Communications*, 228(??):96–99, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300638.

Welsh:2016:CCC

[WR16] T. A. Welsh and D. J. Rowe. A computer code for calculations in the algebraic collective model of the atomic nucleus. *Computer Physics Communications*, 200(??):220–253, March 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003975.

Wolak:2011:PPI

[WRB11] M. J. Wolak, V. G. Rousseau, and G. G. Batrouni. Pairing in population imbalanced fermion systems. *Computer Physics Communications*, 182(9):2021–2024, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005254.

Weyens:2019:CAE

[WRBL19] T. Weyens, J. M. Reynolds-Barredo, and A. Loarte. Computationally advantageous expressions for 3-D MHD stability. *Computer Physics Communications*, 242(??):60–71, September 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301171.

Walsh:2015:OEG

[WRFS15] Jonathan A. Walsh, Paul K. Romano, Benoit Forget, and Kord S. Smith. Optimizations of the energy grid search algorithm in continuous-energy Monte Carlo particle transport codes. *Computer Physics Communications*, 196(??):134–142, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002052.

Winkler:2019:GSM

[WRMR19] Daniel Winkler, Massoud Rezavand, Michael Meister, and Wolfgang Rauch. gpuSPHASE — a shared memory caching implementation for 2D SPH using CUDA (new version announcement). *Computer Physics Communications*, 235(??):514–516, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303126.

Winkler:2018:NLS

[WRR18] Daniel Winkler, Massoud Rezavand, and Wolfgang Rauch. Neighbour lists for smoothed particle hydrodynamics on GPUs. *Computer Physics Communications*, 225(??):140–148, April 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517304198.

Wosniack:2015:PAR

[WRVdL15] M. E. Wosniack, E. P. Raposo, G. M. Viswanathan, and M. G. E. da Luz. A parallel algorithm for random searches. *Computer Physics Communications*, 196(??):390–397, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002830.

Wang:2011:EKS

[WS11a] Kangkang Wang and Arthur R. Smith. Efficient kinematical simulation of reflection high-energy electron diffraction streak patterns for crystal surfaces. *Computer Physics Communications*, 182(10):2208–2212, October 2011. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001603.

Wrobel:2011:MOT

[WS11b] Frédéric Wrobel and Frédéric Saigné. MC–ORACLE: a tool for predicting Soft Error Rate. *Computer Physics Communications*, 182(2):317–321, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000384X.

Winkel:2012:MPM

[WSH+12] Mathias Winkel, Robert Speck, Helge Hübner, Lukas Arnold, Rolf Krause, and Paul Gibbon. A massively parallel, multi-disciplinary Barnes–Hut tree code for extreme-scale N-body simulations. *Computer Physics Communications*, 183(4):880–889, April 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511004012.

Westphal:2014:MCD

[WSH+14] E. Westphal, S. P. Singh, C.-C. Huang, G. Gompper, and R. G. Winkler. Multiparticle collision dynamics: GPU accelerated particle-based mesoscale hydrodynamic simulations. *Computer Physics Communications*, 185(2):495–503, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003317.

Watanabe:2013:HSM

[WSI13] Hiroshi Watanabe, Masaru Suzuki, and Nobuyasu Ito. Huge-scale molecular dynamics simulation of multibubble nuclei. *Computer Physics Communications*, 184(12):2775–2784, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300252X.

Weng:2012:FRR

[WSO+12] Jiantong Weng, Tomoyoshi Shimobaba, Minoru Oikawa, Nobuyuki Masuda, and Tomoyoshi Ito. Fast recurrence relation for computer-generated-hologram. *Computer Physics*

Communications, 183(1):46–49, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511002992`.

Werlich:2015:SAM

[WSTP15] B. Werlich, T. Shakirov, M. P. Taylor, and W. Paul. Stochastic approximation Monte Carlo and Wang–Landau Monte Carlo applied to a continuum polymer model. *Computer Physics Communications*, 186(??):65–70, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003348`.

Williams:2012:EMC

[WT12] Elizabeth Williams and James Tickner. Efficient Monte Carlo simulation of coincidence effects in radioisotope decays including γ–γ angular correlations. *Computer Physics Communications*, 183(9):1869–1876, September 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001336`.

Wu:2015:FFB

[WT15] Jingwen Wu and Hongjiong Tian. Functionally-fitted block methods for second order ordinary differential equations. *Computer Physics Communications*, 197(??):96–108, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515002969`.

Waxenegger:2015:PSM

[WTH15] Jürgen Waxenegger, Andreas Trügler, and Ulrich Hohenester. Plasmonics simulations with the MNPBEM toolbox: Consideration of substrates and layer structures. *Computer Physics Communications*, 193(??):138–150, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001228`.

Wu:2010:EER

[Wu10] Xinyuan Wu. Erratum to “Extended RKN-type methods for numerical integration of perturbed oscillators” [Computer

Physics Communications **180** (2009) 1777–1794]. *Computer Physics Communications*, 181(9):1658, September 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510001876`. See [YWYF09].

Whitehorn:2013:PSS

[WvSL13] Nathan Whitehorn, Jakob van Santen, and Sven Lafebre. Penalized splines for smooth representation of high-dimensional Monte Carlo datasets. *Computer Physics Communications*, 184(9):2214–2220, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001434`.

Wu:2010:MAR

[WW10] Xinyuan Wu and Bin Wang. Multidimensional adapted Runge–Kutta–Nyström methods for oscillatory systems. *Computer Physics Communications*, 181(12):1955–1962, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510003516`.

Wang:2012:TIE

[WW12] Xian-You Wang and Xing-Gang Wu. A trick to improve the efficiency of generating unweighted *Bc* events from BCVEGPY. *Computer Physics Communications*, 183(2):442–445, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511003419`.

Wang:2013:GIV

[WW13] Xian-You Wang and Xing-Gang Wu. GENXICC2.1: an improved version of GENXICC for hadronic production of doubly heavy baryons. *Computer Physics Communications*, 184(3):1070–1074, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003657`.

Wan:2014:FFP

[WW14] Lu-Ping Wan and Jian-Xiong Wang. FDCHQHP: a Fortran package for heavy quarkonium hadroproduction. *Com-*

puter Physics Communications, 185(11):2939–2949, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002276.

Wallraff:2015:COP

[WW15] Marius Wallraff and Christopher Wiebusch. Calculation of oscillation probabilities of atmospheric neutrinos using nuCraft. *Computer Physics Communications*, 197(??):185–189, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002799.

Wang:2016:TDS

[WWC+16] Yue Wang, Jianguo Wang, Zaigao Chen, Guoxin Cheng, and Pan Wang. Three-dimensional simple conformal symplectic particle-in-cell methods for simulations of high power microwave devices. *Computer Physics Communications*, 205(??):1–12, August 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300650.

Wong:2011:EMS

[WWFT11] Hon-Cheng Wong, Un-Hong Wong, Xueshang Feng, and Zesheng Tang. Efficient magnetohydrodynamic simulations on graphics processing units with CUDA. *Computer Physics Communications*, 182(10):2132–2160, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001676.

Wang:2014:SFA

[WWHW14] Hui Wang, Bo Wu, Zhixiang Huang, and Xianliang Wu. A symplectic FDTD algorithm for the simulations of lossy dispersive materials. *Computer Physics Communications*, 185(3):862–872, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004190.

Wong:2011:EPR

[WWL11] Jen-Hsien Wong, Bi-Ru Wu, and Ming-Fa Lin. Electronic properties of rhombohedral graphite. *Computer Physics*

Communications, 182(1):77–80, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002638.

Wong:2014:GMS

[WWM14] Un-Hong Wong, Hon-Cheng Wong, and Yonghui Ma. Global magnetohydrodynamic simulations on multiple GPUs. *Computer Physics Communications*, 185(1):144–152, January 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003007.

Wozniak:2016:GGB

[WWR+16] Bartosz D. Wozniak, Freddie D. Witherden, Francis P. Russell, Peter E. Vincent, and Paul H. J. Kelly. GiMMiK —- generating bespoke matrix multiplication kernels for accelerators: Application to high-order computational fluid dynamics. *Computer Physics Communications*, 202(??):12–22, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004506.

Wagner:2010:ECH

[WWS10] Mathias Wagner, Andrea Walther, and Bernd-Jochen Schaefer. On the efficient computation of high-order derivatives for implicitly defined functions. *Computer Physics Communications*, 181(4):756–764, April 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509004007.

Wilms:2011:MCS

[WWVB11] D. Wilms, A. Winkler, P. Virnau, and K. Binder. Monte Carlo simulations of the 2d-Ising model in the geometry of a long stripe. *Computer Physics Communications*, 182(9):1892–1895, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551000528X.

Wang:2011:ENM

[WX11] Hanquan Wang and Weibiao Xu. An efficient numerical method for simulating the dynamics of coupling Bose–Einstein condensates in optical resonators. *Computer Physics Communications*, 182(3):706–718, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004893.

Wang:2014:PGM

[WX14] Hanquan Wang and Zhiguo Xu. Projection gradient method for energy functional minimization with a constraint and its application to computing the ground state of spin-orbit-coupled Bose–Einstein condensates. *Computer Physics Communications*, 185(11):2803–2808, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001611.

Wang:2013:PSP

[WXL13] Dongling Wang, Aiguo Xiao, and Xueyang Li. Parametric symplectic partitioned Runge–Kutta methods with energy-preserving properties for Hamiltonian systems. *Computer Physics Communications*, 184(2):303–310, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002986.

Wang:2013:ADP

[WXW13] Sibo Wang, Junbo Xu, and Hao Wen. Accelerating dissipative particle dynamics with multiple GPUs. *Computer Physics Communications*, 184(11):2454–2461, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002051.

Wang:2014:ADA

[WXW14] Sibo Wang, Junbo Xu, and Hao Wen. The aggregation and diffusion of asphaltenes studied by GPU-accelerated dissipative particle dynamics. *Computer Physics Communications*, 185(12):3069–3078, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465514002604.

Wei:2019:PES

[WYH19] Ying Wei, Chao Yang, and Jizu Huang. Parallel energy-stable phase field crystal simulations based on domain decomposition methods. *Computer Physics Communications*, 234(??):26–39, January 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303011.

Wu:2010:EIS

[WYSW10] Xinyuan Wu, Xiong You, Wei Shi, and Bin Wang. ERKN integrators for systems of oscillatory second-order differential equations. *Computer Physics Communications*, 181(11):1873–1887, November 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002936.

Wang:2013:ESS

[WZ13] Shanshan Wang and Luming Zhang. An efficient split-step compact finite difference method for cubic-quintic complex Ginzburg–Landau equations. *Computer Physics Communications*, 184(6):1511–1521, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000362.

Wang:2018:DKD

[WZHE18] Han Wang, Linfeng Zhang, Jiequn Han, and Weinan E. DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. *Computer Physics Communications*, 228(??):178–184, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300882.

Wang:2011:ICS

[WZS+11] Gang Wang, Huiyu Zhu, Quanhua Sun, Deliang Zhang, and Kaixin Liu. An improved CE/SE scheme and its application to dilute gas-particle flows. *Computer Physics*

Communications, 182(8):1589–1601, August 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001226.

Wu:2018:WOS

[WZS+18] QuanSheng Wu, ShengNan Zhang, Hai-Feng Song, Matthias Troyer, and Alexey A. Soluyanov. WannierTools: an open-source software package for novel topological materials. *Computer Physics Communications*, 224(??):405–416, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303442.

Xiong:2014:BOS

[XAPK14] Qingang Xiong, Soroush Aramideh, Alberto Passalacqua, and Song-Charng Kong. BIOTC: an open-source CFD code for simulating biomass fast pyrolysis. *Computer Physics Communications*, 185(6):1739–1746, June 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514000459.

Xue:2013:CGF

[XD13] Changfeng Xue and Shaozhong Deng. Coulomb Green's function and image potential near a planar diffuse interface, revisited. *Computer Physics Communications*, 184(1):51–59, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002640.

Xu:2016:IWC

[XD16] Xiaoyang Xu and Xiao-Long Deng. An improved weakly compressible SPH method for simulating free surface flows of viscous and viscoelastic fluids. *Computer Physics Communications*, 201(??):43–62, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004543.

Xu:2019:MCO

[XGH+19] Yingfeng Xu, Wenfeng Guo, Youjun Hu, Lei Ye, Xiaotao Xiao, and Shaojie Wang. Monte Carlo orbit-following simulations including the finite Larmor radius effect based on a phase-space coordinate transform method. *Computer Physics Communications*, 244(??):40–48, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302164.

Xue:2015:CGF

[XHD15] Changfeng Xue, Qiongwei Huang, and Shaozhong Deng. Coulomb Green's function and image potential near a cylindrical diffuse interface. *Computer Physics Communications*, 197(??):153–168, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003264.

Xu:2012:PFL

[XHLM12] Zhijie Xu, Hai Huang, Xiaoyi Li, and Paul Meakin. Phase field and level set methods for modeling solute precipitation and/or dissolution. *Computer Physics Communications*, 183(1):15–19, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002773.

Xaman:2018:XFM

[XHLUF+18] J. Xamán, I. Hernández-López, J. Uriarte-Flores, I. Hernández-Pérez, I. Zavala-Guillén, P. Moreno-Bernal, and J. F. Hinojosa. X-factor: A modified relaxation factor to accelerate the convergence rate of the radiative transfer equation with high-order resolution schemes using the normalized weighting-factor method. *Computer Physics Communications*, 231(??):72–93, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301498.

Xie:2016:NMS

[XJS16] Hang Xie, Feng Jiang, and Wei E. I. Sha. Numerical methods for spin-dependent transport calculations and spin bound states analysis in Rashba waveguides. *Computer Physics Communications*, 198(??):118–127, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S001046551500346X.

Xiong:2014:DSL

[XLCW14] Hailing Xiong, Hang Li, Weiping Chen, and Laosheng Wu. Data structure for on-lattice cluster-cluster aggregation model performance optimization. *Computer Physics Communications*, 185(3):836–840, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004086.

Xu:2015:NMM

[XLL15] Xin Xu, Zhenzhou Lu, and Xiaopeng Luo. A numerical meshless method of soliton-like structures model via an optimal sampling density based kernel interpolation. *Computer Physics Communications*, 192(??):12–22, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000739.

Xiong:2013:GAA

[XLX13] Qingang Xiong, Bo Li, and Ji Xu. GPU-accelerated adaptive particle splitting and merging in SPH. *Computer Physics Communications*, 184(7):1701–1707, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000787.

Xu:2015:SHA

[XLX+15] Zhijie Xu, Dongsheng Li, Wei Xu, Arun Devaraj, Robert Colby, Suntharampillai Thevuthasan, B. P. Geiser, and D. J. Larson. Simulation of heterogeneous atom probe tip shapes evolution during field evaporation using a level set method and different evaporation models. *Computer Physics Communications*, 189(??):106–113, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004366.

Xiao:2016:MPC

[XMLC16] Shuyuan Xiao, Xueli Mu, Tingting Liu, and Hong Chen. A Mathematica program for the calculation of five-body

Moshinsky brackets. *Computer Physics Communications*, 203(??):238–244, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300315.

Xu:2016:EIP

[XNK+16] Junqing Xu, Calogero R. Natoli, Peter Krüger, Kuniko Hayakawa, Didier Sébilleau, Li Song, and Keisuke Hatada. ES2MS: an interface package for passing self-consistent charge density and potential from Electronic Structure codes To Multiple Scattering codes. *Computer Physics Communications*, 203(??):331–338, June 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300467.

Xiao:2019:EHO

[XQ19] Jianyuan Xiao and Hong Qin. Explicit high-order gauge-independent symplectic algorithms for relativistic charged particle dynamics. *Computer Physics Communications*, 241(??):19–27, August 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301158.

Xiao:2015:EVS

[XW15] Bo Xiao and Hao Wang. An extended version of the simple and fast Feynman diagram generator EasyFeynDiag. *Computer Physics Communications*, 186(??):108–109, January 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514003191.

Xiao:2018:LLG

[XWF18] Xufeng Xiao, Kun Wang, and Xinlong Feng. A lifted local Galerkin method for solving the reaction-diffusion equations on implicit surfaces. *Computer Physics Communications*, 231(??):107–113, October 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518301395.

Xiao:2013:SAA

[XWhZ13] Bo Xiao, Hao Wang, and Shou hua Zhu. A simple algorithm for automatic Feynman diagram generation. *Computer Physics Communications*, 184(8):1966–1972, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001124.

Xie:2012:FOC

[XYK12] Shu-Sen Xie, Su-Cheol Yi, and Tae In Kwon. Fourth-order compact difference and alternating direction implicit schemes for telegraph equations. *Computer Physics Communications*, 183(3):552–569, March 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003857.

Xu:2013:NID

[XYM+13] Xinlu Xu, Peicheng Yu, Samual F. Martins, Frank S. Tsung, Viktor K. Decyk, Jorge Vieira, Ricardo A. Fonseca, Wei Lu, Luis O. Silva, and Warren B. Mori. Numerical instability due to relativistic plasma drift in EM–PIC simulations. *Computer Physics Communications*, 184(11):2503–2514, November 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002312.

Xu:2019:ELS

[XYZX19] Zhen Xu, Xiaofeng Yang, Hui Zhang, and Ziqing Xie. Efficient and linear schemes for anisotropic Cahn–Hilliard model using the Stabilized-Invariant Energy Quadratization (S-IEQ) approach. *Computer Physics Communications*, 238(??):36–49, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304417.

Xu:2012:ADI

[XZ12] Yiqiang Xu and Luming Zhang. Alternating direction implicit method for solving two-dimensional cubic nonlinear Schrödinger equation. *Computer Physics Communications*, 183(5):1082–1093, May 2012. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000094.

Xiong:2012:PSH

[XZF12] Wanjie Xiong, Fan Zhong, and Shuangli Fan. Positive specific-heat critical exponent of a three-dimensional three-state random-bond Potts model. *Computer Physics Communications*, 183(6):1162–1171, June 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000331.

Yamaguchi:2016:PCP

[Yam16] Chiaki Yamaguchi. Proposal of a checking parameter in the simulated annealing method applied to the spin glass model. *Computer Physics Communications*, 199(??):47–52, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003914.

Yang:2009:FAM

[Yan09] Hong Wei Yang. A FDTD analysis on magnetized plasma of Epstein distribution and reflection calculation. *Computer Physics Communications*, 180(1):55–60, January 2009. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465508002889. See addendum and comments [Ram10].

Yang:2011:EIB

[Yan11] Chih-Kai Yang. Exploring the interaction between the boron nitride nanotube and biological molecules. *Computer Physics Communications*, 182(1):39–42, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002857.

Yu:2013:DST

[YB13] Wenbin Yu and Maxwell Blair. DNAD, a simple tool for automatic differentiation of Fortran codes using dual numbers. *Computer Physics Communications*, 184(5):1446–1452, May

2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000027`.

Yokota:2011:BEU

[YBK+11] Rio Yokota, Jaydeep P. Bardhan, Matthew G. Knepley, L. A. Barba, and Tsuyoshi Hamada. Biomolecular electrostatics using a fast multipole BEM on up to 512 GPUs and a billion unknowns. *Computer Physics Communications*, 182(6):1272–1283, June 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000750`.

Yokota:2013:PTS

[YBNY13] Rio Yokota, L. A. Barba, Tetsu Narumi, and Kenji Yasuoka. Petascale turbulence simulation using a highly parallel fast multipole method on GPUs. *Computer Physics Communications*, 184(3):445–455, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512002974`.

Yakar:2015:LNA

[YÇÖ15] Yusuf Yakar, Bekir Çakir, and Ayhan Özmen. Linear and nonlinear absorption coefficients of spherical two-electron quantum dot. *Computer Physics Communications*, 188(??):88–93, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003944`.

Yuasa:2012:NCT

[YdDH+12] F. Yuasa, E. de Doncker, N. Hamaguchi, T. Ishikawa, K. Kato, Y. Kurihara, J. Fujimoto, and Y. Shimizu. Numerical computation of two-loop box diagrams with masses. *Computer Physics Communications*, 183(10):2136–2144, October 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512001877`.

Youssef:2014:CNK

[YE14a] Nabil L. Youssef and S. G. Elgendi. Computing nullity and kernel vectors using NF-package: Counterexamples. *Computer Physics Communications*, 185(11):2859–2864, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002471.

Youssef:2014:NFP

[YE14b] Nabil L. Youssef and S. G. Elgendi. New Finsler package. *Computer Physics Communications*, 185(3):986–997, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551300369X.

Yu:2017:CTA

[YFAT17] Haoyu S. Yu, Lucas J. Fiedler, I. M. Alecu, and Donald G. Truhlar. Computational thermochemistry: Automated generation of scale factors for vibrational frequencies calculated by electronic structure model chemistries. *Computer Physics Communications*, 210(??):132–138, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302740.

Yuan:2012:DAV

[YG12] Gary Yuan and François Gygi. A distributed approach to verification and validation of electronic structure simulation data using ESTEST. *Computer Physics Communications*, 183(8):1744–1748, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200121X.

Yang:2015:OPS

[YH15] Han-Xin Yang and Liang Huang. Opinion percolation in structured population. *Computer Physics Communications*, 192(??):124–129, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000946.

Yang:2011:TDS

[YHCS11] Chia-Hei Yang, Ching-Ling Hsu, Nan-Yow Chen, and Chi-Tin Shih. Temporal dynamics of site percolation in nanoparticle assemblies. *Computer Physics Communications*, 182(1):71–73, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002481.

Yang:2011:HCO

[YHL11] Chao-Tung Yang, Chih-Lin Huang, and Cheng-Fang Lin. Hybrid CUDA, OpenMP, and MPI parallel programming on multicore GPU clusters. *Computer Physics Communications*, 182(1):266–269, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510002262.

Yi:2011:PEG

[Yi11] Hongsuk Yi. Performance evaluation of GAIA supercomputer using NPB multi-zone benchmarks. *Computer Physics Communications*, 182(1):263–265, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003437.

Yuan:2011:MGM

[YJK11] Xuefei Yuan, Stephen C. Jardin, and David E. Keyes. Moving grids for magnetic reconnection via Newton–Krylov methods. *Computer Physics Communications*, 182(1):173–176, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001864.

Yang:2010:AWL

[YK10] Jae-Suk Yang and Wooseop Kwak. Application of Wang–Landau sampling to a protein model using SMMP. *Computer Physics Communications*, 181(1):99–104, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509002835.

Yi:2012:FCM

[YK12] Su Do Yi and Beom Jun Kim. Force correlations in molecular and stochastic dynamics. *Computer Physics Communications*, 183(8):1574–1577, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000872.

Yeo:2018:UME

[YK18] Haram Yeo and Hyungson Ki. A unified momentum equation approach for computing thermal residual stresses during melting and solidification. *Computer Physics Communications*, 224(??):230–244, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303533.

Yang:2019:ARM

[YK19] Xiufeng Yang and Song-Charng Kong. Adaptive resolution for multiphase smoothed particle hydrodynamics. *Computer Physics Communications*, 239(??):112–125, June 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300037.

Yamasaki:2019:MAD

[YKK+19] Takahiro Yamasaki, Akiyoshi Kuroda, Toshihiro Kato, Jun Nara, Junichiro Koga, Tsuyoshi Uda, Kazuo Minami, and Takahisa Ohno. Multi-axis decomposition of density functional program for strong scaling up to 82,944 nodes on the K computer: Compactly folded 3D-FFT communicators in the 6D torus network. *Computer Physics Communications*, 244(??):264–276, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301213.

Young:2011:CQA

[YKS11] A. P. Young, S. Knysh, and V. N. Smelyanskiy. The complexity of the Quantum Adiabatic Algorithm. *Computer Physics Communications*, 182(1):27–28, January 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510001785.

Yin:2012:MPW

[YL12] Junqi Yin and D. P. Landau. Massively parallel Wang–Landau sampling on multiple GPUs. *Computer Physics Communications*, 183(8):1568–1573, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000859.

Yang:2010:PFA

[YLK10] Seong-Deog Yang, Hyun Geun Lee, and Junseok Kim. A phase-field approach for minimizing the area of triply periodic surfaces with volume constraint. *Computer Physics Communications*, 181(6):1037–1046, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000494.

Yoo:2017:DIP

[YLKN17] Min-Gu Yoo, Jeongwon Lee, Young-Gi Kim, and Yong-Su Na. Development of 2D implicit particle simulation code for ohmic breakdown physics in a tokamak. *Computer Physics Communications*, 221(??):143–159, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302540.

Yu:2019:MBN

[YLL+19] Jiankai Yu, Hyunsuk Lee, Matthieu Lemaire, Hanjoo Kim, Peng Zhang, and Deokjung Lee. MCS based neutronics/thermal-hydraulics/fuel-performance coupling with CTF and FRAPCON. *Computer Physics Communications*, 238(??):1–18, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300025.

Yan:2013:GPU

[YLO13] Jun Yan, Lin Li, and Christopher O'Grady. Graphics Processing Unit acceleration of the Random Phase Approximation in the projector augmented wave method. *Computer Physics Communications*, 184(12):2728–2733, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002427.

Yang:2017:HPA

[YLQ+17] Sheng-Chun Yang, Zhong-Yuan Lu, Hu-Jun Qian, Yong-Lei Wang, and Jie-Ping Han. A hybrid parallel architecture for electrostatic interactions in the simulation of dissipative particle dynamics. *Computer Physics Communications*, 220(??):376–389, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302126.

Yurchenko:2016:DGP

[YLTS16] Sergei N. Yurchenko, Lorenzo Lodi, Jonathan Tennyson, and Andrey V. Stolyarov. Duo: a general program for calculating spectra of diatomic molecules. *Computer Physics Communications*, 202(??):262–275, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516000023.

Yen:2017:SVS

[YLYL17] Tsung-Wen Yen, Thong-Leng Lim, Tiem-Leong Yoon, and S. K. Lai. Studying the varied shapes of gold clusters by an elegant optimization algorithm that hybridizes the density functional tight-binding theory and the density functional theory. *Computer Physics Communications*, 220(??):143–149, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302096.

Yoshimi:2019:SSM

[YOM+19] Kazuyoshi Yoshimi, Junya Otsuki, Yuichi Motoyama, Masayuki Ohzeki, and Hiroshi Shinaoka. SpM: Sparse modeling tool for analytic continuation of imaginary-time Green's function. *Computer Physics Communications*, 244(??):319–323, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519302103.

Yuste:2012:FDM

[YQM12] Santos B. Yuste and Joaquín Quintana-Murillo. A finite difference method with non-uniform timesteps for fractional diffusion equations. *Computer Physics Communications*, 183(12):2594–2600, December 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002500. See corrigendum [YQM14].

Yuste:2014:CSF

[YQM14] Santos B. Yuste and Joaquín Quintana-Murillo. Corrigendum to "A finite difference method with non-uniform timesteps for fractional diffusion equations" [Comput. Phys. Comm. **183** (12) (2012) 2594–2600]. *Computer Physics Communications*, 185(3):1192, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003822. See [YQM12].

Young:2013:PFE

[YRR13] T. D. Young, E. Romero, and J. E. Roman. Parallel finite element density functional computations exploiting grid refinement and subspace recycling. *Computer Physics Communications*, 184(1):66–72, January 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512002664.

Yu:2017:DCL

[YS17] C. H. Yu and Tony W. H. Sheu. Development of a coupled level set and immersed boundary method for predicting dam break flows. *Computer Physics Communications*, 221(??):1–18, December 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551730214X.

Yang:2019:PRS

[YSLY19] Haijian Yang, Shuyu Sun, Yiteng Li, and Chao Yang. Parallel reservoir simulators for fully implicit complementarity formulation of multicomponent compressible flows. *Computer Physics Communications*, 244(??):2–12, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S001046551930222X.

Young-S:2017:OGI

[YSMA+17] Luis E. Young-S., Paulsamy Muruganandam, Sadhan K. Adhikari, Vladimir Loncar, Dusan Vudragović, and Antun Balaz. OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross–Pitaevskii equation. *Computer Physics Communications*, 220(??):503–506, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302321.

Yahyaoui:2014:ETT

[YSN+14] N. Yahyaoui, N. Sfina, S. Abdi-Ben Nasrallah, J.-L. Lazzari, and M. Said. Electron transport through cubic InGaN/AlGaN resonant tunneling diodes. *Computer Physics Communications*, 185(12):3119–3126, December 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002732.

Young-S:2016:OFP

[YSVM+16] Luis E. Young-S., Dusan Vudragović, Paulsamy Muruganandam, Sadhan K. Adhikari, and Antun Balaz. OpenMP Fortran and C programs for solving the time-dependent Gross–Pitaevskii equation in an anisotropic trap. *Computer Physics Communications*, 204(??):209–213, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630073X.

Yu:2017:SFV

[YTYA17] P. X. Yu, Z. F. Tian, A. Y. Ying, and M. A. Abdou. Stream function-velocity-magnetic induction compact difference method for the 2D steady incompressible full magnetohydrodynamic equations. *Computer Physics Communications*, 219(??):45–69, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301376.

Yuan:2019:PCS

[Yua19] Mingbo Yuan. A predictor–corrector symmetric TVD scheme for magnetogasdynamic flow. *Computer Physics Communications*, 237(??):86–97, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304004.

Yang:2015:HTR

[YvOSM15] Xiaogang Yang, J. Ruud van Ommen, Jasper Schoormans, and Robert F. Mudde. A hybrid tomographic reconstruction algorithm for high speed X-ray tomography. *Computer Physics Communications*, 196(??):27–35, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001885.

Yakovlev:2017:ACV

[YW17] Vladislav S. Yakovlev and Michael S. Wismer. Adiabatic corrections for velocity-gauge simulations of electron dynamics in periodic potentials. *Computer Physics Communications*, 217(??):82–88, August 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517301248.

Yue:2019:CXE

[YWOD19] Changming Yue, Yilin Wang, Junya Otsuki, and Xi Dai. CT-X: an efficient continuous-time quantum Monte Carlo impurity solver in the Kondo regime. *Computer Physics Communications*, 236(??):135–152, March 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303734.

Yang:2013:BEG

[YWW13] Zhi Yang, Xing-Gang Wu, and Xian-You Wang. BEEC: an event generator for simulating the B_c meson production at an e^+e^- collider. *Computer Physics Communications*, 184(12):2848–2855, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002440.

Yu:2011:TDD

[YWX11] Xijun Yu, Di Wu, and Yun Xu. Three dimensional discontinuous Galerkin methods for Euler equations on adaptive conforming meshes. *Computer Physics Communications*, 182(9):1771–1775, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511000063`.

Yang:2009:ERT

[YWYF09] Hongli Yang, Xinyuan Wu, Xiong You, and Yonglei Fang. Extended RKN-type methods for numerical integration of perturbed oscillators. *Computer Physics Communications*, 180(10):1777–1794, October 2009. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509001520`. See erratum [Wu10].

Yu:2015:ENC

[YXD+15] Peicheng Yu, Xinlu Xu, Viktor K. Decyk, Frederico Fiuza, Jorge Vieira, Frank S. Tsung, Ricardo A. Fonseca, Wei Lu, Luis O. Silva, and Warren B. Mori. Elimination of the numerical Cerenkov instability for spectral EM–PIC codes. *Computer Physics Communications*, 192(??):32–47, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515000752`.

Yu:2015:MNC

[YXT+15] Peicheng Yu, Xinlu Xu, Adam Tableman, Viktor K. Decyk, Frank S. Tsung, Frederico Fiuza, Asher Davidson, Jorge Vieira, Ricardo A. Fonseca, Wei Lu, Luis O. Silva, and Warren B. Mori. Mitigation of numerical Cerenkov radiation and instability using a hybrid finite difference-FFT Maxwell solver and a local charge conserving current deposit. *Computer Physics Communications*, 197(??):144–152, December 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003252`.

Yan:2016:NEP

[YZ16] Jinliang Yan and Zhiyue Zhang. New energy-preserving schemes using Hamiltonian Boundary Value and Fourier pseudospectral methods for the numerical solution of the "good" Boussinesq equation. *Computer Physics Communications*, 201(??):33–42, April 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515004518.

Yang:2019:ELS

[YZ19] Xiaofeng Yang and Jia Zhao. Efficient linear schemes for the nonlocal Cahn–Hilliard equation of phase field models. *Computer Physics Communications*, 235(??):234–245, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303084.

Yan:2018:ARP

[YZCS18] Yu-Liang Yan, Dai-Mei Zhou, Xu Cai, and Ben-Hao Sa. Announcement for the replacement of the PACIAE 2.1 and PACIAE 2.2 series. *Computer Physics Communications*, 224(??):417–418, March 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465517303466.

Yang:2014:SNT

[YZWR14] Hongli Yang, Xianyang Zeng, Xinyuan Wu, and Zhengliang Ru. A simplified Nyström-tree theory for extended Runge–Kutta–Nyström integrators solving multi-frequency oscillatory systems. *Computer Physics Communications*, 185(11):2841–2850, November 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514002434.

Yu:2010:CSC

[YZY10] R. Yu, J. Zhu, and H. Q. Ye. Calculations of single-crystal elastic constants made simple. *Computer Physics Communications*, 181(3):671–675, March 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465509003932.

You:2011:TFS

[YZZ11] Xiong You, Yonghui Zhang, and Jinxi Zhao. Trigonometrically-fitted Scheifele two-step methods for perturbed oscillators. *Computer Physics Communications*, 182(7):1481–1490, July 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465511001111`.

Yan:2017:PSO

[YZZ+17] Bailu Yan, Zheng Zhao, Yingcheng Zhou, Wenyan Yuan, Jian Li, Jun Wu, and Daojian Cheng. A particle swarm optimization algorithm with random learning mechanism and Levy flight for optimization of atomic clusters. *Computer Physics Communications*, 219(??):79–86, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551730139X`.

Zaza:2016:CBP

[ZAFAM16] Ayham Zaza, Abeeb A. Awotunde, Faisal A. Fairag, and Mayez A. Al-Mouhamed. A CUDA based parallel multi-phase oil reservoir simulator. *Computer Physics Communications*, 206(??):2–16, September 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516300996`.

Zaghi:2014:OSF

[Zag14] S. Zaghi. OFF, Open source Finite volume Fluid dynamics code: a free, high-order solver based on parallel, modular, object-oriented Fortran API. *Computer Physics Communications*, 185(7):2151–2194, July 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001283`.

Zacares:2010:GTM

[ZAHA10] M. Zacarés, M. Arevalillo-Herráez, and S. Abraham. A group-theory method to find stationary states in nonlinear discrete symmetry systems. *Computer Physics Communications*, 181(1):35–42, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465509002781.

Zeng:2016:MPP

[ZBG+16] Tao Zeng, Nicholas Blinov, Grégoire Guillon, Hui Li, Kevin P. Bishop, and Pierre-Nicholas Roy. MoRiBS-PIMC: a program to simulate molecular rotors in bosonic solvents using path-integral Monte Carlo. *Computer Physics Communications*, 204(??):170–188, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300406.

Zakynthinaki:2011:SOD

[ZBMM11] M. S. Zakynthinaki, R. O. Barakat, C. A. Cordente Martínez, and J. Sampedro Molinuevo. Stochastic optimization for the detection of changes in maternal heart rate kinetics during pregnancy. *Computer Physics Communications*, 182(3):683–691, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004777.

Zolfaghari:2019:HOA

[ZBN+19] Hadi Zolfaghari, Barna Becsek, Maria G. C. Nestola, William B. Sawyer, Rolf Krause, and Dominik Obrist. High-order accurate simulation of incompressible turbulent flows on many parallel GPUs of a hybrid-node supercomputer. *Computer Physics Communications*, 244(??):132–142, November 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL https://www.sciencedirect.com/science/article/pii/S0010465519301997.

Zhen:2012:DFH

[ZC12] Yubao Zhen and Chengbiao Chu. A deformation-fluctuation hybrid method for fast evaluation of elastic constants with many-body potentials. *Computer Physics Communications*, 183(2):261–265, February 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511003249.

Zhao:2019:IAC

[ZCC19] Menglong Zhao, Alex Chankin, and David Coster. An iterative algorithm of coupling the Kinetic Code for Plasma Periphery (KIPP) with SOLPS. *Computer Physics Communications*, 235(??):133–152, February 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518303266`.

Zhu:2017:DOS

[ZCG17] Lianhua Zhu, Songze Chen, and Zhaoli Guo. dugksFoam: an open source OpenFOAM solver for the Boltzmann model equation. *Computer Physics Communications*, 213(??):155–164, April 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516303642`.

Zanotti:2015:HOS

[ZD15] Olindo Zanotti and Michael Dumbser. A high order special relativistic hydrodynamic and magnetohydrodynamic code with space–time adaptive mesh refinement. *Computer Physics Communications*, 188(??):110–127, March 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514003981`.

Zinchenko:2013:NGF

[ZDD+13] O. Zinchenko, H. A. De Raedt, E. Detsi, P. R. Onck, and J. T. M. De Hosson. Nanoporous gold formation by dealloying: a Metropolis Monte Carlo study. *Computer Physics Communications*, 184(6):1562–1569, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000489`.

Zhang:2017:UEB

[ZDWM17] Liming Zhang, Ali Deng, Minghong Wang, and Xianzhu Meng. The use of the edge basis function for non-conformal solution of electric current volume integral equation. *Computer Physics Communications*, 215(??):103–112, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551730070X`.

Zhang:2010:NSN

[ZDWY10] Liming Zhang, Ali Deng, Minghong Wang, and Shaoqing Yang. Numerical study of a novel MFIE formulation using monopolar RWG basis functions. *Computer Physics Communications*, 181(1):52–60, January 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465509002756`.

Zacate:2011:SHI

[ZE11] Matthew O. Zacate and William E. Evenson. Stochastic hyperfine interactions modeling library. *Computer Physics Communications*, 182(4):1061–1077, April 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510005357`.

Zacate:2016:SHI

[ZE16] Matthew O. Zacate and William E. Evenson. Stochastic hyperfine interactions modeling library — Version 2. *Computer Physics Communications*, 199(??):180–181, February 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003938`.

Zerbetto:2015:MIT

[ZF15] Mirco Zerbetto and Diego Frezzato. Multidimensional integration through Markovian sampling under steered function morphing: a physical guise from statistical mechanics. *Computer Physics Communications*, 195(??):129–139, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515001423`.

Zatsarinny:2016:DBS

[ZF16] Oleg Zatsarinny and Charlotte Froese Fischer. DBSR_HF: a B-spline Dirac–Hartree–Fock program. *Computer Physics Communications*, 202(??):287–303, May 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516000047`.

Zilibotti:2011:ICA

[ZFBR11] Giovanna Zilibotti, Mauro Ferrario, Carlo Maria Bertoni, and Maria Clelia Righi. Ab initio calculation of adhesion and potential corrugation of diamond (001) interfaces. *Computer Physics Communications*, 182(9):1796–1799, September 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510005163.

Zhai:2014:NST

[ZFH14] Shuying Zhai, Xinlong Feng, and Yinnian He. Numerical simulation of the three dimensional Allen–Cahn equation by the high-order compact ADI method. *Computer Physics Communications*, 185(10):2449–2455, October 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514001714.

Zhu:2018:GGT

[ZFR18] Ben Zhu, Manaure Francisquez, and Barrett N. Rogers. GDB: a global 3D two-fluid model of plasma turbulence and transport in the tokamak edge. *Computer Physics Communications*, 232(??):46–58, November 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551830208X.

Zhang:2019:AAD

[ZFZ19] S. H. Zhang, Z. H. Fu, and R. F. Zhang. ADAIS: Automatic derivation of anisotropic ideal strength via high-throughput first-principles computations. *Computer Physics Communications*, 238(??):244–253, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518304284.

Zhao:2016:PTL

[ZHC16] Tao Zhao, Feng-Nan Hwang, and Xiao-Chuan Cai. Parallel two-level domain decomposition based Jacobi–Davidson algorithms for pyramidal quantum dot simulation. *Computer Physics Communications*, 204(??):74–81, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465516300674.

Zapata-Herrera:2018:ICP

[ZHCR18] Mario Zapata-Herrera, Ángela S. Camacho, and Hanz Y. Ramírez. Influence of the confinement potential on the size-dependent optical response of metallic nanometric particles. *Computer Physics Communications*, 227(??):1–7, June 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300407.

Zheleznyakova:2015:MDB

[Zhe15] A. L. Zheleznyakova. Molecular dynamics-based triangulation algorithm of free-form parametric surfaces for computer-aided engineering. *Computer Physics Communications*, 190(??):1–14, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000028.

Zhong:2011:PBN

[ZHL11] Jiahang Zhong, Run-Sheng Huang, and Shih-Chang Lee. A program for the Bayesian Neural Network in the ROOT framework. *Computer Physics Communications*, 182(12):2655–2660, December 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002682.

Zhang:2010:RFY

[ZHPS10] Bo Zhang, Jingfang Huang, Nikos P. Pitsianis, and Xiaobai Sun. Revision of FMM–Yukawa: An adaptive fast multipole method for screened Coulomb interactions. *Computer Physics Communications*, 181(12):2206–2207, December 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510003577.

Zhang:2013:SNS

[ZHSL13] Yong Zhang, Ting-Zhu Huang, Wei Shao, and Sheng-Jian Lai. Some new strategies for RCM ordering in solving electromagnetic scattering problems. *Computer Physics*

Communications, 184(4):1161–1164, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512004031.

Ziolkowski:2014:NAN

[Zió14] Andrzej Ziólkowski. A numerical approach to nonlinear propagation of light in photorefractive media. *Computer Physics Communications*, 185(2):504–511, February 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513003329.

Zitko:2011:SMP

[Zit11] Rok Zitko. SNEG — Mathematica package for symbolic calculations with second-quantization-operator expressions. *Computer Physics Communications*, 182(10):2259–2264, October 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511001792.

Zhang:2018:DPA

[ZKG+18] X. Zhang, J. Kang, Z. Guo, S. Xiong, and Q. Han. Development of a Para-AMR algorithm for simulating dendrite growth under convection using a phase-field–lattice Boltzmann method. *Computer Physics Communications*, 223(??):18–27, February 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303260.

Zuniga:2013:MID

[ZKS13] M. Munoz Zuniga, S. Kucherenko, and N. Shah. Metamodelling with independent and dependent inputs. *Computer Physics Communications*, 184(6):1570–1580, June 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000490.

Zhu:2018:DES

[ZKS+18] Guangpu Zhu, Jisheng Kou, Shuyu Sun, Jun Yao, and Aifen Li. Decoupled, energy stable schemes for a phase-field surfactant model. *Computer Physics Communica-*

tions, 233(??):67–77, December 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518302522`.

Zentile:2015:EPC

[ZKW+15] Mark A. Zentile, James Keaveney, Lee Weller, Daniel J. Whiting, Charles S. Adams, and Ifan G. Hughes. ElecSus: a program to calculate the electric susceptibility of an atomic ensemble. *Computer Physics Communications*, 189(??):162–174, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551400407X`.

Zuccaro:2011:MMP

[ZLFM11] G. Zuccaro, G. Lapenta, F. Ferrero, and G. Maizza. Multiphase and multiphysics particle in cell simulation of soot deposition inside a diesel particulate filter single channel. *Computer Physics Communications*, 182(2):347–359, February 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510004066`.

Zhao:2013:IHA

[ZLL13] Yinlong Zhao, Zhiliang Lin, and Shijun Liao. An iterative HAM approach for nonlinear boundary value problems in a semi-infinite domain. *Computer Physics Communications*, 184(9):2136–2144, September 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513001446`.

Zhang:2018:TMM

[ZLL18] Peng Zhang, Hyunsuk Lee, and Deokjung Lee. On the transfer matrix of the modified power method. *Computer Physics Communications*, 222(??):102–112, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517303296`.

Zhang:2017:MAG

[ZLLP17] Xiaoming Zhang, Xin Liu, Xin Li, and Dongyu Pan. MMKG: an approach to generate metallic materials knowledge graph based on DBpedia and Wikipedia. *Computer Physics Communications*, 211(??):98–112, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516301874.

Zhao:2012:MMC

[ZLM12] Yan Zhao, Xuesong Li, and Lin Ma. Multidimensional Monte Carlo model for two-photon laser-induced fluorescence and amplified spontaneous emission. *Computer Physics Communications*, 183(8):1588–1595, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512000896.

Zlokazov:2013:VGD

[Zlo13] V. B. Zlokazov. VACTIV: a graphical dialog based program for an automatic processing of line and band spectra. *Computer Physics Communications*, 184(5):1480–1481, May 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513000106.

Zlokazov:2014:CIO

[Zlo14] V. B. Zlokazov. Confidence interval optimization for testing hypotheses under data with low statistics. *Computer Physics Communications*, 185(3):933–938, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513004281.

Zhang:2019:PAP

[ZLZ19] S. H. Zhang, D. Legut, and R. F. Zhang. PNADIS: an automated Peierls–Nabarro analyzer for dislocation core structure and slip resistance. *Computer Physics Communications*, 240(??):60–73, July 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519300839.

Zheng:2012:MPC

[ZMCT12] Jingjing Zheng, Steven L. Mielke, Kenneth L. Clarkson, and Donald G. Truhlar. MSTor: a program for calculating partition functions, free energies, enthalpies, entropies, and heat capacities of complex molecules including torsional anharmonicity. *Computer Physics Communications*, 183(8):1803–1812, August 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512001129.

Zierenberg:2013:SPP

[ZMJ13] Johannes Zierenberg, Martin Marenz, and Wolfhard Janke. Scaling properties of a parallel implementation of the multicanonical algorithm. *Computer Physics Communications*, 184(4):1155–1160, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551200402X.

Zheng:2013:MVN

[ZMPT13] Jingjing Zheng, Rubén Meana-Pañeda, and Donald G. Truhlar. MSTor version 2013: a new version of the computer code for the multi-structural torsional anharmonicity, now with a coupled torsional potential. *Computer Physics Communications*, 184(8):2032–2033, August 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513001082.

Zwart:2013:MPS

[ZMvE+13] Simon F. Portegies Zwart, Stephen L. W. McMillan, Arjen van Elteren, F. Inti Pelupessy, and Nathan de Vries. Multi-physics simulations using a hierarchical interchangeable software interface. *Computer Physics Communications*, 184(3):456–468, March 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003116.

Zhou:2015:EHO

[ZNT15] K. Zhou, S. H. Ni, and Z. F. Tian. Exponential high-order compact scheme on nonuniform grids for the steady MHD duct flow problems with high Hartmann numbers. *Computer Physics Communications*, 196(??):194–211, November 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515002519.

Zouros:2018:CEA

[Zou18] Grigorios P. Zouros. CCOMP: an efficient algorithm for complex roots computation of determinantal equations. *Computer Physics Communications*, 222(??):339–350, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303302.

Zhang:2013:VME

[ZOZ13] Lin Zhang, Jie Ouyang, and Xiaohua Zhang. The variational multiscale element free Galerkin method for MHD flows at high Hartmann numbers. *Computer Physics Communications*, 184(4):1106–1118, April 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465512003980.

Zhang:2015:PAS

[ZPH+15] Bo Zhang, Bo Peng, Jingfang Huang, Nikos P. Pitsianis, Xiaobai Sun, and Benzhuo Lu. Parallel AFMPB solver with automatic surface meshing for calculation of molecular solvation free energy. *Computer Physics Communications*, 190(??):173–181, May 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000089.

Zhu:2018:AGV

[ZPS+18] Xiaojue Zhu, Everett Phillips, Vamsi Spandan, John Donners, Gregory Ruetsch, Joshua Romero, Rodolfo Ostilla-Mónico, Yantao Yang, Detlef Lohse, Roberto Verzicco, Massimiliano Fatica, and Richard J. A. M. Stevens. AFiD-GPU: A versatile Navier–Stokes solver for wall-bounded turbulent flows on GPU clusters. *Computer Physics Communications*, 229(??):199–210, August 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518300985.

Zheng:2016:EOF

[ZPvR16] Dawei Zheng, Gisela Pöplau, and Ursula van Rienen. Efficiency optimization of a fast Poisson solver in beam dynamics simulation. *Computer Physics Communications*, 198(??):82–96, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515003434.

Zhang:2012:SSS

[ZRS12] Chuan-Hui Zhang, Qiong Ran, and Jiang Shen. Structural stability of silicene-like nanotubes. *Computer Physics Communications*, 183(1):30–33, January 2012. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465511002815.

Zheleznyakova:2013:MDB

[ZS13] A. L. Zheleznyakova and S. T. Surzhikov. Molecular dynamics-based unstructured grid generation method for aerodynamic applications. *Computer Physics Communications*, 184(12):2711–2727, December 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465513002415.

Zhu:2011:MSW

[ZST11] Huajun Zhu, Songhe Song, and Yifa Tang. Multi-symplectic wavelet collocation method for the nonlinear Schrödinger equation and the Camassa–Holm equation. *Computer Physics Communications*, 182(3):616–627, March 2011. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510004492.

Zhang:2017:UVM

[ZSW$^+$17a] Hanqing Zhang, Tim Stangner, Krister Wiklund, Alvaro Rodriguez, and Magnus Andersson. UmUTracker: a versatile MATLAB program for automated particle tracking of 2D light microscopy or 3D digital holography data. *Computer Physics Communications*, 219(??):390–399, October 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517301820`.

Zhang:2017:NIL

[ZSW+17b] Jilin Zhang, Chaoqun Sha, Yusen Wu, Jian Wan, Li Zhou, Yongjian Ren, Huayou Si, Yuyu Yin, and Ya Jing. The novel implicit LU–SGS parallel iterative method based on the diffusion equation of a nuclear reactor on a GPU cluster. *Computer Physics Communications*, 211(??):16–22, February 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465516301965`.

Zhong:2013:MCD

[ZTG13] Zhaopeng Zhong, Alberto Talamo, and Yousry Gohar. Monte Carlo and deterministic computational methods for the calculation of the effective delayed neutron fraction. *Computer Physics Communications*, 184(7):1660–1665, July 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513000660`. See corrigendum [ZTG14].

Zhong:2014:CSC

[ZTG14] Zhaopeng Zhong, Alberto Talamo, and Yousry Gohar. Corrigendum to "Monte Carlo and deterministic computational methods for the calculation of the effective delayed neutron fraction" [Comput. Phys. Commun. **184** (2013) 1660–1665]. *Computer Physics Communications*, 185(3):1193, March 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465513004001`. See [ZTG13].

Zlokazov:2013:VPA

[ZUT13] V. B. Zlokazov, V. K. Utyonkov, and Yu. S. Tsyganov. VSHEC — a program for the automatic spectrum calibration. *Computer Physics Communications*, 184(2):428–431, February 2013. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465512003104`.

Zhao:2015:NMN

[ZW15] Deng Zhao and R. E. Waltz. Numerical methods for nonlinear simulations of cyclokinetics illustrating the breakdown of gyrokinetics at high turbulence levels. *Computer Physics Communications*, 195(??):23–34, October 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001447.

Zhu:2019:GAI

[ZWC+19] Lianhua Zhu, Peng Wang, Songze Chen, Zhaoli Guo, and Yonghao Zhang. GPU acceleration of an iterative scheme for gas-kinetic model equations with memory reduction techniques. *Computer Physics Communications*, 245(??):Article 106861, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302486.

Zhang:2017:WIC

[ZWLZ17] Lei Zhang, Jizeng Wang, Xiaojing Liu, and Youhe Zhou. A wavelet integral collocation method for nonlinear boundary value problems in physics. *Computer Physics Communications*, 215(??):91–102, June 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517300693.

Zhao:2010:VIM

[ZX10] Yongxiang Zhao and Aiguo Xiao. Variational iteration method for singular perturbation initial value problems. *Computer Physics Communications*, 181(5):947–956, May 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465510000202.

Zhang:2016:NVC

[ZXL16] Kebo Zhang, Hailing Xiong, and Chao Li. A new version of code Java for 3D simulation of the CCA model. *Computer Physics Communications*, 204(??):214–215, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300741.

Zhang:2019:DBM

[ZXZ+19] Yudong Zhang, Aiguo Xu, Guangcai Zhang, Zhihua Chen, and Pei Wang. Discrete Boltzmann method for non-equilibrium flows: Based on Shakhov model. *Computer Physics Communications*, 238(??):50–65, May 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518304405`.

Zhang:2019:ESO

[ZY19a] Jun Zhang and Xiaofeng Yang. Efficient second order unconditionally stable time marching numerical scheme for a modified phase-field crystal model with a strong nonlinear vacancy potential. *Computer Physics Communications*, 245(??):Article 106860, December 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302371`.

Zhang:2019:NAN

[ZY19b] Jun Zhang and Xiaofeng Yang. Numerical approximations for a new L_2 -gradient flow based phase field crystal model with precise nonlocal mass conservation. *Computer Physics Communications*, 243(??):51–67, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301559`.

Yu:2018:EUS

[zYCG+18] Victor Wen zhe Yu, Fabiano Corsetti, Alberto García, William P. Huhn, Mathias Jacquelin, Weile Jia, Björn Lange, Lin Lin, Jianfeng Lu, Wenhui Mi, Ali Seifitokaldani, Álvaro Vázquez-Mayagoitia, Chao Yang, Haizhao Yang, and Volker Blum. ELSI: a unified software interface for Kohn–Sham electronic structure solvers. *Computer Physics Communications*, 222(??):267–285, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465517302941`.

Zhou:2015:UIP

[ZYL+15] Dai-Mei Zhou, Yu-Liang Yan, Xing-Long Li, Xiao-Mei Li, Bao-Guo Dong, Xu Cai, and Ben-Hao Sa. An upgraded issue of the parton and hadron cascade model, PACIAE 2.2. *Computer Physics Communications*, 193(??):89–94, August 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000429.

Zheng:2019:GDO

[ZYL+19] Hongxia Zheng, Xinning Yu, Wanli Lu, Jack Ng, and Zhifang Lin. GCforce: Decomposition of optical force into gradient and scattering parts. *Computer Physics Communications*, 237(??):188–198, April 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465518303941.

Zhang:2015:DFD

[ZYZ15] Bin Zhang, Jianmin Yuan, and Zengxiu Zhao. DMTDHF: a full dimensional time-dependent Hartree–Fock program for diatomic molecules in strong laser fields. *Computer Physics Communications*, 194(??):84–96, September 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515001393.

Zhang:2015:SSL

[ZZ15] Bin Zhang and Zengxiu Zhao. SLIMP: Strong laser interaction model package for atoms and molecules. *Computer Physics Communications*, 192(??):330–341, July 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465515000934.

Zhang:2017:AAE

[ZZ17a] S. H. Zhang and R. F. Zhang. AELAS: Automatic ELAStic property derivations via high-throughput first-principles computation. *Computer Physics Communications*, 220(??):403–416, November 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517302400.

Zheng:2017:PUP

[ZZ17b] Fawei Zheng and Ping Zhang. Phonon Unfolding: a program for unfolding phonon dispersions of materials. *Computer Physics Communications*, 210(??):139–144, January 2017. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302752.

Zheng:2015:QUP

[ZZD15] Fawei Zheng, Ping Zhang, and Wenhui Duan. Quantum unfolding: a program for unfolding electronic energy bands of materials. *Computer Physics Communications*, 189(??):213–219, April 2015. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465514004172.

Zhang:2016:VCJ

[ZZD+16] Kebo Zhang, Junsen Zuo, Yifeng Dou, Chao Li, and Hailing Xiong. Version 3.0 of code Java for 3D simulation of the CCA model. *Computer Physics Communications*, 207(??):547–548, October 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551630176X.

Zhang:2016:STM

[ZZG+16] Peng Zhang, Na Zhang, Chao Gao, Li Zhang, Yuxiang Gao, Yuefan Deng, and Danny Bluestein. Scalability test of multiscale fluid–platelet model for three top supercomputers. *Computer Physics Communications*, 204(??):132–140, July 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516300777.

Zhang:2016:MCT

[ZZH+16] R. F. Zhang, S. H. Zhang, Z. J. He, J. Jing, and S. H. Sheng. Miedema Calculator: a thermodynamic platform for predicting formation enthalpies of alloys within framework of Miedema's theory. *Computer Physics Communications*, 209(??):58–69, December 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465516302430.

Zhang:2018:MSN

[ZZHG18] Chenglong Zhang, Mingcan Zhao, Chaofeng Hou, and Wei Ge. A multilevel-skin neighbor list algorithm for molecular dynamics simulation. *Computer Physics Communications*, 222(??):59–69, January 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465517303041.

Zhang:2019:PFC

[ZZSW19] Z. Zhang, D.-B. Zhang, T. Sun, and R. M. Wentzcovitch. phq: a Fortran code to compute phonon quasiparticle properties and dispersions. *Computer Physics Communications*, 243(??):110–120, October 2019. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519301523.