CS205b/CME306

Lecture 11

1 Discrete Conservation Form

Supplementary Reading: Osher and Fedkiw, §14.2, §14.3.2-4, §14.4-5; Leveque §4.1, §12.9-10

To ensure that shocks and other steep gradients are captured by our scheme (i.e. they move at the right speed even if they are unresolved) we must write the equation in a discrete conservation form. That is, a form in which the rate of change of conserved quantities is equal to a difference of fluxes. This form guarantees that we discretely conserve the total amount of the states of ϕ (e.g. mass, momentum and energy) that are present, analogously with the integral form given by

$$\frac{d}{dt}\int_{\Omega}\phi\,dV + \int_{\partial\Omega}\mathbf{f}(\phi)\cdot dA = \int_{\Omega}s(\phi)\,dV.$$

More importantly, this can be shown to imply that steep gradients or jumps in the discrete profiles propagate at the physically correct speeds.

Usually, conservation form is derived for control volume methods, that is, methods that evolve cell average values in time rather than nodal values. In this approach, a grid node x_i is assumed to be the center of a grid cell $(x_{i-1/2}, x_{i+1/2})$, which is taken as the control volume. We integrate the conservation law across this control volume to obtain

$$\int_{x_{i-1/2}}^{x_{i+1/2}}\phi_t + f(\phi)_x\,dx = \frac{d}{dt}\int_{x_{i-1/2}}^{x_{i+1/2}}\phi\,dx + f(\phi_{i+1/2}) - f(\phi_{i-1/2}) = 0.$$

If we let $\hat{\phi}_i$ denote the total quantity of ϕ in the i^{th} grid cell, i.e.

$$\hat{\phi}_i = \int_{x_{i-1/2}}^{x_{i+1/2}}\phi\,dx$$

then we can write this as

$$(\hat{\phi}_i)_t + f(\phi_{i+1/2}) - f(\phi_{i-1/2}) = 0. \tag{1}$$

We will refer to values computed at the x_i as grid point or cell center values, and values computed at the $x_{i\pm1/2}$ as half grid point, cell wall, or flux values. We also define the cell average value of ϕ in the grid cell i as

$$\overline{\phi}_i = \frac{1}{\Delta x}\hat{\phi}_i = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}}\phi\,dx.$$

Equation (1) has the desired conservation form in that the rate of change of the cell average is a difference of fluxes. The difficulty with this formulation is that it requires transforming between cell averages of ϕ (which are directly evolved in time by the scheme) and cell wall values of ϕ (which must be reconstructed) to evaluate the needed fluxes. We would like to avoid reconstructing pointwise values of ϕ from the cell average values. The distinction between cell average and midpoint values can be ignored for schemes whose accuracy is no higher than second order, since the cell average and the midpoint value differ by only $O(\Delta x^2)$. This can be seen if we write ϕ in terms of its Taylor series expansion about the point x_i

$$\phi(x) = \phi(x_i) + (x - x_i)\phi'(x_i) + \frac{(x - x_i)^2}{2}\phi''(x_i) + \cdots .$$

Then,

$$\begin{aligned}
\overline{\phi}_i &= \frac{1}{(x_{i+1/2} - x_{i-1/2})} \int_{x_{i-1/2}}^{x_{i+1/2}} \phi(x)\, dx \\
&= \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \left[\phi(x_i) + (x - x_i)\phi'(x_i) + \frac{(x - x_i)^2}{2}\phi''(x_i) + \cdots \right] dx \\
&= \frac{1}{\Delta x} \left[\phi(x_i)\Delta x + \left. \frac{(x - x_i)^2}{2} \right|_{x_{i-1/2}}^{x_{i+1/2}} \phi'(x_i) + \left. \frac{(x - x_i)^3}{6} \right|_{x_{i-1/2}}^{x_{i+1/2}} \phi''(x_i) + \cdots \right] \\
&= \phi(x_i) + \frac{\Delta x^2}{24}\phi''(x_i) + O(\Delta x^4).
\end{aligned}$$

We also assume that we have a uniform grid, so that

$$x_{i+1/2} - x_{i-1/2} = \Delta x_i = \Delta x.$$

For $i \in \{1, \ldots, m\}$, we have

$$(\hat{\phi}_i)_t + f(\phi_{i+1/2}) - f(\phi_{i-1/2}) = 0.$$

Summing over i, the fluxes cancel except for the ones on either side of the domain, so we get

$$\sum_{i=1}^{m} (\hat{\phi}_i)_t + f(\phi_{m+1/2}) - f(\phi_{1/2}) = 0,$$

or, equivalently,

$$\sum_{i=1}^{m} (\overline{\phi}_i \Delta x_i)_t + f(\phi_{m+1/2}) - f(\phi_{1/2}) = 0.$$

When using the weak form of the conservation law we evolve cell average values of ϕ in time, but require pointwise values of ϕ at the half grid cells in order to evaluate the flux functions. As noted above, if we only wanted a second order accurate scheme, we could simply approximate the cell average value with the value of ϕ at the cell center. However, we would like to use the pointwise values of ϕ while still getting better than second order accuracy. To achieve this, we replace the physical flux function with a *numerical flux* function. We define the numerical flux function $\mathscr{F}$ such that

$$f(\phi)_x = \frac{\mathscr{F}(x + \Delta x/2) - \mathscr{F}(x - \Delta x/2)}{\Delta x} \tag{2}$$

We call $\mathscr{F}$ the numerical flux since we require it in our numerical scheme, and also to distinguish it from the closely related "physical flux", $f(\phi)$. It is not obvious that the numerical flux function exists, but from relationship (2) one can solve for its Taylor expansion to obtain

$$\mathscr{F} = f(\phi) - \frac{\Delta x^2}{24} f(\phi)_{xx} + \frac{7\Delta x^4}{5760} f(\phi)_{xxxx} - \cdots .$$

In summary, we start with the conservation law

$$\phi_t + f(\phi)_x = 0.$$

Integrating over a grid cell, we have

$$(\overline{\phi}_i \Delta x)_t + f(\phi_{i+1/2}) - f(\phi_{i-1/2}) = 0.$$

Replacing $\overline{\phi}_i$ with the pointwise value ϕ_i we make an $O(\Delta x^2)$ error

$$(\phi_i \Delta x)_t + f(\phi_{i+1/2}) - f(\phi_{i-1/2}) = O(\Delta x^2).$$

Introducing the numerical flux function instead of the physical flux function eliminates the error

$$(\phi_i)_t + \frac{\mathscr{F}\left(x_{i+1/2}\right) - \mathscr{F}\left(x_{i-1/2}\right)}{\Delta x} = 0.$$

This is the desired conservation form.

1.1 Constructing the Numerical Flux Function

We define the numerical flux function through the relation

$$f(\phi_i)_x = \frac{\mathscr{F}\left(x_{i+1/2}\right) - \mathscr{F}\left(x_{i-1/2}\right)}{\Delta x}.$$

To obtain a convenient algorithm for computing this numerical flux function, we define $h(x)$ implicitly through the following equation

$$f(\phi(x)) = \frac{1}{\Delta x} \int_{x-\Delta x/2}^{x+\Delta x/2} h(y)\ dy$$

and note that taking a derivative on both sides of this equation yields

$$f(\phi(x))_x = \frac{h(x+\Delta x/2) - h(x-\Delta x/2)}{\Delta x}$$

which shows that h is identical to the numerical flux function at the cell walls. That is $\mathscr{F}_{i\pm 1/2} = h(x_{i\pm 1/2})$ for all i. We calculate h by finding its primitive

$$H(x) = \int_{x_{-1/2}}^{x} h(y) dy$$

using polynomial interpolation, and then take a derivative to get h. We build a divided difference table to construct H.

zeroth order	$D^0_{i+1/2}H$	at cell walls
first order	$D^1_i H$	at cell centers
second order	$D^2_{i+1/2}H$	at cell walls
third order	$D^3_i H$	at cell centers
$\vdots$	$\vdots$	$\vdots$

That is, the even divided differences of H are at the cell walls, and the odd divided differences of H are at the cell centers. Since we are actually interested in determining h, we do not need the zeroth order divided differences of H as they will drop out when we differentiate to obtain h. Therefore, we can ignore the zeroth level of the divided difference table and construct it starting at the first level. The first level is given by

$$D^1_i H = \frac{H\big(x_{i+1/2}\big) - H\big(x_{i-1/2}\big)}{\Delta x} = f(\phi_i) = D^0_i f.$$

This is because

$$\begin{aligned} H(x_{i+1/2}) &= \int_{x_{-1/2}}^{x_{i+1/2}} h(y)dy \\ &= \sum_{j=0}^{i} \left(\int_{x_{j-1/2}}^{x_{j+1/2}} h(y)dy \right) \\ &= \Delta x \sum_{j=0}^{i} f(\phi(x_j)). \end{aligned}$$

And similarly,

$$H(x_{i-1/2}) = \Delta x \sum_{j=0}^{i-1} f(\phi(x_j)).$$

so that

$$H(x_{i+1/2}) - H(x_{i-1/2}) = \Delta x f(\phi(x_i)).$$

The higher divided differences are

$$D^2_{i+1/2}H = \frac{f(\phi(x_{i+1})) - f(\phi(x_i))}{2\Delta x} = \frac{1}{2}D^1_{i+1/2}f$$

$$D^3_i H = \frac{1}{3}D^2_i f$$

continuing in that manner.

According to the rules of polynomial interpolation, we can take any path along the divided difference table to construct H, although they do not all give good results. ENO reconstruction comprises two important features. First, choose $D^1_i H$ in the upwind direction. Second, choose higher order divided differences by taking the smaller (in absolute value) of the possible choices. Once we construct $H(x)$, we evaluate $H'(x_{i+1/2})$ to get the numerical flux $\mathscr{F}_{i+1/2}$.