Finite Volume Method for Computational Hydrodynamics

Hsi-Yu Schive & Kuo-Chuan Pan

Numerical Astrophysics Summer School 2019: Astrophysical Fluid Dynamics
Advection of a Scalar

- Governing eq. \[ \frac{\partial u(x, t)}{\partial t} = -v \frac{\partial u(x, t)}{\partial x} \]
  - Scalar \( u \) is simply transported with a velocity \( v \)
  - Assuming \( v \) is constant
  - \( u \) is conserved \( \rightarrow \int u(x, t) \, dx = \text{constant} \)
Finite Difference Approximation

- Discretize space and time
  \[ u(x, t) \Rightarrow u_j^n \]
  \[ x_j = x_0 + j\Delta x \]
  \[ t_n = t_0 + n\Delta t \]

- Given \( u_j^n \), solve \( u_j^{n+1} \)

- Taylor expansion
  \[ f(\alpha + \Delta \alpha) = f(\alpha) + f'(\alpha)\Delta \alpha + \frac{1}{2!} f''(\alpha)\Delta \alpha^2 + \frac{1}{3!} f'''(\alpha)\Delta \alpha^3 + \ldots \]
  - Use it to approximate partial derivatives by discrete \( u_j^n \)
  - That’s what differentiates different schemes
    - May NOT be as trivial as you think!
Forward-Time Central-Space Scheme

- Advection eq.
  \[
  \frac{\partial u(x, t)}{\partial t} = -v \frac{\partial u(x, t)}{\partial x}
  \]

- FTCS scheme:
  \[
  \frac{\partial u(x_j, t_n)}{\partial t} \rightarrow \frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} + O(\Delta t)
  \]
  \[
  \frac{\partial u(x_j, t_n)}{\partial x} \rightarrow \frac{u_{j+1}^{n} - u_{j-1}^{n}}{2\Delta x} + O(\Delta x^2)
  \]
  
  \[
  u_{j}^{n+1} = u_{j}^{n} - \frac{v\Delta t}{2\Delta x}(u_{j+1}^{n} - u_{j-1}^{n})
  \]
Forward-Time Central-Space Scheme

- **Explicit** scheme
  - $u_{j}^{n+1}$ for each $j$ can be computed explicitly from values at $t = t_n$
  - $u_{j}^{n+1}$ for different $j$ be computed independently (and thus in parallel)
  - In comparison, **implicit** schemes solve equations coupling $u_{j}^{n+1}$ with different $j$

- FTCS scheme is very simple. But, it is **UNSTABLE** in general for hyperbolic equations!
Governing Equations of Ideal Hydro

- Euler eqs.
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \leftarrow \text{mass conservation}
  \]
  \[
  \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + P \mathbf{I}) = 0 \quad \leftarrow \text{momentum conservation}
  \]
  \[
  \frac{\partial E}{\partial t} + \nabla \cdot [(E + P)\mathbf{v}] = 0 \quad \leftarrow \text{energy conservation}
  \]

- \(\rho\): mass density, \(\mathbf{v}\): velocity, \(P\): pressure, \(E\): total energy density, \(\mathbf{I}\): identity matrix
  \[E = e + \frac{1}{2} \rho \mathbf{v}^2, \text{ where } e \text{ is the internal energy density}\]

- 6 variables, 5 equations \(\rightarrow\) need equation of state to compute \(P\)
  - For example, ideal gas: \(e = \frac{P}{\gamma - 1}, \text{ where } \gamma \text{ is the ratio of specific heat}\)
Conserved vs. Primitive Variables

Conserved variables

\[ U = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ E \end{bmatrix} \]

Primitive variables

\[ W = \begin{bmatrix} \rho \\ v_x \\ v_y \\ v_z \\ P \end{bmatrix} \]
Flux-Conservative Form in 1D

- Euler eqs. in a compact flux-conservative form:

\[
\frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0
\]

- \( F_x, F_y, F_z \): fluxes along different directions

\[
F_x = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P \\ \rho v_x v_y \\ \rho v_x v_z \\ (E + P)v_x \end{bmatrix}, \quad F_y = \begin{bmatrix} \rho v_y \\ \rho v_y v_x \\ \rho v_y^2 + P \\ \rho v_y v_z \\ (E + P)v_y \end{bmatrix}, \quad F_z = \begin{bmatrix} \rho v_z \\ \rho v_z v_x \\ \rho v_z v_y \\ \rho v_z^2 + P \\ (E + P)v_z \end{bmatrix}
\]
Finite-Volume Scheme

- Divergence theorem: \[ \int_V \frac{\partial U}{\partial t} dV = - \int_V (\nabla \cdot F) dV = - \oint_S (F \cdot n) dS \]

- Integrate over the cell volume \( \Delta x \Delta y \Delta z \) and time interval \( \Delta t = t^{n+1} - t^n \)

\[
U^n_{i,j,k} \equiv \frac{1}{\Delta x \Delta y \Delta z} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, y, z, t^n) \, dx \, dy \, dz
\]

\[
F^{n+1/2}_{x,i-1/2,j,k} \equiv \frac{1}{\Delta y \Delta z \Delta t} \int_{t^n}^{t^{n+1}} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} F(x_{i-1/2}, y, z, t) \, dy \, dz \, dt
\]

similar for \( F^{n+1/2}_{y,i,j-1/2,k} \) and \( F^{n+1/2}_{z,i,j,k-1/2} \)
Finite-Volume Scheme

- Euler eqs. can be casted into the following form:

\[
U_{i,j,k}^{n+1} = U_{i,j,k}^n - \frac{\Delta t}{\Delta x} \left( F_{x,i+1/2,j,k}^{n+1/2} - F_{x,i-1/2,j,k}^{n+1/2} \right) \\
- \frac{\Delta t}{\Delta y} \left( F_{y,i,j+1/2,k}^{n+1/2} - F_{y,i,j-1/2,k}^{n+1/2} \right) \\
- \frac{\Delta t}{\Delta z} \left( F_{z,i,j,k+1/2}^{n+1/2} - F_{z,i,j,k-1/2}^{n+1/2} \right)
\]

- Note that this form is EXACT!
  - i.e., no approximation has been made

- \( U_{i,j,k}^n \): volume-averaged conserved variables

- \( F_{x,i-1/2,j,k}^{n+1/2} \): time- and area-averaged fluxes
Lax-Wendroff Scheme

- Two-step approaches
  - Step 1: evaluate $U_{j+1/2}^{n+1/2}$ defined at the half time-step $n+1/2$ and the cell interface $j+1/2$ with the Lax scheme
    \[
    U_{j+1/2}^{n+1/2} = \frac{1}{2} (U_{j+1}^n + U_j^n) - \frac{\Delta t}{2\Delta x} \left[ F(U_{j+1}^n) - F(U_j^n) \right]
    \]
  - Step 2: use $U_{j+1/2}^{n+1/2}$ to evaluate the half-step fluxes for the full-step update
    \[
    U_{j}^{n+1} = U_j^n - \frac{\Delta t}{\Delta x} \left[ F(U_{j+1/2}^{n+1/2}) - F(U_{j-1/2}^{n+1/2}) \right]
    \]
Ghost Zones are used for setting the boundary conditions:
- Physical boundaries (e.g., periodic, outflow, inflow)
- Numerical boundaries between different parallel processes

Number of ghost zones depends on the stencil size:
- Lax-Wendroff: 1
Acoustic Wave Test

- How to test a hydrodynamic scheme?
  - Euler eqs. are coupled nonlinear eqs. → no trivial analytical solution

- Example: acoustic (sound) wave solution
  - Perturb the Euler eqs.
    - Let \( \rho = \rho_0 + \delta\rho, v = \delta v, P = P_0 + \delta P \)
    - Ignore all high-order terms
    - Insert the plane wave solution and solve the dispersion relation

\[
C_s^2 = \frac{\gamma P_0}{\rho_0} \\
\delta v_k = C_s \delta \rho_k / \rho_0 \\
\delta P_k = \delta \rho_k C_s^2
\]
How about Nonlinear Solutions?

- Example: acoustic wave steepening:

\[
\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = -\frac{1}{\rho} \frac{\partial P}{\partial x}
\]

nonlinear convection term for wave steepening

- How does Lax-Wendroff scheme work in this case?
  - Try Increasing the \texttt{d_amp} parameter from 1e-6 to 1e-1 in the acoustic wave demo
Sod Shock Tube Problem

Initial condition

\[
\begin{bmatrix}
\rho_L \\
v_L \\
P_L
\end{bmatrix} = \begin{bmatrix} 1.0 \\
0.0 \\
0.125 \end{bmatrix}, \quad \begin{bmatrix}
\rho_R \\
v_R \\
P_R
\end{bmatrix} = \begin{bmatrix} 0.125 \\
0.0 \\
0.1 \end{bmatrix}
\]
Demo

lec4-demo2-shock-tube-lax-wendroff
Sod Shock Tube Problem

- Lax-Wendroff scheme
- Unphysical oscillations
- Motivate high-resolution shock-capturing schemes
High-Resolution Shock-Capturing Methods

- Godunov method
  - Approximate data with a **piecewise constant** distribution
    \[ U(x, t) \]
    
    ![Riemann problems](image)
    
    \[ U_i^n = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t^n) \, dx \]
  
  - Solve the local Riemann problems
    - Piecewise constant data with a single discontinuity (like shock tube)
    - Apply either exact or approximate solutions
  
  - Update data by averaging the Riemann problem solution over each cell
    - Equivalently, we can solve the intercell fluxes
    - Avoid wave interaction within each cell
Riemann Problem in 1D Hydro

- Euler eqs. in 1D: \[
\frac{\partial U}{\partial t} + \frac{\partial F_x(U)}{\partial x} = 0, \quad U = \begin{bmatrix} \rho \\ \rho v_x \\ E \end{bmatrix}, \quad F_x = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P \\ (E + P)v_x \end{bmatrix}
\]

- Riemann problem:

\[
U(x, t = 0) = \begin{cases} 
U_L & = \begin{bmatrix} \rho_L \\ \rho_L v_{xL} \\ E_L \end{bmatrix}, \quad x \leq 0 \\
U_R & = \begin{bmatrix} \rho_R \\ \rho_R v_{xR} \\ E_R \end{bmatrix}, \quad x > 0
\end{cases}
\]
Riemann Problem in 1D Hydro

- Exact solution of the Riemann problem involves three waves
  - Contact discontinuity
  - Shock wave
  - Rarefaction wave

- Decompose the entire domain into four regions $W_L$, $W_{*L}$, $W_{*R}$, $W_R$
Riemann Problem in 1D Hydro

- Riemann problem can be solved analytically
  - Known: $W_L, W_R$
  - Unknowns: $W^*_L, W^*_R$
    - In fact, we always have $P^*_L = P^*_R$ and $v_{x,*L} = v_{x,*R}$ (because the middle wave is always a contact discontinuity)
    - So only 4 unknown variables: $\rho^*_L, \rho^*_R, P^*, v_{x^*}$

- However, exact Riemann solver is very computationally expensive
  - Approximate Riemann solvers are usually accurate enough
    - All we need is the interface fluxes
    - Examples
      - Roe solver
      - HLLE solver
      - HLLC solver
Higher-Order Godunov Methods

- **MUSCL** (*Monotone Upstream–centred Scheme for Conservation Laws*)

- Data reconstruction within each cell
  - Original Godunov’s scheme: piecewise constant method (PCM)
  - Piecewise linear method (PLM)
  - Piecewise parabolic method (PPM)
Higher-Order Godunov Methods

- Avoid introducing new local extrema during data reconstruction
  - Reduce spurious (i.e., unphysical) oscillations
  - Avoid unphysical values such as negative density/pressure

- Slope limiters
  - $U_j(x) = U_j + \frac{(x - x_j)}{\Delta x} \tilde{\delta}_i, \quad |x - x_j| \leq \Delta x/2$

  where $\tilde{\delta}_i = \bar{\delta}_i(\delta_{i-1/2}, \delta_{i+1/2}), \quad \delta_{i-1/2} = U_i - U_{i-1}$

  limited slope satisfying the TVD (Total Variation Diminishing) condition

- Examples: van Leer: $\bar{\delta}_i = \left\{ \begin{array}{ll}
  \frac{2\delta_{i-1/2}\delta_{i+1/2}}{\delta_{i-1/2} + \delta_{i+1/2}}, & \delta_{i-1/2}\delta_{i+1/2} \geq 0 \\
  0, & \delta_{i-1/2}\delta_{i+1/2} < 0
\end{array} \right.$

MinMod: $\bar{\delta}_i = \left\{ \begin{array}{ll}
  \text{sign}(\delta_{i-1/2}) \min(|\delta_{i-1/2}|, |\delta_{i+1/2}|), & \delta_{i-1/2}\delta_{i+1/2} \geq 0 \\
  0, & \delta_{i-1/2}\delta_{i+1/2} < 0
\end{array} \right.$
Higher-Order Godunov Methods

- Effects of various slope limiters
  - Diffusiveness (resolution) vs. robustness

- Left and right states are not equal unless the flow is smooth
  - Define Riemann problems

- Data reconstruction on the **primitive variables** usually results in better results (less oscillatory) than on the **conserved variables**
  - It may be even better to reconstruct the **characteristic variables**
    - Diagonalize the linearized eqs. of motion in the primitive variables
    - Determine eigenvectors
    - Perform eigen-decomposition on $\delta_{i-1/2}$ and $\delta_{i+1/2}$ to get the characteristic variables
    - Compute limited slopes on these characteristic variables
Second-Order Accuracy in Time

Example: MUSCL-Hancock scheme

1. Data reconstruction → obtain the face-centered data (i.e., data on the left and right edges of each cell) at $t^n$
   \[ U_{i,L}^n = U_i^n - \frac{1}{2} \delta_i, \quad U_{i,R}^n = U_i^n + \frac{1}{2} \delta_i \]

2. Evolve the face-centered data by $\Delta t/2$ using
   \[ U_{i,L}^{n+1/2} = U_{i,L}^n - \frac{\Delta t}{2\Delta x} \left[ F_x(U_{i,R}^n) - F_x(U_{i,L}^n) \right] \]
   \[ U_{i,R}^{n+1/2} = U_{i,R}^n - \frac{\Delta t}{2\Delta x} \left[ F_x(U_{i,R}^n) - F_x(U_{i,L}^n) \right] \]

   ... exactly the same fluxes; no ghost zones are required ...

3. Riemann solver → compute the inter-cell fluxes
   \[ F_{x,i-1/2}^{n+1/2} = Riemann(U_L, U_R), \text{ where } U_L = U_{i-1,R}^{n+1/2} \text{ and } U_R = U_{i,L}^{n+1/2} \]

4. Evolve the volume-averaged data by $\Delta t$
   \[ U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left[ F_{x,i+1/2}^{n+1/2} - F_{x,i-1/2}^{n+1/2} \right] \]
Sod Shock Tube with MUSCL-Hancock

MUSCL-Hancock $\rightarrow$ much better!

Lax-Wendroff $\rightarrow$ unphysical oscillations...

Graphs showing comparisons at $t = 0.100$.