Part I. Compressible flow (cont'd)

2. Nonlinear scalar problems

Consider the nonlinear PDE for the scalar function *u:*

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \tag{1}$$

where $f(u)$, $u \in \Re$ and $f(u)$ is a convex function (e.g., the inviscid Berger's equation, for which $f(u) = \frac{1}{2}u^2$). Assume that equation (-1) satisfies the initial condition

$$u(x, 0) = \phi(x) \tag{2}$$

Let the wavespeed *a* be defined by $a(u) = \frac{\partial f}{\partial u}$ with $\frac{\partial a}{\partial u} > 0$. Assuming that $u(x,t)$ is differentiable, equation (-2) can be written in quasilinearized form:

$$\frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0 \tag{3}$$

If the wavespeed is $\frac{\partial x}{\partial t} = a(u(x,t),t)$ with initial locations prescribed at $x(0) = x_o$, then the solution is $u(x(t),t) = u(x-at,0) = \phi(x_o - at)$.

We now need to introduce the concept of characteristics. These beasts can be thought of as either a trajectory in space or as a curve in space/time along which information propagates.

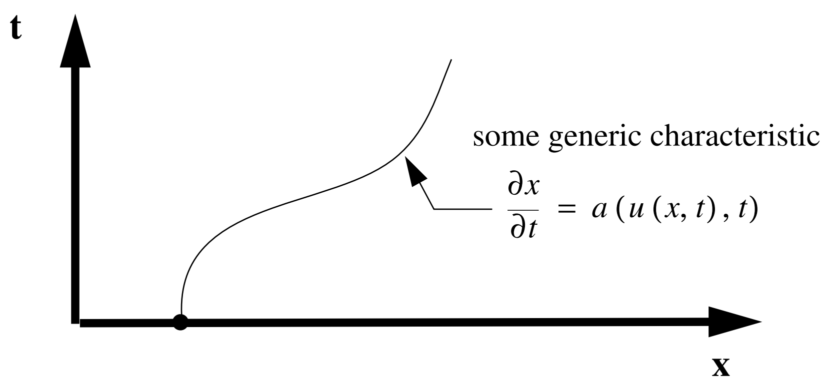

FIGURE 1. Characteristic curve in space/time.

Let's examine what happens to *u* along characteristics.Using the chain rule, the material derivative of $u(x(t),t)$ is:

$$\frac{d}{dt}(u(x(t),t)) = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{\partial x}{\partial t}$$

$$\frac{d}{dt}(u(x(t),t)) = \frac{\partial u}{\partial t} + a(u(x,t),t)\frac{\partial u}{\partial x} \quad (4)$$

However, the differential equation (-2) tells us that the r.h.s. of equation (-1) vanishes. Therefore, the substantial derivative of *u* nets out to be a big fat goose egg (i.e., zero). This indicates that *u* is constant along characteristics.

What can we say about the wavespeed *a* along characteristics?

$$\frac{dx}{dt} = a(u(x,t),t) = a(u(x_o,0))$$

$$\frac{dx}{dt} = \phi(x_o) \quad (5)$$

For this problem, the characteristics in space/time are therefore straight lines with slope $\phi(x_o)$, and the information which propagates along the characteristics is $u(x_o,0)$. The difference between the linear and nonlinear cases is that the slopes of the characteristics are not necessarily constant for the latter case, e.g., consider figure (+1).

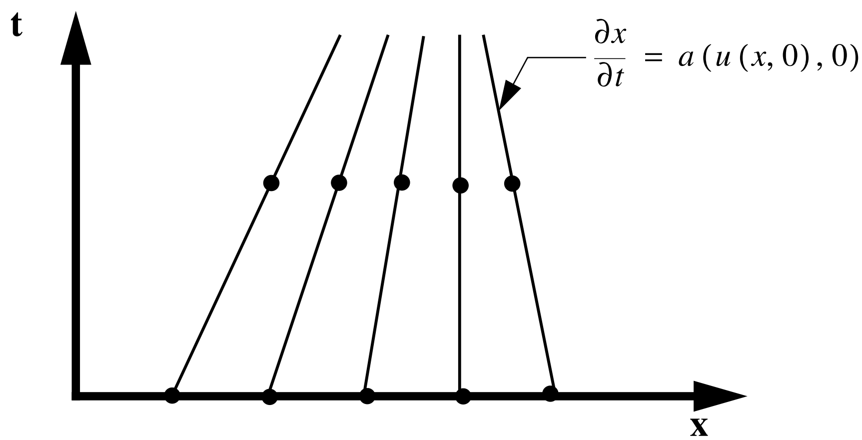

FIGURE 2. Characteristic curves for the nonlinear scalar problem

The astute observer might note that there is potential danger up ahead for the characteristics above in figure -1. If the lines are extended further in time, it is graphically apparent that they will cross. So, if at time $t = 0$, there are some *u*'s (a/k/a $\phi(x_o)$) which are positive and some which are negative, then they will cross at some finite time. In more rigorous terminology, assuming that $\phi(x_o)$ is smooth and of compact support (i.e., constant outside of some finite interval), then there will be some time $t_{KA\text{-}BOOM}$ at which the solution blows up because the solution is multiply valued. For example

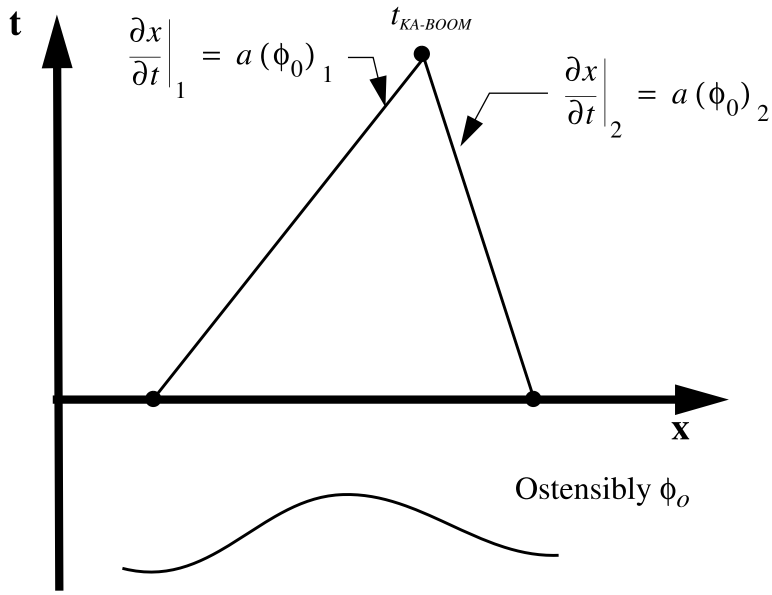

FIGURE 3. Trouble afoot.

At $t_{KA\text{-}BOOM}$, is the value of $a(\phi)$ equivalent to the value carried with the left-running characteristic? Or the right-running characteristic? Or both?

To examine this more closely, consider the behavior of u in space. We know that the exact solution at any time t is given by:

$$u(x, t) = \phi(x - a(u(x, t))t) \tag{6}$$

The partial derivative of $u(x(t),t)$ with respect to x is:

$$\frac{\partial u}{\partial x} = \phi' - t\frac{\partial a(u(x, t))}{\partial x}\phi'$$

where the prime indicates differentiation with respect to x. Next use the chain rule to obtain

$$\frac{\partial u}{\partial x} = \phi' - t\frac{da}{du}\frac{\partial u}{\partial x}\phi'$$

or

$$\frac{\partial u}{\partial x} = \frac{\phi'}{1 + t\frac{da}{du}\phi'} \tag{7}$$

If $\phi' < 0$ anywhere, then the solution blows up because the denominator of equation (-1) goes to zero at time $t_{KA\text{-}BOOM}$ where

$$t_{KB} = -\frac{1}{\frac{da}{du}\phi'} \tag{8}$$

This mathematical analysis would thus indicate that the solution blows up at finite time. However, from a physical standpoint, we know that real solutions do not simply blow up. Although the profile of u may steepen in time, gradients are finite and u is bounded when the terms which were heretofore neglected, e.g., viscous terms, are included. This is precisely why weak solutions were invented.

2.1 Weak solutions to nonlinear data

A weak solution to the nonlinear scalar equation described above satisfies

$$\int_{x_L}^{x_R} u(x, t^N)\, dx = \int_{x_L}^{x_R} u(x, t^0)\, dx + \int_{t^0}^{t^N} f(u(x_L, t))\, dt - \int_{t^0}^{t^N} f(u(x_R, t))\, dt \tag{9}$$

between initial time t^0 and a later time t^N and between the left and right boundaries of the physical domain, x_L and x_R respectively. Consider the particular case of a discontinuous solution, specifically, an isolated discontinuity propagating at speed s.

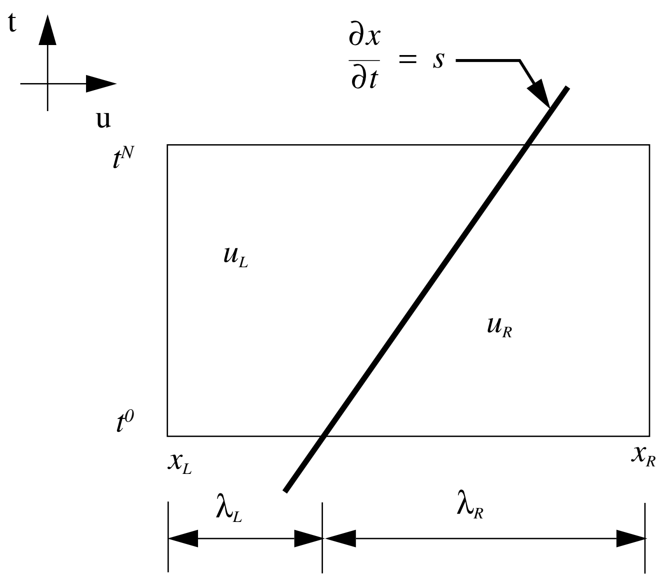

FIGURE 4. Cartoon of a discontinuity propagating in space/time

From the graphical depiction above in figure (-1), we can evaluate the integrals:

$$\int_{x_L}^{x_R} (u(x, t^N) - u(x, t^0))\, dx = u_L(\lambda_L - s(t^N - t^0)) + u_R(\lambda_R - s(t^N - t^0)) - (u_L\lambda_L + u_L\lambda_L)$$

or

$$\int_{x_L}^{x_R} (u(x, t^N) - u(x, t^0))\, dx = (u_L - u_R)\, s(t^N - t^0) \tag{10}$$

Similarly

$$\int_{t^0}^{t^N} (f(u(x_L, t)) - f(u(x_R, t)))\, dt = (f(u_L) - f(u_R))\,(t^N - t^0) \tag{11}$$

Using equations (-1, -2) above, we can solve for the propagation speed which the discontinuity is traveling at:

$$s = \frac{f(u_L) - f(u_R)}{u_L - u_R} \tag{12}$$

This is the infamous Rankine-Hugoniot relation. If f is a smooth function, then by the mean value theorem

$$\frac{f(u_L) - f(u_R)}{u_L - u_R} = \left.\frac{\partial f}{\partial u}\right|_{\xi} \tag{13}$$

where ξ is some intermediate value between u_L and u_R. Thus we see that as $u_L \to u_R$, then

$$s \to \left.\frac{df}{du}\right|_{\frac{u_L + u_R}{2}} = a\left(\frac{u_L + u_R}{2}\right) \tag{14}$$

This indicates that weak waves are propagated along characteristics.

2.1.1 Nonuniqueness of weak solutions

One problem with weak solutions is that they are not unique, i.e., for the same initial data, we can obtain more than one weak solution. For example, consider Berger's equation for which $f(u) = \frac{1}{2}u^2$ with the following initial data:

$$u(x, 0) = \begin{cases} -1 \ldots (x < 0) \\ 1 \ldots (x > 0) \end{cases}$$

The trivial solution is $s = 0$, shown in figure +1(a). Another weak solution is presented in figure (+1(b)) for which characteristics fan out from a point

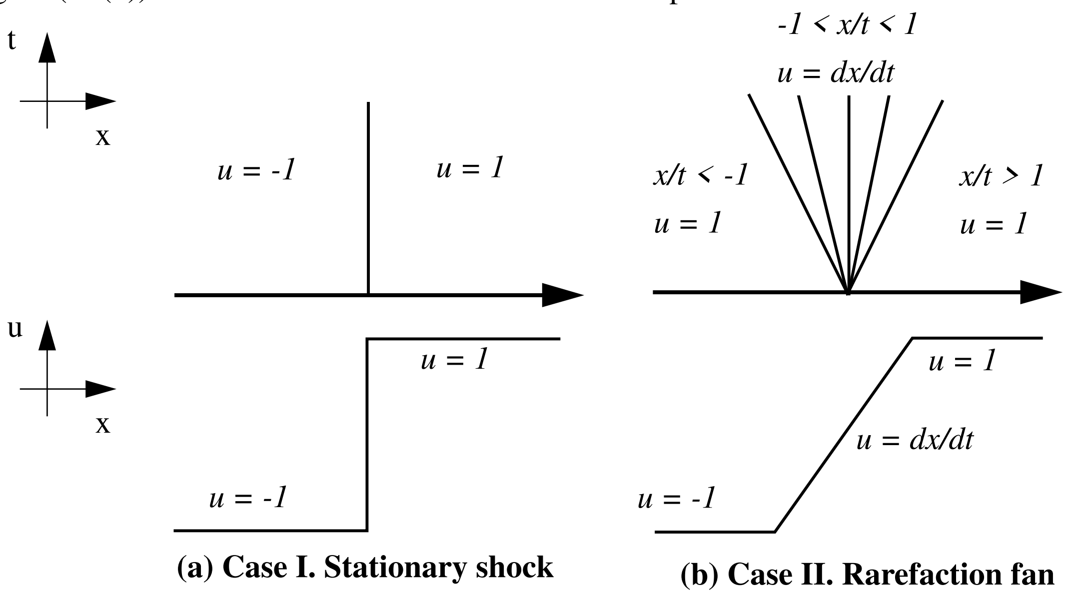

FIGURE 5. Two weak solutions which satisfy Berger's equation: (a) Stationary shock; (b) Rarefaction fan

For the expansion fan in figure -1(b), the solution $u(x,t)$ is a weak solution since it is smooth enough to integrate. It is continuous for $t > 0$, and, using integration by parts, we can show that the discontinuity in derivative at the boundary of the fan is not a problem.

2.1.2 The entropy condition

We are then left with the dilemma of deciding how to choose the physically realizable solution. The answer to this conundrum is to require the weak solution to be the limit of the viscous solution, which is a statement of the entropy condition. So, given the viscous solution, u^{ε}, which satisfies:

$$\frac{\partial u^{\varepsilon}}{\partial t} + \frac{\partial f(u^{\varepsilon})}{\partial x} = \varepsilon \frac{\partial^2 u^{\varepsilon}}{\partial x^2} \tag{15}$$

with ε being the viscosity, we require u to also satisfy the following condition:

$$\lim_{\varepsilon \to 0} u^{\varepsilon}(x, t) = u(x, t) \tag{16}$$

We claim that a weak solution which satisfies the entropy condition leads to a well-posed problem, i.e., the solution exists, is unique, and has continuous dependence on initial data.

Let's examine what this implies for a discontinuity. We can locally define the speed of propagation of a discontinuity, s, by

$$s = \frac{f(u_L) - f(u_R)}{u_L - u_R} \tag{17}$$

where L and R denote left and right sides of the wave. If $\frac{\partial^2 f}{\partial u^2} > 0$, the entropy condition is satisfied if:

$$a(u_L) > s > a(u_R) \tag{18}$$

(For Berger's equation, recall that $a(u) = u$.) Geometrically, this means that the information must propagate forward in time:

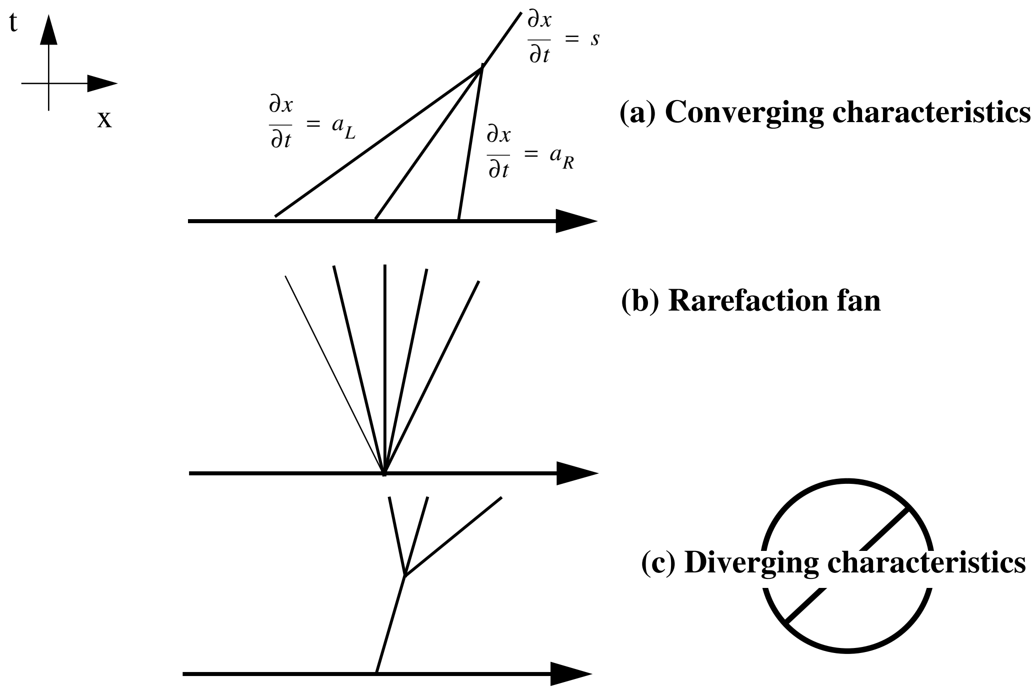

FIGURE 6. Weak solutions to Berger's equation which satisfy the entropy condition: (a) Converging characteristics; and (b) Rarefaction fan; and a weak solution which violates the entropy condition: (c) Diverging characteristics

This means that this entropy condition is really good stuff; it gets us from an infinitude of solutions to a single one, depending on initial conditions.

2.2 Strategies to enforce the entropy condition

To summarize our story to this point, in order to develop an adequate numerical scheme to solve the nonlinear scalar equation, we need:

- a weak solution (the discretized analog to the governing equations in conservation form);
- reasonable accuracy in the smooth regions, using the design criteria for linear advection;
- more stringent requirements on the stability of the scheme for the case of nonlinear discontinuities (e.g., LW4 is stable for purely linear problems, but it spreads out the Fourier components of the wave since they travel at different speeds. This may cause nasty things like mode-mode coupling in nonlinear problems);
- satisfaction of the entropy condition.

Let's examine what happens when the entropy condition is not satisfied. Consider the simple case of upwind differencing. The discretized form of the governing equation in conservation form is:

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x}\left(F^n_{j-\frac{1}{2}} - F^n_{j+\frac{1}{2}}\right) \tag{19}$$

where

$$F_{j+\frac{1}{2}} = \begin{cases} f(u_j)\ \ldots if \ldots a\left(\frac{u_j + u_{j+1}}{2}\right) > 0 \\ f(u_{j+1})\ \ldots if \ldots a\left(\frac{u_j + u_{j+1}}{2}\right) \le 0 \end{cases} \tag{20}$$

Desirable properties of this scheme include the facts that it is stable and total-variation-diminishing; however, it does not satisfy the entropy condition. Suppose we have the initial data at $t = 0$:

$$u_j^0 = \begin{cases} -1 \ldots j < 0 \\ 1 \ldots j \ge 0 \end{cases}$$

Since this particular discontinuity violates the entropy condition, we would like the numerical simulation to dissipate the discontinuity with time. For Berger's equation, $f(u_j) = u_j^2/2$ and $a(u_j) = \partial f/\partial u = u_j$. A simple calculation shows that all the fluxes cancel each other, and the solution reproduces itself at each time step. As Δx and Δt go to zero, we would converge to an entropy-violating shock using upwind differencing.

2.2.1 Addition of artificial viscosity

There are a number of ways to cope with this nuisance. One solution is to add in a small amount of artificial viscosity, ε. The error in smooth regions is of order ε, while it is of order $\sqrt{\varepsilon}$ at discontinuities. The advice of von Neumann and Richtmeyer, and Lax and Wendroff is to let $\varepsilon = O(\Delta x)$. This works. Although we could choose to keep ε fixed, this would wipe out all of the careful improvements we have made in designing a higher-order numerical scheme. So, to preserve the accuracy, we would like $\varepsilon = O(\Delta x)$ at the discontinuities, and $\varepsilon = O(\Delta x^p)$ in smooth regions, where p is the order of the scheme. The truncation error for upwinding is:

$$\frac{\partial u_{MOD}}{\partial t} + \frac{\partial f(u_{MOD})}{\partial x} = a(u_{MOD}) \left(\frac{1-\sigma}{2}\right) \Delta x \frac{\partial^2 u_{MOD}}{\partial x^2} \tag{21}$$

What happens as $a \to 0$?

2.2.2 Godunov's method (first order)

Another strategy is to utilize Godunov's method, a "real" geometric upwinding scheme. The solution process is broken down into three steps:

(1) Interpolate $u_I(x)$ from u_j^n. Choose a piecewise linear interpolation function so that $u_I(x) = u_j^n$ for $(j-\frac{1}{2})\Delta x < x < (j+\frac{1}{2})\Delta x$. (See figure 2 of section 1);

(2) Solve the above exactly, i.e., solve the Riemann problem at each discontinuity, with the left and right states given by u_j and u_{j+1} respectively. This is always solvable because $\partial^2 f/\partial u^2 > 0$ and $da/du > 0$. We will obtain compression waves or expansion fans as shown by figure -1(a) and (b) of section 2.1.2;

(3) Average the results back on to the grid.

Step (2) above meets the entropy condition, while step (3) adds artificial viscosity. We will later prove that if we start out with something which satisfies the entropy condition and average it, the result will still satisfy the entropy condition.

Each piece of the solution satisfies the entropy condition by itself and is a weak solution to the governing equation:

Let's define our terminology. We want to solve the nonlinear scalar problem:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \tag{22}$$

The finite-difference scheme for first-order Godunov is laid out by:

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x}\left(F_{j-\frac{1}{2}} - F_{j+\frac{1}{2}}\right) \tag{23}$$

where the flux is defined by

$$F_{j+\frac{1}{2}} = f\left(\hat{u}_{j+\frac{1}{2}}\right) \tag{24}$$

and $\hat{u}_{j+\frac{1}{2}}$ is the solution to the Riemann problem, i.e.,

$$\hat{u}_{j+\frac{1}{2}} = \left\{ \begin{array}{l} u_j \ldots (x < 0) \\ u_{j+1} \ldots (x < 0) \end{array} \right. \tag{25}$$

evaluated along the ray *x/t = 0*. This satisfies the entropy condition because any rarefaction shock would get spread out by the Riemann solver.

Let's compare Godunov's method to classical upwinding. The flux for the latter is:

$$F^{upwind}_{j+\frac{1}{2}} = \begin{cases} f(u_j) \ldots if \ldots \left(\dfrac{a(u_j) + a(u_{j+1})}{2} > 0\right) \\ f(u_{j+1}) \ldots if \ldots \left(\dfrac{a(u_j) + a(u_{j+1})}{2} < 0\right) \end{cases} \tag{26}$$

For cases in which the entropy condition is not violated, the result reduces to the same answer as upwinding would give. If $a(u_j) > 0 > a(u_{j+1})$, the Riemann problem would choose

$$F^{Godunov}_{j+\frac{1}{2}} = \left\{ \begin{array}{l} f(u_j) \ldots if \ldots (s > 0) \\ f(u_{j+1}) \ldots if \ldots (s < 0) \end{array} \right. \tag{27}$$

By the Rankine-Hugoniot relation for Berger's equation, $f(u_j) = u_j^2/2$, the speed is simply:

$$s = \frac{u_j + u_{j+1}}{2} \tag{28}$$

as for upwinding. On the other hand, if $a(u_j) < 0 < a(u_{j+1})$, solving the Riemann problem looks something like adding a viscous flux at the transonic point, so that we can write

$$F^{Godunov}_{j+\frac{1}{2}} = F^{upwind}_{j+\frac{1}{2}} + \alpha (u_{j+1} - u_j) \tag{29}$$

where $\alpha > 0$ and is of order $|u_j|$ and $|u_{j+1}|$. This adds a flux in the *-x* direction which tends to smooth out rarefaction shocks. Godunov's method modifies the direction of information transfer, depending on the sign of the wavespeed, just as upwinding does. However, Godunov's method also tends to smooth out physically unrealistic rarefaction shocks.

2.2.3 Godunov's method (second order)

The second-order Godunov's method is a two-sided predictor/corrector scheme. This allows information to travel from both sides of the cell. First we must develop the concept of the approximate Riemann problem.

For convex functions,[1] consider the case where the wavespeed in adjacent cells is increasing as $a(u_j) < 0 < a(u_{j+1})$. We would like to obtain $\hat{u}_{j+\frac{1}{2}}$, which we define as the exact solution to $a\left(\hat{u}_{j+\frac{1}{2}}\right) = 0$. We can approximate the solution by linear interpolation:

$$\hat{u}_{j+\frac{1}{2}} \approx u_j^n - \frac{a\left(u_j^n\right)}{a\left(u_{j+1}^n\right) - a\left(u_j^n\right)}\left(u_j^n - u_{j+1}^n\right) \tag{30}$$

For this case, there will be only one value of u for which $a(u) = 0$, as shown in figure +1, below.

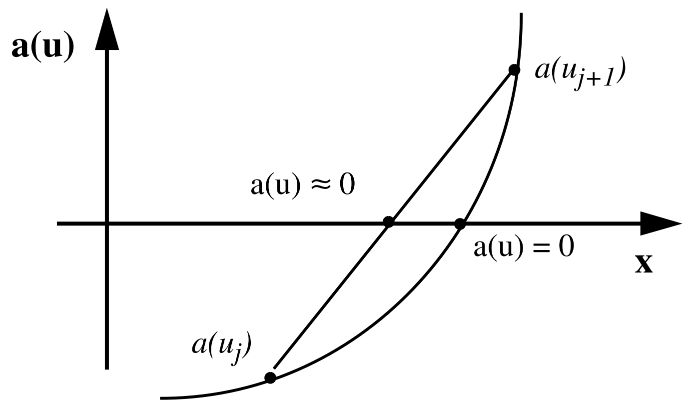

FIGURE 7. Geometric representation of approximate solution

Then the flux can be written

$$f\left(\hat{u}_{j+\frac{1}{2}}\right) = F^{upwind}_{j+\frac{1}{2}} + \alpha\left(u_j - u_{j+1}\right) \tag{31}$$

where $\alpha > 0$, and is of order u_j and u_{j+1}. To make this scheme second-order, we follow the same guidelines as for linear equations. Given u_j^n at time t^n, we must find the interpolation function; solve the initial-value problem for $u_I(x)$ exactly; and average the results back down to the grid.

1. In other words, $f'' > 0$. This condition is met for the case of gasdynamics, but almost everything else in the real world is not convex.Examples of nonconvex functions are solutions to flow through porous media, magnetohydrodynamics, shocks in solids and phase change.

2.2.3.1 Outline of second-order Godunov's method

Let's handle each of these steps sequentially. Assume that we know u_j^n at the cell centers, and that Δx and Δt are constants. We would like to evolve u such that

$$u_j^{n+1} = \pounds(u^n) \tag{32}$$

where £ is a nonlinear operator.

(1) **Find the interpolation function $u_I(x)$**. The constraint on $u_I(x)$ is that

$$u_j^n = \frac{1}{\Delta x} \int_{(j-\frac{1}{2})\Delta x}^{(j+\frac{1}{2})\Delta x} u_I(x)\, dx$$

To find $u_I(x)$, calculate

$$u_I(x) = u_j^n + \frac{(x - j\Delta x)}{\Delta x} \Delta^{VL} u_j \tag{33}$$

where Δ^{VL} is the van Leer slope. To construct the van Leer slopes, recall the definition from the discussion of geometric limiters for the linear scalar problem:

$$\Delta^{VL} u_j = \begin{cases} S_j \cdot min\,(2|u_{j+1} - u_j|, 2|u_j - u_{j-1}|, \frac{1}{2}|u_{j+1} - u_{j-1}|) \ldots if \ldots (\varphi > 0) \\ 0 \ldots otherwise \end{cases} \tag{34}$$

where

$$S_{j+\frac{1}{2}} = sign\,(u_{j+1} - u_{j-1}) \tag{35}$$

and

$$\varphi = (u_{j+1} - u_j) \cdot (u_j - u_{j-1}) \tag{36}$$

The usage of flux limiters makes the scheme second order and, furthermore, helps us to avoid the nuisance of Gibb's phenomenon at discontinuities.

(2) **Solve the initial-value problem for $u_I(x)$ exactly.** To accomplish this, calculate the left and right states for the Riemann problem, depending on the sign of the wavespeed:

$$u_{j+\frac{1}{2},L} = \begin{cases} u_j^n + \frac{1}{2}\,(1 - a\,(u_j^n)\,\frac{\Delta t}{\Delta x})\,\Delta^{VL} u_j \ldots if \ldots (a\,(u_j) > 0) \\ u_j^n + \frac{1}{2}\Delta^{VL} u_j \ldots if \ldots (a\,(u_j) < 0) \end{cases} \tag{37}$$

$$u_{j+\frac{1}{2},R} = \begin{cases} u^n_{j+1} - \frac{1}{2}\left(1 + a\left(u^n_{j+1}\right)\frac{\Delta t}{\Delta x}\right)\Delta^{VL} u_{j+1} \ldots if \ldots \left(a\left(u_j\right) < 0\right) \\ u^n_{j+1} - \frac{1}{2}\Delta^{VL} u_{j+1} \ldots if \ldots \left(a\left(u_j\right) > 0\right) \end{cases} \quad (38)$$

Where do these magical formulas come from? The construction of the left and right states comes from upstream-centered Taylor expansions from both sides. Consider a Taylor's expansion for $u_{j+1/2,L}$.

$$u_{j+\frac{1}{2},L} = u^n_j + \frac{\Delta x}{2}\frac{\partial u}{\partial x}\bigg|_{j\Delta x} + \frac{\Delta t}{2}\frac{\partial u}{\partial t}\bigg|_{j\Delta x} + \ldots$$

Transform the temporal derivative to a spatial one by using the PDE in nonconservation form:

$$u_{j+\frac{1}{2},L} = u^n_j + \left(\frac{\Delta x}{2} - a\left(u^n_j\right)\frac{\Delta t}{2}\right)\frac{\partial u}{\partial x}\bigg|_{j\Delta x}$$

where $a(u_j^n) > 0$ and finally

$$u_{j+\frac{1}{2},L} = u^n_j + \frac{1}{2}\left(1 - a\left(u^n_j\right)\frac{\Delta t}{\Delta x}\right)\Delta^{VL} u_j \quad (39)$$

Had we been traveling to the left, $a(u_j^n) < 0$, and

$$u_{j+\frac{1}{2},R} = u^n_{j+1} - \frac{1}{2}\left(1 + a\left(u^n_{j+1}\right)\frac{\Delta t}{\Delta x}\right)\Delta^{VL} u_{j+1} \quad (40)$$

After having calculated the left and right states, solve the Riemann problem, i.e., find the half-step value $u^{n+1/2}_{j+1/2}$ along $x/t = 0$.

(3) **Average the results back down to the grid.** To find the equivalent flux form, compute $u_{j+1/2}$ for $t^n < t < t^n + \Delta t$ and find

$$F_{j+\frac{1}{2}} = \frac{1}{\Delta t}\int_{t^n}^{(t^n+\Delta t)} f\left(u^{n+\frac{1}{2}}_{j+\frac{1}{2}}\right) dt \quad (41)$$

Finally, calculate the updated value of the solution by conservative differencing

$$u^{n+1}_j = u^n_j + \frac{\Delta t}{\Delta x}\left(F_{j-\frac{1}{2}} - F_{j+\frac{1}{2}}\right) \quad (42)$$

Et voilà! The scheme has *life* !!!

2.2.3.2 Analysis of second-order Godunov's method

Before putting our final stamp of approval on this scheme, however, let's examine more carefully what this method does in the following general categories of solution regimes:

- if all of the wave speeds are moving in one direction, will this scheme do the right thing? Will the wavespeeds $a(u_j^n)$'s have unambiguous sign?
- what happens at shocks?
- what happens at transonic expansions? Could this scheme generate an entropy-violating discontinuity?

Chugging through the procedure outlined in the section above will show that the upwind state is always chosen by this method. When the wavespeed is positive, information propagates from the left; conversely, when $a(u_j^n) < 0$.

At shocks, nothing terribly nasty happens. Imagine the situation shown below in figure +1. The wavespeed a changes sign across the shock. To deal with this, extrapolate to the cell edge from both sides using a Taylor expansion. This yields two different states at the cell edge. Next, treating these two extrapolated values as the left and right states of the Riemann problem, let the Riemann solver sort out the appropriate upwind value.

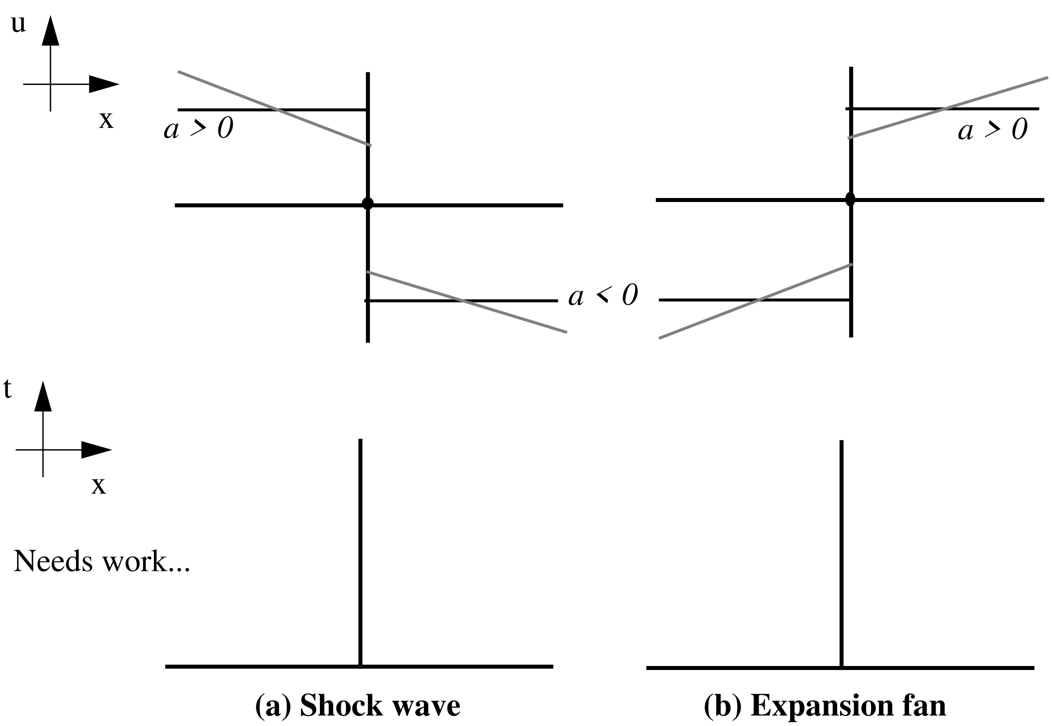

FIGURE 8. Geometrical interpretation of Godunov's method at discontinuities

Now let's examine the accuracy issue. Can we apply our concept of local truncation error to smooth regions of the solution?

Assume that the exact solution at cell center is given by $u^n_{E,j} = u_E(j\Delta x, n\Delta t)$ which satisfies the PDE

$$\frac{\partial u_E}{\partial t} + a(u_E)\frac{\partial u_E}{\partial x} = 0 \tag{43}$$

Further assume that u_E has enough derivatives (say, two or three) and $a(u_E) > 0$. So far, we will make no restrictions on the convexity of u_E. We claim that, for second-order Godunov:

$$u_E^{n+1} - £u_E^{n} = O(\Delta x^3) \tag{44}$$

Define the predictor step by

$$\tilde{u}_{E_{j+\frac{1}{2}}} = u^n_{E_j} + \frac{1}{2}\left(1 - a(u^n_{E_j})\frac{\Delta t}{\Delta x}\right)\Delta u^n_{E_j} \tag{45}$$

and define

$$u_{E_{j+\frac{1}{2}}}^{n+\frac{1}{2}} = u_E\left(\left(j+\frac{1}{2}\right)\Delta x,\ \left(n+\frac{1}{2}\right)\Delta t\right) \tag{46}$$

or, rewriting as a Taylor series expansion about $j\Delta x,\ n\Delta t$:

$$u_{E_{j+\frac{1}{2}}}^{n+\frac{1}{2}} = u^n_{E_j} + \frac{\Delta x}{2}\frac{\partial u_E}{\partial x}\bigg|_{j\Delta x,\ n\Delta t} + \frac{\Delta x^2}{8}\frac{\partial^2 u_E}{\partial x^2}\bigg|_{j\Delta x,\ n\Delta t} + \frac{\Delta t}{2}\frac{\partial u_E}{\partial t}\bigg|_{j\Delta x,\ n\Delta t} +$$
$$\frac{\Delta t^2}{8}\frac{\partial^2 u_E}{\partial t^2}\bigg|_{j\Delta x,\ n\Delta t} + \frac{\Delta x \Delta t}{4}\frac{\partial^2 u_E}{\partial x \partial t}\bigg|_{j\Delta x,\ n\Delta t} + O(\Delta x^3, \Delta t^3) \tag{47}$$

Since u_E is a smooth function and satisfies the PDE:

$$\frac{\partial u_E}{\partial t}\bigg|_{j\Delta x,\ n\Delta t} = -a(u_E)\frac{\partial u_E}{\partial x}\bigg|_{j\Delta x,\ n\Delta t} \tag{48}$$

Then, substituting equation (-1) into (-2) and regrouping:

$$u_{E_{j+\frac{1}{2}}}^{n+\frac{1}{2}} = u^n_{E_j} + \left(\frac{\Delta x}{2} - a(u^n_{E_j})\frac{\Delta t}{2}\right)\frac{\partial u_E}{\partial x}\bigg|_{j\Delta x,\ n\Delta t} + \left(\frac{\Delta x^2}{8} - a(u^n_{E_j})\frac{\Delta t^2}{8}\right)\frac{\partial^2 u_E}{\partial x^2}\bigg|_{j\Delta x,\ n\Delta t} +$$

$$\frac{\Delta x \Delta t}{4}\frac{\partial^2 u_E}{\partial x \partial t}\bigg|_{j\Delta x,\, n\Delta t} + O(\Delta x^3, \Delta t^3) \tag{49}$$

We know that as $\Delta x \to 0$ and $\Delta t \to 0$, the ratio of Δt to Δx goes to a constant value so that $O(\Delta t^3) \to O(\Delta x^3)$. Comparing the expressions for (-1) and twiddle (-5) above, and noting that

$$\Delta u^n_{E_j} - (\Delta x)\frac{\partial u_E}{\partial x}\bigg|_{j\Delta x,\, n\Delta t} \approx O(\Delta x^3) \tag{50}$$

if the derivative is approximated with central differencing, we conclude that

$$u_{E_{j+\frac{1}{2}}}^{n+\frac{1}{2}} - \tilde{u}_{E_{j+\frac{1}{2}}} = C\left[\left(\left(j+\frac{1}{2}\right)\Delta x\right)\Delta x^2 + O(\Delta x^3)\right] \tag{51}$$

where C indicates some smooth function. Notice that the term in brackets is of order Δx^3. Now we need to show that the local truncation error of the evolved solution is of order Δx^3. Using central differencing, we know that:

$$\frac{u^{n+1}_{E_j} - u^n_{E_j}}{\Delta t} = \frac{\partial u_E}{\partial t}\bigg|_{j\Delta x,\ (n+1/2)\Delta t} + O(\Delta t^2) \tag{52}$$

and

$$f(u^{n+1/2}_{E_{j+1/2}}) - f(u^{n+1/2}_{E_{j-1/2}}) = \frac{\partial f}{\partial x}\bigg|_{(j+1/2)\Delta x,\ (n+1/2)\Delta t} + O(\Delta x^2) \tag{53}$$

Then the evolved solution is

$$L(u^n_{E_j}) = u^n_{E_j} + \frac{\Delta t}{\Delta x}\left[f(\tilde{u}_{j-1/2}) - f(\tilde{u}_{j+1/2})\right]$$

$$L(u^n_{E_j}) = u^n_{E_j} + \frac{\Delta t}{\Delta x}\left[f(u^{n+1/2}_{E_{j-1/2}}) - f(u^{n+1/2}_{E_{j+1/2}})\right] + C_1\left[\left(\left(j+\frac{1}{2}\right)\Delta x\right)\Delta x^2\right] + C_2\left[\left(\left(j-\frac{1}{2}\right)\Delta x\right)\Delta x^2\right] + O(\Delta x^3) \tag{54}$$

This is all fairly muddled

2.2.4 Convexification of the Riemann problem

The next question to ask is what happens if f'' changes sign? (If $f'' > 0$, the condition for convexity is not met.) The answer is that weak solutions still exist, but entropy conditions become much harder to enforce. The Lax entropy condition ($a(u_L)$ s $a(u_R)$) is a necessary but not sufficient condition.

Let's examine the Riemann problem with some $f(u)$ which is monotonically increasing but has a change in curvature. In pictures:

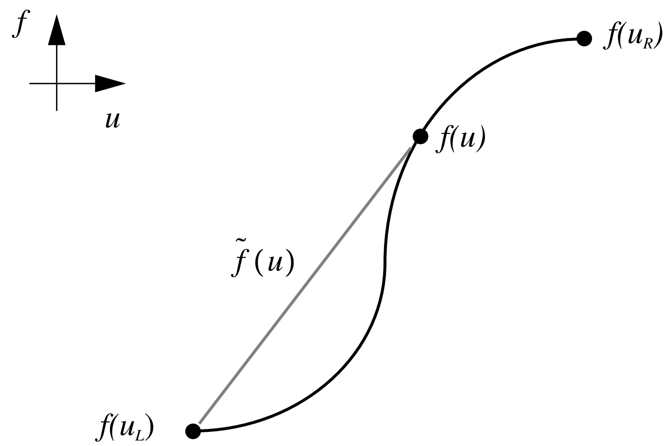

FIGURE 9. Pictorial representation of $f(u)$

The goal is to construct a new function, $\tilde{f}(u)$ between u_L and u_R which is the smallest convex function which is greater than or equal to f. Then solve the Riemann problem with the Lax entropy condition on the new convex function $\tilde{f}(u)$.

This function $\tilde{f}(u)$ turns out to be either equivalent to f or is linear. For example,

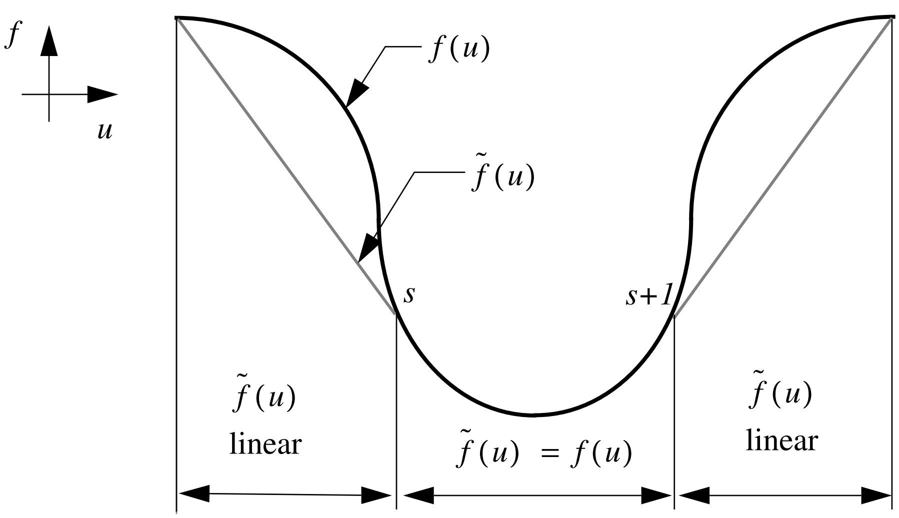

FIGURE 10. Convexification of the function $f(u)$

Next, place discontinuities at the intersections between the regions where $\tilde{f}(u)$ follows f and where it blazes new territory (locations s and $s+1$, above in figure (-1)). The wavespeed of the discontinuity is

$$\frac{d\tilde{f}}{du} = \frac{f(u_{s+1}) - f(u_s)}{u_{s+1} - u_s} \tag{55}$$

If $u_L > u_R$, this will look like a shock; if the opposite holds true, then $\tilde{f}(u) = f$ and behavior like an expansion fan will be seen. This may, however, seem like a lot of work (it is). Another alternative follows in the next section.

2.2.5 The Engquist-Osher flux

Consider the flux obtained for first-order Godunov:

$$u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x} [f(u_{RP_{j-1/2}}) - f(u_{RP_{j-1/2}})] \tag{56}$$

where u_{RP} is the solution for the Riemann problem with left and right states u_j^n and u_{j+1}^n. We would like to find a flux function that is:

- upwind when the sign of a is unambiguous;
- always more dissipative than Godunov;
- easier to deal with than Godunov.

One solution is to use the Engquist-Osher flux, f_{EO}, where

$$f_{EO} = f(u_L) + \int_{u_L}^{u_R} min\,(a(u), 0)\, du \tag{57}$$

Let's back up a second to remind ourselves that $a(u) = df/du$. The term f_G is the Godunov flux. This indicates that f_{EO} is simply the Godunov flux plus some diffusive function of $(u_L\text{-}u_R)$. Let's examine the specific cases which arise when $f(u)$ is convex $(f'' > 0)$:

- $a(u) > 0$: $f_{EO} = f_G = f(u_L)$
- $a(u) < 0$: $f_{EO} = f_G = f(u_R)$
- $a(u_L) < 0 < a(u_R)$: $f_{EO} = f_G = f(a^{-1}(0))$ where $a^{-1}(0)$ is the value corresponding to u=0?
- $a(u_L) > 0 > a(u_R)$: This transonic case is the interesting one. For this case, $f_G = f(u_L)$ or $f(u_R)$, depending on the sign of s. However f_{EO} is given by:

$$f_{EO} = f(u_L) + \int_{u_L}^{u_R} min\,(a(u), 0)\, du$$

$$f_{EO} = f(u_L) + \underbrace{\int_{u_L}^{a^{-1}(0)} min\,(a(u), 0)\, du}_{0} + \int_{a^{-1}(0)}^{u_R} min\,(a(u), 0)\, du$$

$$f_{EO} = f(u_L) + \int_{a^{-1}(0)}^{u_R} min(a(u), 0)\, du$$

$$f_{EO} = f(u_L) + f(u_R) - f(a^{-1}(0)) \qquad (58)$$

Note that for this case $f_{EO} \neq f_G$. For Berger's equation, $f(u) = u^2/2$ and

$$f_G = \begin{cases} \frac{u_L^2}{2} \ldots if \ldots (s > 0) \\ \frac{u_R^2}{2} \ldots if \ldots (s < 0) \end{cases} \qquad (59)$$

and

$$f_{EO} = \frac{u_L^2}{2} + \frac{u_R^2}{2} \qquad (60)$$

Since f_{EO} is larger than f_G, it is more diffusive and can push more "stuff" down gradients. This indicates that the Engquist-Osher flux will spread out discontinuities, but only for the case of transonic flow; however, the numerical diffusion will be somewhat muted by the characteristics will drive the discontinuities back in. This is advantageous over the previous convexification approach described in the last section, since there is much less logic involved. In addition, the logic that is involved is simply algebra; once we find *a(0)* for the first time, we can simply store it and we're set. For further details, see Bell, Colella and Trangenstein (1989) **J Comp Phys ___:___-___** "... Something ... for general systems of hyperbolic conservation laws".

Potpourri: The big drawback to this approach is its extension to higher order. According to Osher (ref??), the only known schemes which are known to produce entropy-satisfying shocks for a general *f* are first order. Bell and Shubin (ref??) have made the empirical observation that using van Leer flux limiting will lead to entropy-violating discontinuities. We know that for convex *f*, entropy violations are very unstable; for nonconvex *f*, entropy violations can actually steepen the shock. The answer will lie in changing the limiter. For example, we might try some kind of modified van Leer approach. If either $f'' > 0$ or $f'' < 0$ over large intervals of *u*, one might be able to knock the scheme down to first order only near the points where $f'' = 0$ and retain higher-order accuracy elsewhere.