Finite Volume Method for Computational Hydrodynamics

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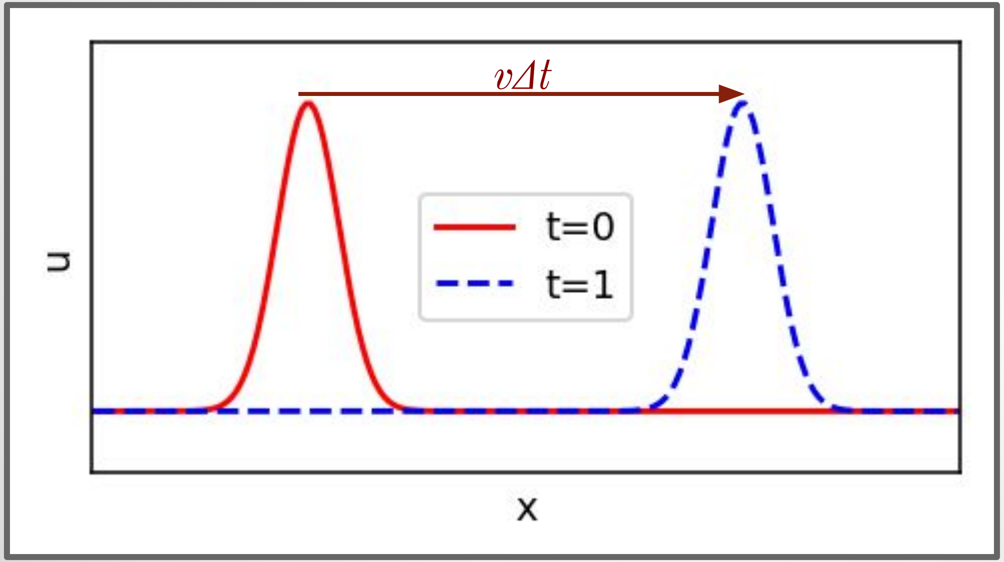
Astrophysical Fluid Dynamics

Advection of a Scalar

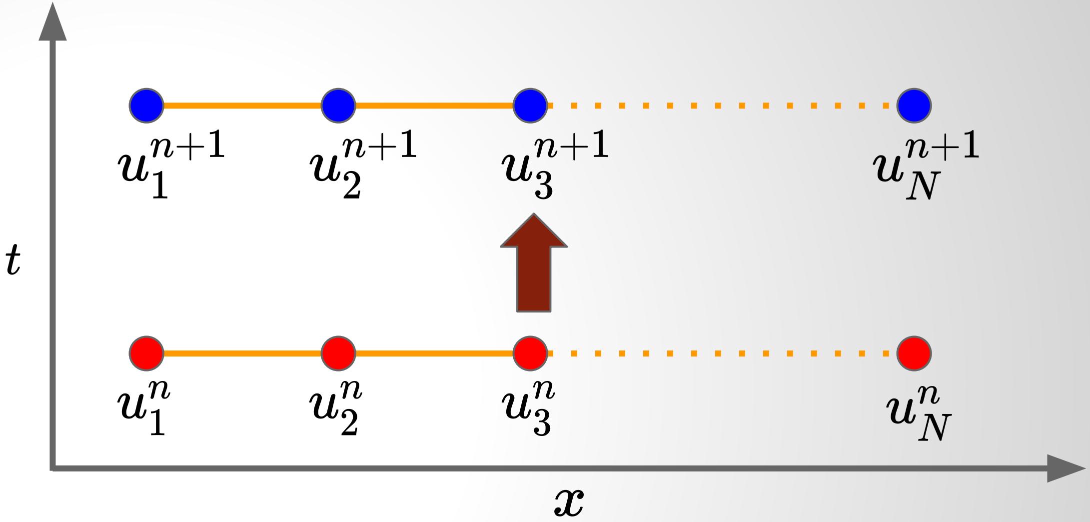
- **Governing eq.** $$\frac{\partial u(x,t)}{\partial t} = -v\frac{\partial u(x,t)}{\partial x}$$
  - **Scalar** u **is simply transported with a velocity** v
  - **Assuming** v **is constant**
  - u **is conserved →** $\int u(x,t)dx = constant$



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:**

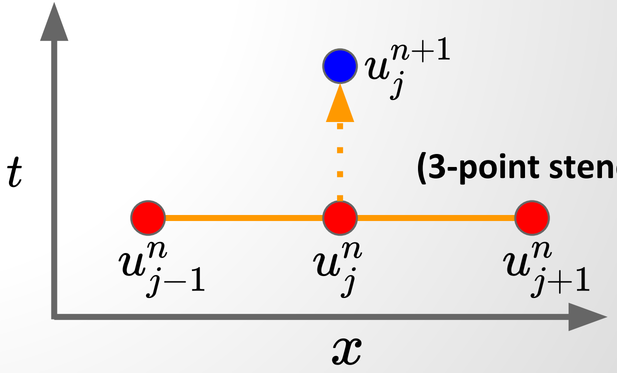
$$\frac{\partial u(x_j,t_n)}{\partial t} \rightarrow \frac{u_j^{n+1}-u_j^n}{\Delta t} + O(\Delta t)$$

↙ forward-time

$$\frac{\partial u(x_j,t_n)}{\partial x} \rightarrow \frac{u_{j+1}^{n}-u_{j-1}^n}{2\Delta x} + O(\Delta x^2)$$

↖ central-space

$$u_j^{n+1} = u_j^n - \frac{v\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n)$$



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.**

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0 \quad \leftarrow \text{mass conservation}$$

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v} \boldsymbol{v} + P \boldsymbol{I}) = 0 \quad \leftarrow \text{momentum conservation}$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot [(E + P) \boldsymbol{v}] = 0 \quad \leftarrow \text{energy conservation}$$

- ρ: **mass density,** v: **velocity,** P: **pressure,** E: **total energy density,** I: **identity matrix**

  $E = e + \frac{1}{2}\rho v^2$ **, where** e **is the internal energy density**

- **6 variables, 5 equations → need <u>equation of state</u> to compute** P
  - **For example, ideal gas:** $e = \frac{P}{\gamma - 1}$**, where** γ **is the ratio of specific heat**

Conserved vs. Primitive Variables

Conserved variables

$$\boldsymbol{U} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ E \end{bmatrix}$$

Primitive variables

$$\boldsymbol{W} = \begin{bmatrix} \rho \\ v_x \\ v_y \\ v_z \\ P \end{bmatrix}$$

Flux-Conservative Form in 1D

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

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

  - $\boldsymbol{F}_x$, $\boldsymbol{F}_y$, $\boldsymbol{F}_z$: **fluxes along different directions**

$$\boldsymbol{F_x} = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P \\ \rho v_x v_y \\ \rho v_x v_z \\ (E+P)v_x \end{bmatrix} \qquad \boldsymbol{F_y} = \begin{bmatrix} \rho v_y \\ \rho v_y v_x \\ \rho v_y^2 + P \\ \rho v_y v_z \\ (E+P)v_y \end{bmatrix} \qquad \boldsymbol{F_z} = \begin{bmatrix} \rho v_z \\ \rho v_z v_x \\ \rho v_z v_y \\ \rho v_z^2 + P \\ (E+P)v_z \end{bmatrix}$$

Finite-Volume Scheme

- **Divergence theorem:** $\int_V \frac{\partial \boldsymbol{U}}{\partial t} dV = -\int_V (\boldsymbol{\nabla} \cdot \boldsymbol{F}) dV = -\oint_S (\boldsymbol{F} \cdot \boldsymbol{n}) dS$
- **Integrate over the cell volume** $\Delta x \Delta y \Delta z$ **and time interval** $\Delta t = t^{n+1} - t^n$

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

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

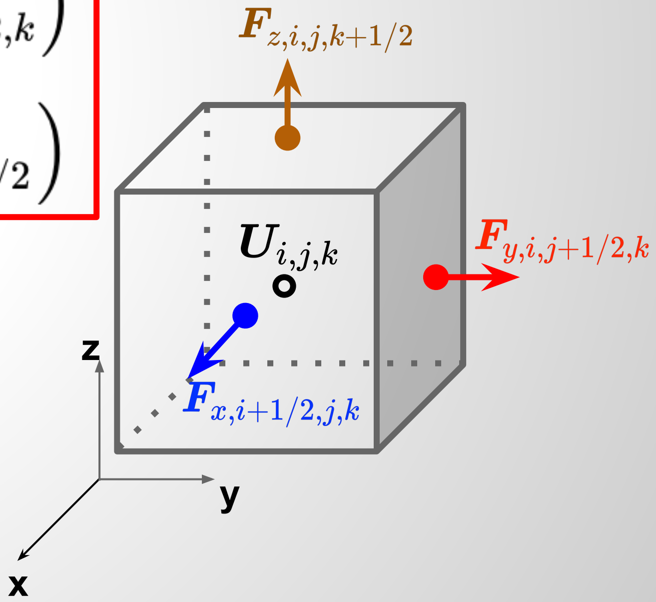
similar for $\boldsymbol{F}^{n+1/2}_{y,i,j-1/2,k}$ and $\boldsymbol{F}^{n+1/2}_{z,i,j,k-1/2}$

Finite-Volume Scheme

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

$$
\begin{aligned}
\boldsymbol{U}^{n+1}_{i,j,k} = \boldsymbol{U}^{n}_{i,j,k} &- \frac{\Delta t}{\Delta x}\left(\boldsymbol{F}^{n+1/2}_{x,i+1/2,j,k} - \boldsymbol{F}^{n+1/2}_{x,i-1/2,j,k}\right) \\
&- \frac{\Delta t}{\Delta y}\left(\boldsymbol{F}^{n+1/2}_{y,i,j+1/2,k} - \boldsymbol{F}^{n+1/2}_{y,i,j-1/2,k}\right) \\
&- \frac{\Delta t}{\Delta z}\left(\boldsymbol{F}^{n+1/2}_{z,i,j,k+1/2} - \boldsymbol{F}^{n+1/2}_{z,i,j,k-1/2}\right)
\end{aligned}
$$

  - Note that this form is EXACT!
    - i.e., no approximation has been made
  - $\boldsymbol{U}^{n}_{i,j,k}$: volume-averaged conserved variables
  - $\boldsymbol{F}^{n+1/2}_{x,i-1/2,j,k}$: time- and area-averaged fluxes



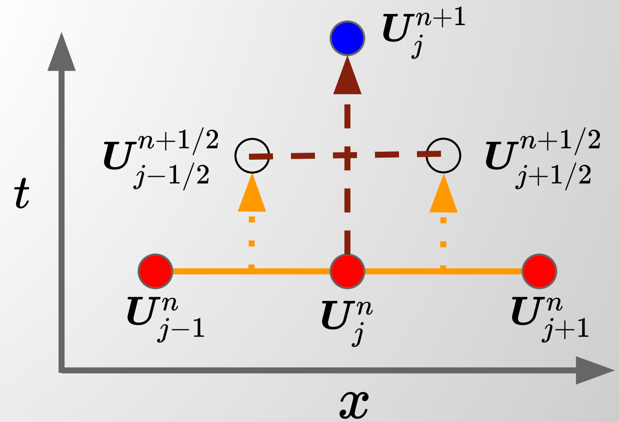
Lax-Wendroff Scheme

- Two-step approaches
  - Step 1: evaluate $\boldsymbol{U}_{j+1/2}^{n+1/2}$ defined at the half time-step $n+1/2$ and the cell interface $j+1/2$ with the Lax scheme

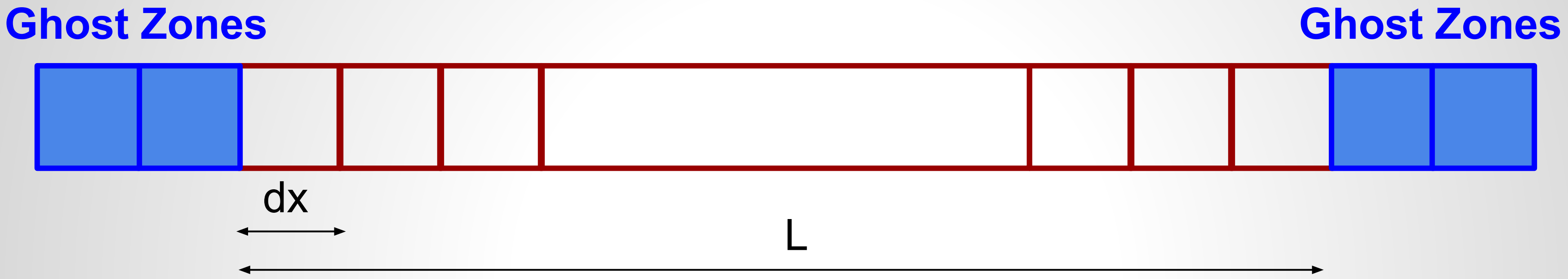
$$\boldsymbol{U}_{j+1/2}^{n+1/2} = \frac{1}{2}(\boldsymbol{U}_{j+1}^{n} + \boldsymbol{U}_{j}^{n}) - \frac{\Delta t}{2\Delta x}\left[\boldsymbol{F}(\boldsymbol{U}_{j+1}^{n}) - \boldsymbol{F}(\boldsymbol{U}_{j}^{n})\right]$$

  - Step 2: use $\boldsymbol{U}_{j+1/2}^{n+1/2}$ to evaluate the half-step fluxes for the full-step update

$$\boldsymbol{U}_{j}^{n+1} = \boldsymbol{U}_{j}^{n} - \frac{\Delta t}{\Delta x}\left[\boldsymbol{F}(\boldsymbol{U}_{j+1/2}^{n+1/2}) - \boldsymbol{F}(\boldsymbol{U}_{j-1/2}^{n+1/2})\right]$$



Ghost Zones



- Ghost zones are used for setting the <u>boundary conditions</u>
  - 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

$$C_s^2 = \gamma P_0 / \rho_0$$
$$\delta v_k = C_s \delta\rho_k / \rho_0$$
$$\delta P_k = \delta\rho_k C_s^2$$

Demo

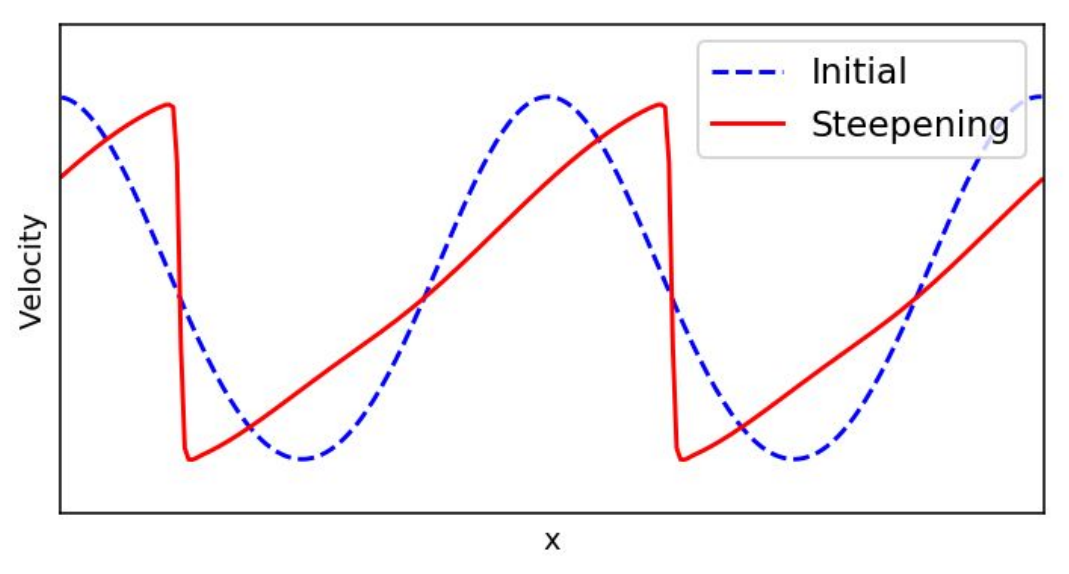
lec4-demo1-acoustic-wave-lax-wendroff

How about Nonlinear Solutions?

- **Example: acoustic wave steepening:**

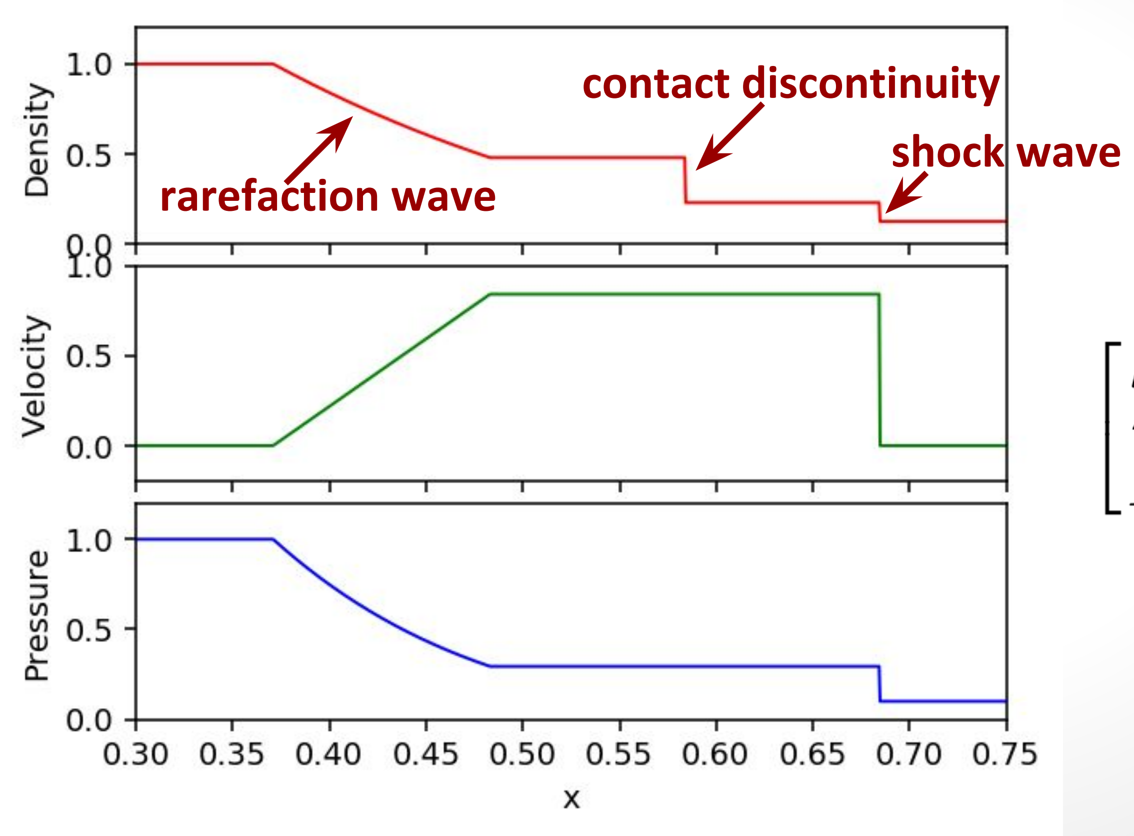
$$\frac{\partial v}{\partial t} + \boxed{v\frac{\partial v}{\partial x}} = -\frac{1}{\rho}\frac{\partial P}{\partial x}$$

nonlinear convection term for wave steepening



- **How does Lax-Wendroff scheme work in this case?**
  - **Try Increasing the `d_amp` parameter from 1e-6 to 1e-1 in the acoustic wave demo**

Sod Shock Tube Problem



Initial condition

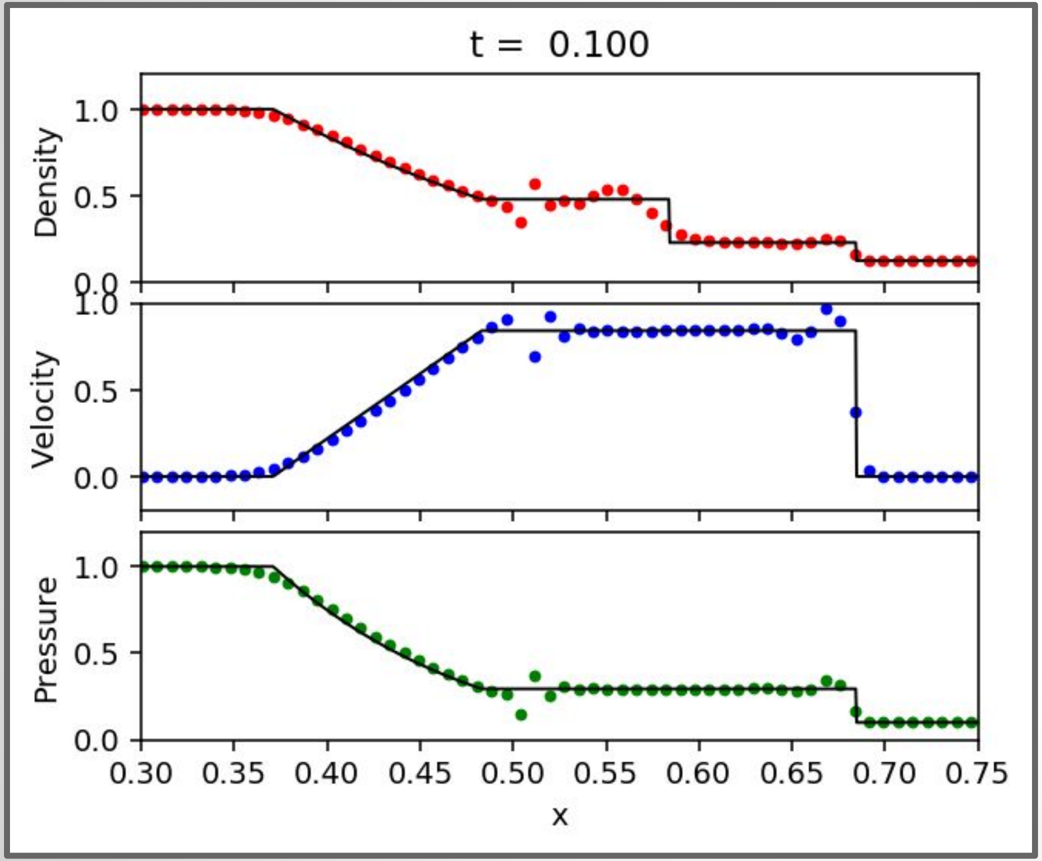
Left state **Right state**

$$\begin{bmatrix} \rho_L \\ v_L \\ P_L \end{bmatrix} = \begin{bmatrix} 1.0 \\ 0.0 \\ 0.125 \end{bmatrix}, \begin{bmatrix} \rho_R \\ v_R \\ P_R \end{bmatrix} = \begin{bmatrix} 0.125 \\ 0.0 \\ 0.1 \end{bmatrix}$$

Demo

lec4-demo2-shock-tube-lax-wendroff

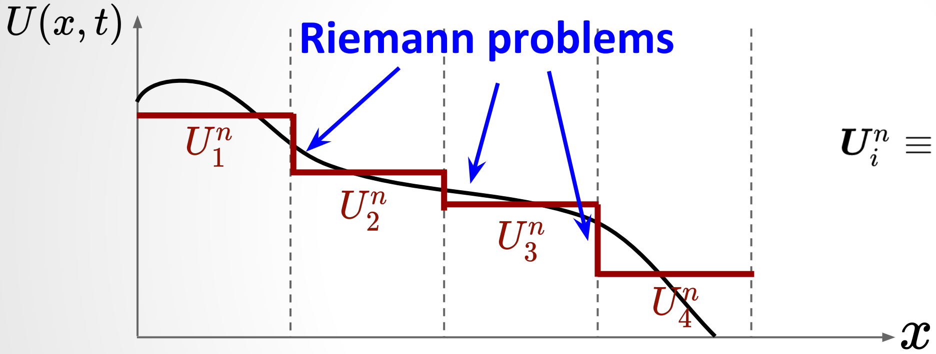
Sod Shock Tube Problem



- **Lax-Wendroff scheme**
- **Unphysical oscillations**
- **Motivate <u>high-resolution shock-capturing</u> schemes**

High-Resolution Shock-Capturing Methods

- Godunov method
  - Approximate data with a <u>piecewise constant</u> distribution



$$\boldsymbol{U}_i^n \equiv \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \boldsymbol{U}(x, t^n)dx$$

  - 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

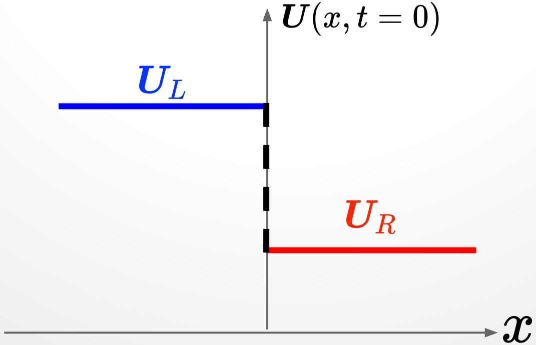
Riemann Problem in 1D Hydro

- **Euler eqs. in 1D:** $\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}_x(\boldsymbol{U})}{\partial x} = 0,\ \boldsymbol{U} = \begin{bmatrix} \rho \\ \rho v_x \\ E \end{bmatrix},\ \boldsymbol{F}_x = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P \\ (E+P) v_x \end{bmatrix}$

- **Riemann problem:** $\boldsymbol{U}(x, t=0) = \begin{cases} \boldsymbol{U}_L = \begin{bmatrix} \rho_L \\ \rho_L v_{xL} \\ E_L \end{bmatrix}, & x \leq 0 \\ \boldsymbol{U}_R = \begin{bmatrix} \rho_R \\ \rho_R v_{xR} \\ E_R \end{bmatrix}, & x > 0 \end{cases}$

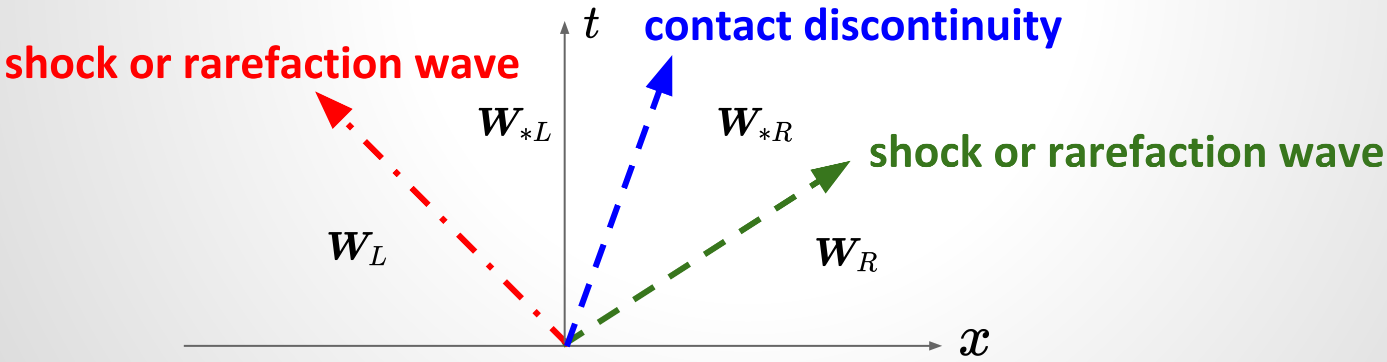
left state

right state



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

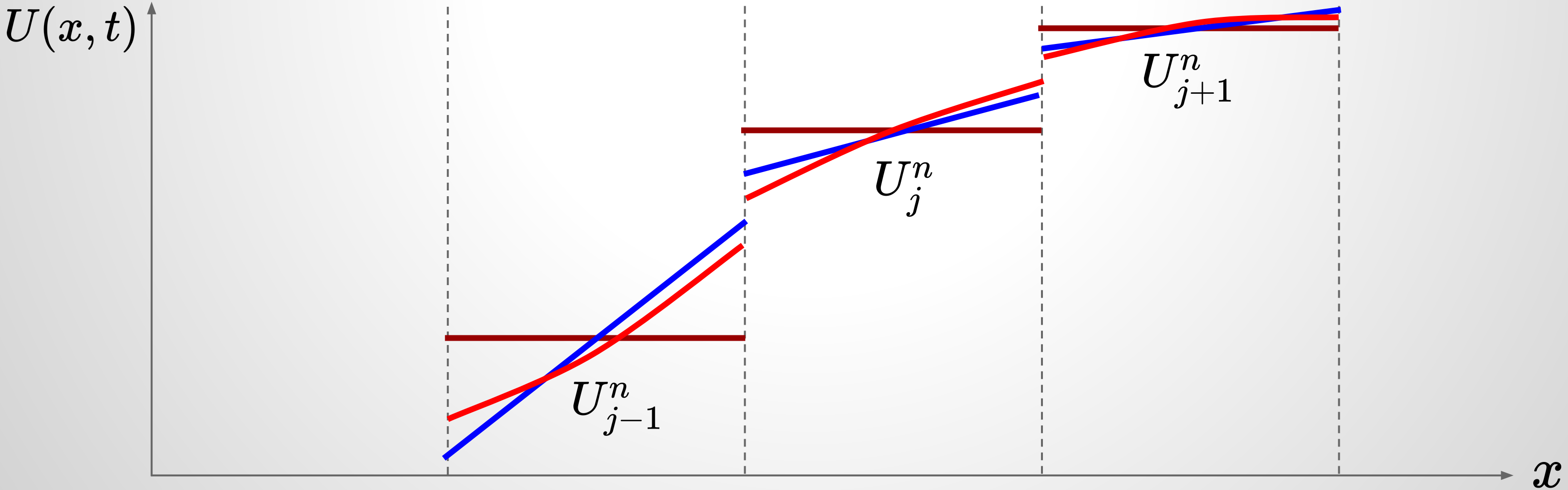


Riemann Problem in 1D Hydro

- **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**
  - $\boldsymbol{U}_j(x) = \boldsymbol{U}_j + \frac{(x - x_j)}{\Delta x}\bar{\boldsymbol{\delta}}_i, \quad |x - x_j| \le \Delta x/2$

    where $\bar{\boldsymbol{\delta}}_i = \bar{\boldsymbol{\delta}}_i(\boldsymbol{\delta}_{i-1/2}, \boldsymbol{\delta}_{i+1/2}), \quad \boldsymbol{\delta}_{i-1/2} \equiv \boldsymbol{U}_i - \boldsymbol{U}_{i-1}$

    limited slope satisfying the TVD (Total Variation Diminishing) condition
  - **Examples:** van Leer: $\bar{\boldsymbol{\delta}}_i = \begin{cases} \frac{2\boldsymbol{\delta}_{i-1/2}\boldsymbol{\delta}_{i+1/2}}{\boldsymbol{\delta}_{i-1/2} + \boldsymbol{\delta}_{i+1/2}}, & \boldsymbol{\delta}_{i-1/2}\boldsymbol{\delta}_{i+1/2} \ge 0 \\ 0, & \boldsymbol{\delta}_{i-1/2}\boldsymbol{\delta}_{i+1/2} < 0 \end{cases}$

    MinMod: $\bar{\boldsymbol{\delta}}_i = \begin{cases} sign(\boldsymbol{\delta}_{i-1/2})\, min(|\boldsymbol{\delta}_{i-1/2}|, |\boldsymbol{\delta}_{i+1/2}|), & \boldsymbol{\delta}_{i-1/2}\boldsymbol{\delta}_{i+1/2} \ge 0 \\ 0, & \boldsymbol{\delta}_{i-1/2}\boldsymbol{\delta}_{i+1/2} < 0 \end{cases}$

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**

$$\boldsymbol{U}_{i,L}^n = \boldsymbol{U}_i^n - \frac{1}{2}\bar{\boldsymbol{\delta}}_i, \quad \boldsymbol{U}_{i,R}^n = \boldsymbol{U}_i^n + \frac{1}{2}\bar{\boldsymbol{\delta}}_i$$

2. **Evolve the face-centered data by $\Delta t/2$ using**

$$\boldsymbol{U}_{i,L}^{n+1/2} = \boldsymbol{U}_{i,L}^n - \frac{\Delta t}{2\Delta x}\left[\boldsymbol{F}_x(\boldsymbol{U}_{i,R}^n) - \boldsymbol{F}_x(\boldsymbol{U}_{i,L}^n)\right]$$

$$\boldsymbol{U}_{i,R}^{n+1/2} = \boldsymbol{U}_{i,R}^n - \frac{\Delta t}{2\Delta x}\left[\boldsymbol{F}_x(\boldsymbol{U}_{i,R}^n) - \boldsymbol{F}_x(\boldsymbol{U}_{i,L}^n)\right]$$

exactly the same fluxes;
no ghost zones are required

3. **Riemann solver → compute the inter-cell fluxes**

$\boldsymbol{F}_{x,i-1/2}^{n+1/2} = Riemann(\boldsymbol{U}_L, \boldsymbol{U}_R)$, where $\boldsymbol{U}_L = \boldsymbol{U}_{i-1,R}^{n+1/2}$ and $\boldsymbol{U}_R = \boldsymbol{U}_{i,L}^{n+1/2}$

4. **Evolve the volume-averaged data by Δt**

$$\boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\Delta x}\left[\boldsymbol{F}_{x,i+1/2}^{n+1/2} - \boldsymbol{F}_{x,i-1/2}^{n+1/2}\right]$$

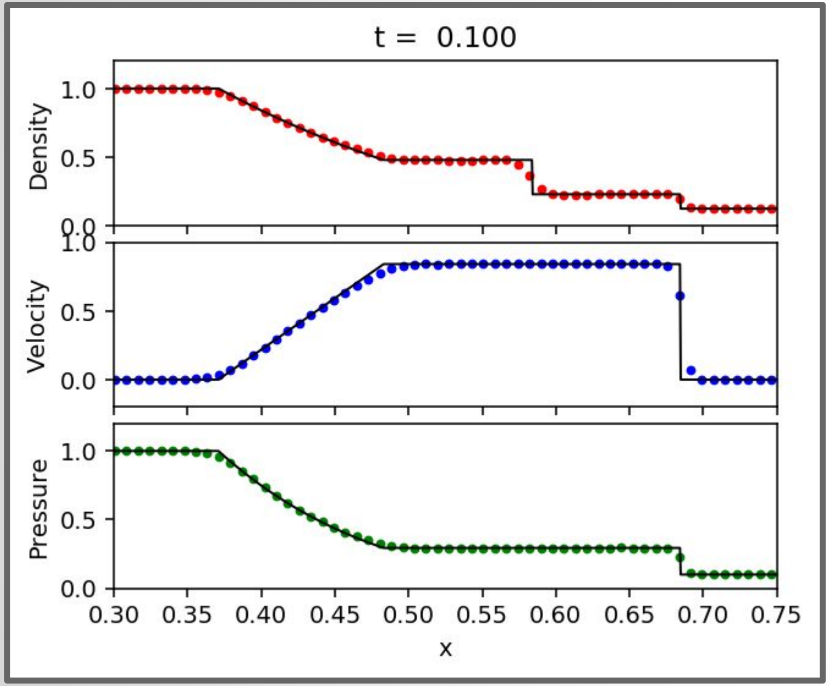
Demo

lec4-demo3-acoustic-wave-muscl-hancock

lec4-demo4-shock-tube-muscl-hancock

Sod Shock Tube with MUSCL-Hancock

MUSCL-Hancock → much better!



Lax-Wendroff → unphysical oscillations...