Hyperbolic Conservation Laws: Computation

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A conservation law is a first-order system of PDEs in divergence form

$$\partial_t U(x,t) + \partial_x G(U(x,t)) = 0, \qquad t \geq 0, x \in \mathbb{R}, \tag{1}$$

describing the evolution of conserved quantities $U \in \mathbb{R}^n$ according to flux function $G : \mathbb{R}^n \to \mathbb{R}^n$. (Herein, we only consider the 1D case for brevity.) Solutions of (1) admit various kinds of nonlinear and discontinuous waves. Numerical methods developed to accurately compute such waves have significantly influenced developments in modern computational science. Methods come in two forms: *shock-fitting methods* in which discontinuities are introduced explicitly in the solution and *shock-capturing methods* in which numerical dissipation is used to capture discontinuities within a few grid cells.

1. Classical Shock-Capturing Methods

Equation (1) is not valid in the classical pointwise sense for discontinuous solutions. Instead, we will work with the integral form of (1). Introducing the sliding average $\bar{U}(x,t) = \frac{1}{\Delta x}\int_{x-\Delta x/2}^{x+\Delta x/2} U(\xi,t)\,d\xi$ gives the system of evolution equations

$$\bar{U}(x,t+\Delta t) = \bar{U}(x,t) - \frac{1}{\Delta x}\int_t^{t+\Delta t} \big[G\big(U(x+\tfrac{\Delta x}{2},\tau)\big) - G\big(U(x-\tfrac{\Delta x}{2},\tau)\big)\big]\,d\tau. \tag{2}$$

Next, we partition the physical domain Ω into a set of grid cells $\Omega_i = [x_{i-1/2}, x_{i+1/2}]$ and set $t^n = n\Delta t$. This suggests a numerical scheme

$$U_i^{n+1} = U_i^n - r\big(G_{i+1/2}^n - G_{i-1/2}^n\big), \qquad r_i = \Delta t/\Delta x, \tag{3}$$

where $U_i^n = \bar{U}_i(x_i, t^n)$ are unknown *cell averages* and the numerical flux functions $G_{i\pm1/2}^n$ are approximations to the average flux over each cell interface,

$$G_{i\pm1/2}^n \approx \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} G\big(U(x_{i\pm1/2},\tau)\big)\,d\tau. \tag{4}$$

Because (1) has finite speed of propagation, the numerical fluxes are given in terms of neighboring cell averages; i.e., $G_{i+1/2}^n = G(U_{i-p}^n, \ldots, U_{i+q}^n) = G(U^n; i+1/2)$.

Schemes on the form (3) are called *conservative*. If a sequence of approximations computed by a consistent and conservative scheme converges to some limit, then this limit is a weak solution of the conservation law [4].

Centered Schemes. Assume that $U(x,t^n)$ is piecewise constant and equals U_i^n inside Ω_i. The integrand of (4) can then be approximated by $\frac{1}{2}(G(U_{i\pm1}^n)+G(U_i^n))$. This yields a centered scheme that unfortunately is notoriously unstable. To stabilize, we add artificial diffusion, $\frac{\Delta x^2}{\Delta t}\partial_x^2 U$ discretized using standard centered differences and obtain the classical first-order Lax–Friedrichs scheme [3]

$$U_i^{n+1} = \frac{1}{2}\Big(U_{i+1}^n + U_{i-1}^n\Big) - \frac{1}{2}r\Big[G(U_{i+1}^n) - G(U_{i-1}^n)\Big] \tag{5}$$

which is very robust and will always converge, although sometimes painstakingly slow. To see this, consider the trivial case of a stationary discontinuity satisfying $\partial_t U = 0$. In this case, (5) will simply compute U_i^{n+1} as the arithmetic average of the cell averages in the two neighboring cells. The Lax–Friedrichs scheme can be written in conservative form (3) using the numerical flux

$$G(U^n; i+1/2) = \frac{1}{2r}\big(U_i^n - U_{i+1}^n\big) + \frac{1}{2}\big[G(U_i^n) + G(U_{i+1}^n)\big]. \tag{6}$$

The second-order Lax–Wendroff scheme is obtained by using the midpoint rule to evaluate (4), with midpoint values predicted by (5) with grid spacing $\frac{1}{2}\Delta x$.

Upwind and Godunov Schemes. In the scalar case, we obtain a particularly simple two-point scheme by using one-sided differences in the *upwind* direction from which the characteristics are pointing; i.e., setting $G_{i+1/2}^n = G(U_i^n)$ if $G'(U) \geq 0$, or $G_{i+1/2}^n = G(U_{i+1}^n)$ if $G'(U) < 0$.

Upwind differencing is the design principle underlying *Godunov schemes* [2]. If $U(x,t^n) := U_i^n$ in each grid cell Ω_i, the evolution of U can be decomposed into a set of local *Riemann problems*

$$\partial_t V + \partial_x G(V) = 0, \qquad V(x,0) = \begin{cases} U_i^n, & x < x_{i+1/2}, \\ U_{i+1}^n, & x \geq x_{i+1/2}, \end{cases} \tag{7}$$

each which admits a self-similar solution $V(x/t)$. Cell averages can now be correctly evolved by (3) a time step Δt if we use $V(0)$, or a good approximation thereof, to evaluate G in (4). The time step Δt is restricted by the time it takes the fastest Riemann wave to cross a single cell,

$$\frac{\Delta t}{\Delta x}\ \max_j |\lambda_j| \leq 1, \tag{8}$$

where $\lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of the Jacobian matrix $DG(U)$. The inequality (8) is called the *CFL condition*, named after Courant, Friedrichs, and Lewy, who wrote one of the first papers on finite difference methods in 1928 [1]. If Δt satisfies (8), the numerical scheme (3) will be stable. An alternative interpretation of (8) is that the domain of dependence for the PDE should be contained within the domain of dependence for (3) so that all information that will influence U_i^{n+1} has time to travel into Ω_i.

Example 1. *Consider the advection of a scalar quantity in a periodic domain. Figure 1 shows the profile evolved for ten periods by the upwind, Lax–Friedrichs, and Lax–Wendroff schemes. The first-order schemes smear the smooth and the discontinuous part of the advected profile. The second-order scheme preserves the smooth profile quite well, but introduces spurious oscillations around the two discontinuities.*

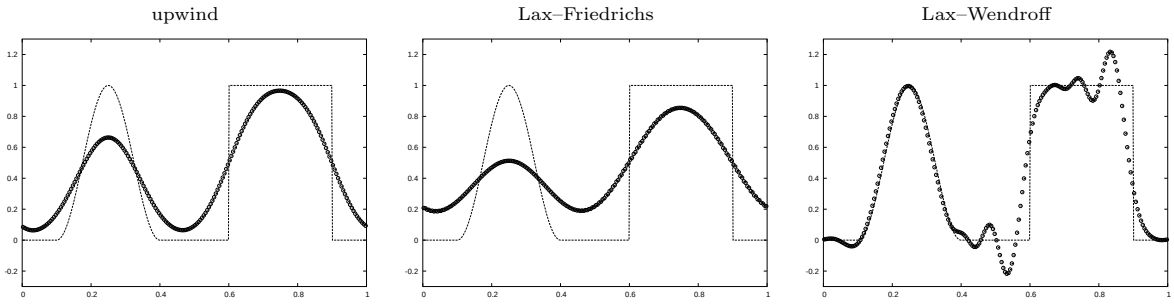

FIGURE 1. Approximate solutions after ten periods of linear advection within a periodic domain.

2. High-Resolution Schemes

High-resolution schemes are designed to have second order spatial accuracy or higher in smooth parts and high accuracy around shocks and other discontinuities (i.e., a small number of cells containing the wave). They use nonlinear dissipation mechanisms to provide solutions without spurious oscillations.

Flux-Limiter Schemes. Let $G_L(U^n; i+1/2)$ be a low-order flux (e.g., (6)) and $G_H(U^n; i+1/2)$ be a high-order flux (e.g., the Lax–Wendroff flux). Then, using the flux

$$G^n_{i+1/2} = G_L(U^n; i+1/2) + \theta^n_i \big[G_H(U^n; i+1/2) - G_L(U^n; i+1/2)\big] \tag{9}$$

in (3) gives a high-resolution scheme for an appropriate *limiter function* $\theta^n_i = \theta(U^n; i)$ that is close to unity if U is smooth and close to zero if U is discontinuous.

Slope-Limiter Schemes. Shock-capturing schemes can be constructed using the general REA algorithm:

(1) Starting from known cell averages U^n_i, **reconstruct** a piecewise polynomial function $\hat{U}(x, t^n)$ defined for all x. Constant reconstruction in each cell gives a first-order scheme, linear gives second order, quadratic gives third order, etc.
(2) Next, we **evolve** the differential equation, exactly or approximately, using $\hat{U}(x, t^n)$ as initial data.
(3) Finally, we **average** the evolved solution $\hat{U}(x, t^{n+1})$ onto the grid again to obtain new cell averages U^{n+1}_i.

In the reconstruction, care must be taken to avoid introducing spurious oscillations. Using a linear reconstruction [9],

$$\hat{U}(x, t^n) = U^n_i + \Phi(U^n_i - U^n_{i-1}, U^n_{i+1} - U^n_i)\frac{(x - x_i)}{\Delta x}, \qquad x \in \Omega_i,$$

one can ensure that the resulting scheme is *total-variation diminishing* (TVD) under certain assumptions on the nonlinear *slope limiter* Φ. Likewise, higher-order reconstructions can be designed to satisfy an *essentially non-oscillatory* (ENO) property.

For the averaging, there are two fundamentally different choices, see Figure 2. In upwind methods ($x = x_i$), the temporal integrals in (2) are evaluated at points $x_{i\pm1/2}$ where $\hat{U}(x, t)$ is discontinuous. Hence, one cannot apply standard integration and extrapolation techniques. Instead, one must resolve the wave structure arising due to the discontinuity,

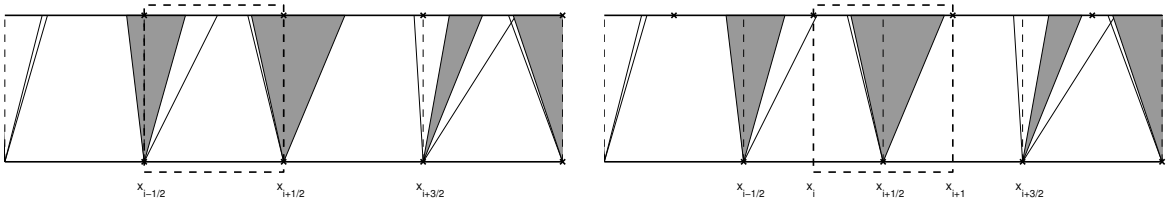

FIGURE 2. Computation of sliding average for upwind methods (left) and central methods (right).

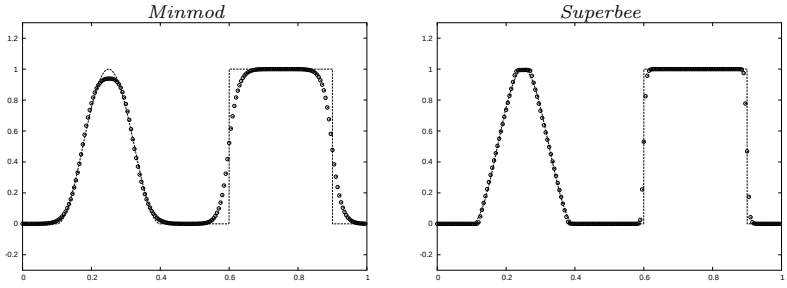

FIGURE 3. Linear advection problem computed by a second-order scheme with two different limiters.

solving a Riemann problem or generalizations thereof. For central methods ($x = x_{i+1/2}$), the sliding average is computed over a *staggered* grid cell $[x_i, x_{i+1}]$. Under a CFL condition of one half, the integrand will remain smooth so that standard integration and extrapolation techniques can be applied.

EXAMPLE 2. *Figure 3 shows the advection problem from Example 1 computed by a second-order non-oscillatory central scheme [6] with two different limiters. The dissipative minmod limiter always chooses the lesser slope and thus behaves more like a first-order scheme. The compressive superbee limiter picks steeper slopes and flattens the top of the smooth wave.*

Computational Efficiency. Explicit high-resolution schemes are essentially stencil computations that have an inherent parallelism that can be exploited to ensure computational efficiency. Moreover, high arithmetic intensity (i.e., large number of computations per data fetch) for high-order methods means that these methods can relatively easily exploit both message-passing systems and many-core hardware accelerators (GPUS and alike).

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