Shock-capturing fluctuation-splitting wave-propagation for conservation laws

by E. Alec Johnson, July 2008

We recount the shock-capturing flux-difference-splitting wave propagation algorithm described in [Bale03].

1 Background

In one dimension, this algorithm seeks to solve the generic hyperbolic conservation law

$$q_t + f(q)_x = 0.$$

Integrated over a single cell and a single time step, this conservation law says that the change in the amount of stuff in a cell over one time step equals the net amount of stuff that flowed into the cell. So the state variables Q_i^n are updated using flux differencing:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}[F_{i+1/2} - F_{i-1/2}]; \tag{1.1}$$

here Q_i^n denotes the average amount of stuff in cell i at time step n, $F_{i-1/2}$ denotes the average rate of flow of stuff across the boundary between cells $i-1$ and i, Δt denotes the time step length, and Δx denotes the width of a mesh cell.

Conservative numerical methods are based on estimating fluxes at cell interfaces. Approximate Riemann solvers estimate these fluxes by linearizing the PDE at each cell interface.

In quasilinear form the PDE reads

$$q_t + f_q \cdot q_x = 0.$$

Muliplying by f_q shows that the flux satisfies the same PDE:

$$f_t + f_q \cdot f_x = 0.$$

We will estimate the average flux rate at a cell interface by approximating the state (or flux) with a linear function of position and advecting it with this equation. Let A be an approximation of f_q at a cell boundary centered at $x = 0$. Assume linear initial conditions:

$$q^0(x) = q_0 + (q_x)_0 \cdot x,$$
$$f^0(x) = f_0 + (f_x)_0 \cdot x,$$

where by the linear approximation we have that $(f_x)_0 = f_q \cdot (q_x)_0$. We solve by eigenvector decomposition. Assume

$$(q_x)_0 = \sum_p (q_x)_0^p,$$
$$A \cdot (q_x)_0 = s^p (q_x)_0^p.$$

Multiplying both sides by A,

$$(f_x)_0 = \sum_p (f_x)_0^p, \qquad A \cdot (f_x)_0 = s^p (f_x)_0^p,$$

where

$$(f_x)_0^p := A(q_x)_0^p = s^p (q_x)_0^p,$$
$$(f_x)_0 := A(q_x)_0 = \sum_p s^p (q_x)_0^p.$$

The general solution simply advects the initial conditions:

$$q(x,t) = q_0 + \sum_p (q_x)_0^p \cdot (x - ts^p),$$
$$f(x,t) = f_0 + \sum_p (f_x)_0^p \cdot (x - ts^p).$$

For this linear solution, flux changes at a constant rate, so the average value of the flux at position zero over a time step is simply the value at the half time-step:

$$f^{t=\Delta t/2} = f_0 - \frac{\Delta t}{2} \sum_p s^p (f_x)_0^p.$$

Call this the *advected linear flux value model.*

For Lax-Wendroff, the initial conditions $f^0(x)$ are a linear function connecting the flux values at the center of the adjacent cell; this implies that $f^0 := \frac{f(Q_L)+f(Q_R)}{2}$, where Q_L and Q_R are left and right states, $(f_x)_0 = \frac{f(Q_R)-f(Q_L)}{\Delta x}$. So

$$\begin{aligned} f^{t=\Delta t/2} &= f_0 - \frac{\Delta t}{2} \sum_p s^p (f_x)_0^p \\ &= f_0 - \frac{\Delta t}{2} A \cdot \sum_p (f_x)_0^p \\ &= f_0 - \frac{\Delta t}{2} A \cdot (f_x)_0 \\ &= \frac{1}{2}(f_R + f_L) - \frac{\Delta t}{2\Delta x} A \cdot (f_R - f_L) \end{aligned} \tag{1.2}$$

For the approximate Riemann solver we first split the flux jumps ("fluctuations") into left- and right-going fluctuations:

$$f_R - f_L = \sum_p Z^p$$

We denote the total left-propagating flux jump by

$$f|_L^0 := \sum_{s^p<0} Z^p \quad (=: A^- \Delta Q)$$

and the total right-propagating flux jump by

$$f|_0^R := \sum_{s^p>0} Z^p \quad (=: A^+ \Delta Q)$$

The Riemann flux is the intermediate state:

$$\begin{aligned} F^R &:= f_L + f|_L^0 = f_R - f|_0^R \\ &= \frac{1}{2}(f_{i-1} + f_i) - \frac{1}{2}\Big(\sum_p \mathrm{sgn}(s^p) Z^p\Big) \end{aligned}$$

The Godunov solver takes this Riemann flux as the flux over a time step; i.e., for the advected linear flux value model, the Godunov solver assumes that the flux values are constant.

$$f_0 = F^R, \qquad (f_x)_0 = 0;$$

High-order corrections modify these constant fluxes by applying "limiters" to the Lax-Wendroff slopes. For right-propagating limited flux jumps $\tilde{Z}^p$ we add to the constant flux value a linear perturbation which is zero at the center of the left cell and has slope $\tilde{Z}^p/\Delta x$. For left-propagating limited flux jumps $\tilde{Z}^p$ we add to the constant flux value a linear perturbation which is zero at the center of the right cell and has slope $\tilde{Z}^p/\Delta x$. This yields initial condition parameters

$$f_0 = F^R + \frac{1}{2}\sum_p \operatorname{sgn}(s^p)\tilde{Z}^p, \qquad (f_x)_0^p = \frac{1}{\Delta x}\tilde{Z}^p.$$

Thus the interface flux is

$$\begin{aligned} f^{t=\Delta t/2} &= f_0 - \frac{\Delta t}{2}\sum_p s^p (f_x)_0^p \\ &= F^R + \frac{1}{2}\Big(\sum_p \operatorname{sgn}(s^p)\tilde{Z}^p - \frac{\Delta t}{\Delta x} s^p \tilde{Z}^p\Big) \\ &= F^R + \frac{1}{2}\sum_p \operatorname{sgn}(s^p)\Big(1 - \frac{\Delta t}{\Delta x}|s^p|\Big)\tilde{Z}^p \end{aligned}$$

2 Summary of algorithm

To summarize the algorithm and discuss limiters, we generalize notation and locate quantities about a cell interface $i-1/2$.

The fluxes are computed as

$$F_{i-1/2} = F^R_{i-1/2} + \tilde{F}_{i-1/2},$$

where $F^R_{i-1/2}$ is the Riemann flux and $\tilde{F}_{i-1/2}$ is a second-order limited correction flux.

$$\begin{aligned} F^R_{i-1/2} \quad &= \quad \frac{1}{2}\Big(f(Q_{i-1}) + f(Q_i)\Big) \\ &\quad + \frac{1}{2}\Big(\sum_{s_p<0} Z^p_{i-1/2} - \sum_{s_p>0} Z^p_{i-1/2}\Big), \end{aligned} \qquad (2.1)$$

where the "flux waves" $Z^p_{i-1/2}$ are defined by a decomposition of the flux jump in terms of the eigenvalues s^p and corresponding eigenvectors of $\hat{A}_{i-1/2}$, an approximation to $f'(Q_{i-1/2})$:

$$f(Q_i) - f(Q_{i-1}) =: \sum_p Z^p_{i-1/2}\Big(=: \sum_p s^p_{i-1/2} W^p_{i-1/2}\Big).$$

Typically

$$\hat{A}_{i-1/2} = f'\Big(\frac{Q_{i-1}+Q_i}{2}\Big).$$

The correction flux is

$$\tilde{F}_{i-1/2} = \frac{1}{2}\sum_p \operatorname{sgn}(s^p_{i-1/2})\Big(1 - \frac{\Delta t}{\Delta x}|s^p_{i-1/2}|\Big)\tilde{Z}^p_{i-1/2}$$

where

$$\tilde{Z}^p_{i-1/2} = \text{vectorLimiter}(Z^p_{i-1/2}, Z^p_{I^p-1/2})$$

where I^p is the upwind index in the p-th eigenvalue:

$$I^p = i - \operatorname{sgn}(s^p)$$

The vectorLimiter function is typically computed by projecting the second argument onto the first and applying a scalar limiter function:

$$\text{vectorLimiter}(U,V) = \text{scalarLimiter}\Big(1, \frac{U\cdot V}{U\cdot U}\Big)U.$$

Some common high-resolution choices for scalarLimiter(a,b) follow. Each limiter immediately returns 0 if the signs of the arguments disagree. Else each limiter if necessary caps the magnitude of the value it initially computes by twice the magnitude of the smaller of its arguments in order to avoid overshoot. The value that each limiter initially computes is:

- minmod: the minimum-sized argument (which makes capping unnecessary).
- superbee: the larger of the two arguments.
- MC (monotonized central-difference limiter): the average of the two arguments
- van Leer: twice the product divided by the sum (which makes capping unnecessary).

So explicit formulas are:

$$\text{minmod}(a,b) = \begin{cases} a & \text{if } |a| \le |b| \text{ and } ab > 0 \\ b & \text{if } |b| \le |a| \text{ and } ab > 0 \\ 0 & \text{if } ab \le 0 \end{cases}$$

$$\text{maxmod}(a,b) = \begin{cases} b & \text{if } |a| \le |b| \text{ and } ab > 0 \\ a & \text{if } |b| \le |a| \text{ and } ab > 0 \\ 0 & \text{if } ab \le 0 \end{cases}$$

$$\text{superbee}(a,b) = \text{maxmod}\big(\text{minmod}(a,2b), \text{minmod}(2a,b)\big)$$

$$\text{MC}(a,b) = \text{minmod}\big(\frac{a+b}{2}, 2a, 2b\big)$$

$$\text{van Leer}(a,b) = \begin{cases} 0 & \text{if } ab \le 0 \\ \frac{2ab}{a+b} & \text{otherwise} \end{cases}$$

And in particular,

$$\text{minmod}(1,\theta) = \begin{cases} 1 & \text{if } 1 \le |\theta| \\ \theta & \text{if } 0 < \theta| \le 1 \\ 0 & \text{if } \theta \le 0 \end{cases},$$

$$\text{superbee}(1,\theta) = \max\big(0, \text{minmod}(1,2\theta), \text{minmod}(2,\theta)\big),$$

$$\text{MC}(1,\theta) = \max\left(0, \min\left(\frac{1+\theta}{2}, 2, 2\theta\right)\right), \text{ and}$$

$$\text{van Leer}(1,\theta) = \begin{cases} 0 & \text{if } \theta \le 0 \\ \frac{2\theta}{1+\theta} & \text{otherwise} \end{cases}$$

2.1 LeVeque notation

Formulas to translate this algorithm into the language of LeVeque:

$$A^{+}\Delta Q_{i-1/2} = \sum_{s^p>0} Z^p_{i-1/2}$$
$$A^{-}\Delta Q_{i-1/2} = \sum_{s^p<0} Z^p_{i-1/2}$$

So we can write the Riemann flux formula (2.1) as

$$F^R_{i-1/2} = \frac{1}{2}\Big(f(Q_{i-1}) + f(Q_i)\Big) + \frac{1}{2}\Big(A^{-}\Delta Q_{i-1/2} - A^{+}\Delta Q_{i-1/2}\Big),$$

which agrees with LeVeque Equ. (4.61). Observe that differences of the Riemann fluxes require only the left and right flux *jumps*, not the fluxes themselves:

$$F^R_{i+1/2} - F^R_{i-1/2} = A^{+}\Delta Q_{i-1/2} + A^{-}\Delta Q_{i+1/2}.$$

A Lax-Wendroff

The Lax-Wendroff method is a second-order method for the conservation law

$$q_t + f(q)_x = 0$$

derived by Taylor series expansion:

$$\begin{aligned} q^{t=\Delta t} &\approx q_{t=0} + \Delta t\, q_t + \frac{\Delta t^2}{2} q_{tt} && + O(\Delta t^3) \\ &= q_0 \quad - \Delta t\, f_x - \frac{\Delta t^2}{2} f_{tx} && + O(\Delta t^3) \\ &= q_0 \quad - \Delta t \left(f + \frac{\Delta t}{2}(f_q \cdot q_t)\right)_x && + O(\Delta t^3) \\ &= q_0 \quad - \Delta t \Big(\underbrace{f - \frac{\Delta t}{2}(f_q \cdot f_x)}_{\text{call } \mathcal{F}}\Big)_x && + O(\Delta t^3) \end{aligned}$$

In order to fit the flux-differencing framework (1.1), we seek a second-order accurate expression for $\mathcal{F}_x$ of the form $(\mathcal{F}_x)_i = \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x}$ in terms of flux function values at cell centers. So we need a second-order accurate estimate for the Riemann problem flux,

$$\begin{aligned} (f_x)_i &= \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} + O(\Delta x^2) \\ &= \frac{1}{\Delta x}\Big(\frac{f_{i+1} + f_i}{2} - \frac{f_{i-1} + f_i}{2}\Big) + O(\Delta x^2), \end{aligned}$$

and a first-order accurate estimate for the correction flux:

$$\begin{aligned} ((f_q \cdot f_x)_x)_i &= \frac{(f_q \cdot f_x)_{i+1/2} - (f_q \cdot f_x)_{i-1/2}}{\Delta x} + O(\Delta x^2) \\ &= \hat{A}_{i+1/2} \cdot \frac{f_{i+1} - f_i}{\Delta x^2} - \hat{A}_{i-1/2} \cdot \frac{f_i - f_{i-1}}{\Delta x^2} + O(\Delta x), \end{aligned}$$

where $\hat{A}_{i-1/2}$ and $\hat{A}_{i+1/2}$ are estimates of $(f_q)_{i-1/2}$ and $(f_q)_{i+1/2}$ which (1) are first-order accurate, i.e. $\hat{A}_{i+1/2} = (f_q)_i + O(\Delta x) = \hat{A}_{i-1/2}$, and (2) whose discrete derivative is first-order accurate, i.e. $\frac{\hat{A}_{i+1/2} - \hat{A}_{i-1/2}}{\Delta x} = ((f_q)_x)_i + O(\Delta x)$. For example, $\hat{A}_{i-1/2} := (f_q)_{i+n}$ for any constant n, or more commonly, $\hat{A}_{i-1/2} := (f_q)_{q=q_{i-1/2}+O(\Delta x)}$.

To verify this claim, the product rule and addition and subtraction of the same quantity are handy:

$$((f_q \cdot f_x)_x)_i = ((f_q)_x)_i \cdot (f_x)_i + (f_q)_i \cdot ((f)_{xx})_i$$

From the other end,

$$\begin{aligned} &\hat{A}_{i+1/2} \cdot \frac{f_{i+1} - f_i}{\Delta x^2} - \hat{A}_{i-1/2} \cdot \frac{f_i - f_{i-1}}{\Delta x^2} \\ =&\hat{A}_{i+1/2} \cdot \frac{f_{i+1} - f_i}{\Delta x^2} - \hat{A}_{i-1/2} \cdot \frac{f_{i+1} - f_i}{\Delta x^2} \\ &+ \hat{A}_{i-1/2} \cdot \frac{f_{i+1} - f_i}{\Delta x^2} - \hat{A}_{i-1/2} \cdot \frac{f_i - f_{i-1}}{\Delta x^2} \\ =&\frac{\hat{A}_{i+1/2} - \hat{A}_{i-1/2}}{\Delta x} \cdot \frac{f_{i+1} - f_i}{\Delta x} \\ &+ \hat{A}_{i-1/2} \cdot \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \\ =&((f_q)_x)_i \cdot (f_x)_i + (f_q)_i \cdot ((f)_{xx})_i + O(\Delta x) \end{aligned}$$

To sum up, the Lax-Wendroff flux here agrees with (1.2) and is given by

$$\begin{aligned} &\mathcal{F}_{i-1/2} + O(\Delta x^2) = F_{i-1/2} \\ :=&\frac{f_{i-1} + f_i}{2} + \frac{\Delta t}{2\Delta x}\hat{A}_{i-1/2}(f_i - f_{i-1}) \end{aligned}$$

where it is sufficient that $\hat{A}_{i-1/2}$ satisfies $\hat{A}_{i-1/2} = (f_q)_{i-1/2} + O(\Delta x^2)$.

We verify that in case no limiters are applied to the correction fluxes (i.e., $\tilde{Z}^p = Z^p$), high-order corrections reconstruct the Law-Wendroff flux:

$$\begin{aligned} f_0 &= F^R + \frac{1}{2}\sum_p \operatorname{sgn}(s^p)\tilde{Z}^p \\ &= f_L + \sum_{s^p<0} Z^p + \frac{1}{2}\sum_{s^p>0}\tilde{Z}^p - \frac{1}{2}\sum_{s^p<0}\tilde{Z}^p \\ &= f_L + \frac{1}{2}\sum_{s^p} Z^p. \end{aligned}$$

References

[Bale03] D.S. Bale, R.J. LeVeque, S. Mitran, and J.A. Rossmanith. *A wave propagation method for conservation laws and balance laws with spatially varying flux functions*, SIAM J. Sci. Comp., 24: 955-978, 2003.

[LeVeque02] R. LeVeque, *Finite Volume Methods for Hyperbolic Problems*, Cambridge University Press, 2002.