Unit 3. Introduction to Computational Fluid Dynamics (CFD)

Lecture 312: Accuracy, conservation and boundary conditions of finite-volume methods

Reference book:

“Introduction to Computational Astrophysical Hydrodynamics” by Zingale.
http://bender.astro.sunysb.edu/hydro_by_example/CompHydroTutorial.pdf

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Introduction to CFD: accuracy and stencils

3.3.1 Differences and order of accuracy

In practice, when computing derivatives in a finite-volume discretization, we can use the second-order centered difference from § 1.2.2 treating the finite-volume data as living at the cell-centers and still be second-order accurate. For higher accuracy, we can fit a *conservative interpolant* (as illustrated in exercise 3.2) to a collection of points and then differentiate the interpolant itself.

Notice that the righthand side of all derivative approximations involve some linear combinations of f_i's. We call this the *stencil*. The *width* of the stencil is a measure of how many zones on either side of zone i we reach when computing our approximation.

For example, a second derivative can be discretized as:

$$\left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \tag{3.10}$$

The stencil on the righthand side encompasses 3 zones.

3.3.2 Conservation

The finite-volume grid is useful when dealing with conservation laws. Consider the following system:

$$\frac{\partial \boldsymbol{\mathcal{U}}}{\partial t} + \nabla \cdot \mathbf{F}(\boldsymbol{\mathcal{U}}) = 0 \tag{3.11}$$

where $\boldsymbol{\mathcal{U}}$ is a vector of conserved quantities and $\mathbf{F}(\boldsymbol{\mathcal{U}})$ is the flux of each quantity. This type of system arises, for example, in fluid flow, where the system will represent conservation of mass, momentum, and energy.

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Consider one-dimension. Integrating this system over a zone, and normalizing by Δx, we have:

$$\frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \boldsymbol{\mathcal{U}}}{\partial t} dx = -\frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \mathbf{F}}{\partial x} dx \tag{3.12}$$

On the left, we can take the time derivative out of the integral, and we are left with the definition of a zone average, so this becomes simply $\partial \langle \boldsymbol{\mathcal{U}} \rangle_i / \partial t$. On the right, we apply the divergence theorem, giving:

$$\frac{\partial \langle \boldsymbol{\mathcal{U}} \rangle_i}{\partial t} = -\frac{1}{\Delta x}\left\{ \mathbf{F}(\boldsymbol{\mathcal{U}})|_{x_{i+1/2}} - \mathbf{F}(\boldsymbol{\mathcal{U}})|_{x_{i-1/2}} \right\} \tag{3.13}$$

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$$\frac{\partial \langle \mathcal{U} \rangle_i}{\partial t} = -\frac{1}{\Delta x} \left\{ \mathbf{F}(\mathcal{U})|_{x_{i+1/2}} - \mathbf{F}(\mathcal{U})|_{x_{i-1/2}} \right\} \tag{3.13}$$

Independent of how we discretize in time, notice that we have the cell-average on the left and that the righthand side is simply a difference of fluxes through the interfaces of the zone. For the $i+1$ zone, the update would be:

$$\frac{\partial \langle \mathcal{U} \rangle_{i+1}}{\partial t} = -\frac{1}{\Delta x} \left\{ \mathbf{F}(\mathcal{U})|_{x_{i+3/2}} - \mathbf{F}(\mathcal{U})|_{x_{i+1/2}} \right\} \tag{3.14}$$

Notice that this shares the flux at the $x_{i+1/2}$ interface, but with the opposite sign. When all of the updates are done, the flux through each boundary adds to one zone and subtracts from its neighbor, exactly conserving (to round-off error) the quantity $\mathcal{U}$.

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This cancellation of the sums is an example of a *telescoping property*, and is the main reason why finite-volume methods are attractive—conserved quantities are conserved to machine (roundoff) precision.

Note that conservation is not the same as accuracy. We can construct the fluxes for our discretized equation by calling a random number generator and we'd still be conservative, but not at all accurate.

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3.3.3 Boundary conditions with finite-volume grids

Imagine that we wish to compute the derivative in every zone using:

$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{f_i - f_{i-1}}{\Delta x} \quad . \tag{3.15}$$

If we denote the index corresponding to the leftmost zone in our domain as 'lo', then when we try to compute $\partial f/\partial x|_{\rm lo}$, we will "fall-off" the grid, i.e., we need a value of f for zone $\rm lo - 1$, which is outside the domain. This is where boundary conditions for our grid come into play.

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We implement boundary conditions by extending the computational grid beyond the physical domain (see Figure 3.2). These additional zones are called *ghost cells*. They exist solely to handle the boundary conditions and allow us to use the same update equation (e.g. Eq. 3.15) for all zones in the domain.

Figure 3.2: A simple 1-d finite-volume grid with a single ghost cell at each end of the domain. The domain boundaries are indicated by the heavy vertical lines. Here there are hi − lo + 1 zones used in the discretization of the domain, with the first zone in the domain labeled lo and the last in the domain labeled hi.

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The number of ghostcells needed for the grid depends on how wide the stencils used in the computation are. The wider the stencil, the more ghostcells are needed.

Periodic boundary conditions would be implemented as:

$$f_{\mathrm{hi}+1} = f_{\mathrm{lo}} \tag{3.16}$$

$$f_{\mathrm{lo}-1} = f_{\mathrm{hi}} \tag{3.17}$$

A simple outflow (zero-gradient) boundary condition would be implemented as:

$$f_{\mathrm{hi}+1} = f_{\mathrm{hi}} \tag{3.18}$$

$$f_{\mathrm{lo}-1} = f_{\mathrm{lo}} \tag{3.19}$$

3.4 Numerical implementation details

The computational grids used for finite-volume techniques maps nicely onto multi-dimensional arrays. For the cell-average data, a typical array would be dimensioned as

```
ilo = ng
ihi = nx + ng - 1
state = np.zeros((nx + 2*ng, nvar))
```

in python (using NumPy), where nx is the number of zones in the domain and ng is the number of ghost cells.

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For some problems, there might be more than one state variable, so `nvar`, is the number of state variables that live in each zone. We would then loop from `ilo` to `ihi` to access the state data in the grid interior.

Fluxes are also stored in arrays, but since we cannot index an array with half-integer indices, the standard convention is that the index `i` in an array refers to the flux on the *left* edge of that zone. I.e.,

$$\texttt{flux[i]} \quad \longleftrightarrow \quad F_{i-1/2}$$