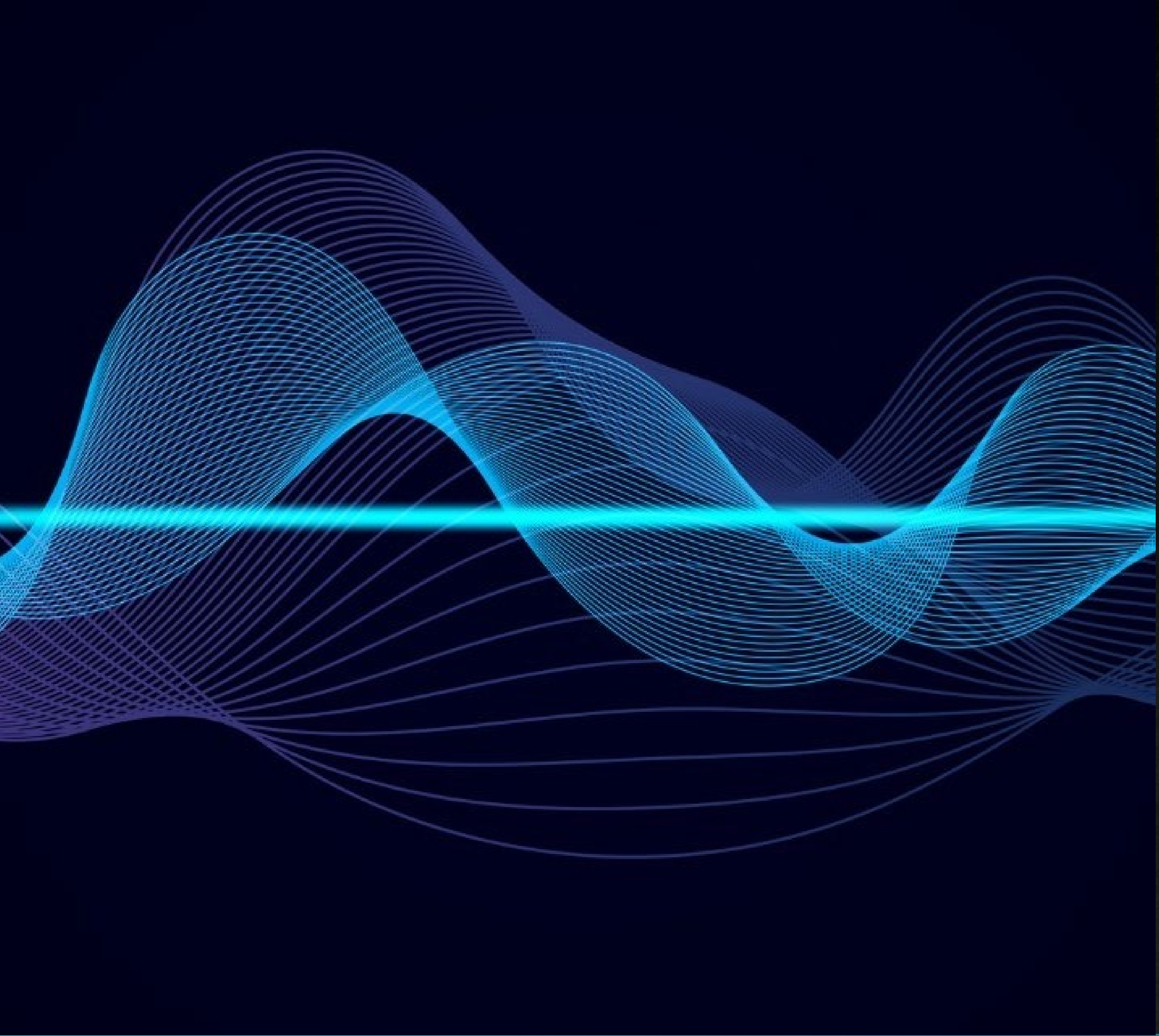


Computational Physics

PHYS 6260

Fluid Dynamics

Announcements:

- Last class!
- Term project paper: Due Thursday May 2

Lecture Outline

We will skim these topics

- Fluid dynamics equations
- Eulerian vs Lagrangian
- Shocks: Riemann Problem
- Fluid advection
- Reconstruction of cell interfaces
- Conservative system
- Primitive system
- Jumps across waves

Euler’s equations

- Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

- Momentum equation

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} + \frac{1}{\rho}\nabla P = 0$$

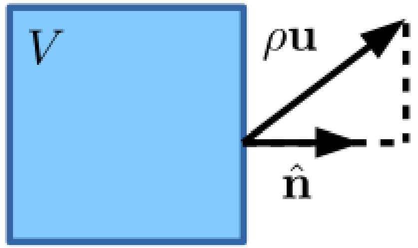
- Energy equation

$$\frac{\partial \epsilon}{\partial t} + \vec{u} \cdot \nabla \epsilon + \frac{P}{\rho}\nabla \cdot \vec{v} = 0$$

$$\int dV\, \frac{\partial \rho}{\partial t} = -\int dV\, \nabla \cdot (\rho \mathbf{u})$$

$$\frac{d}{dt}\int dV\, \rho = -\int dA\, \rho \mathbf{u} \cdot \hat{\mathbf{n}}$$

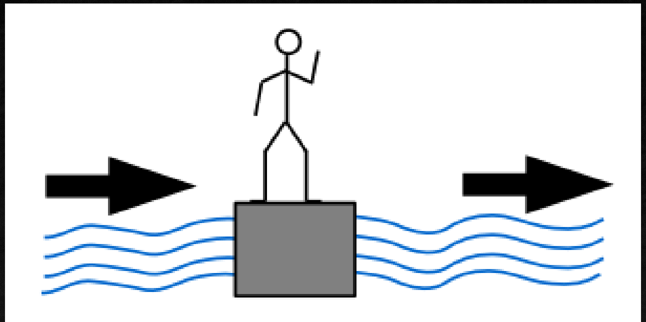
$$\frac{dM}{dt} = \text{net rate of inflow}$$



Choice of reference frame

- Eulerian: stand still as fluid moves by
  - Fluid quantities are functions of position and time

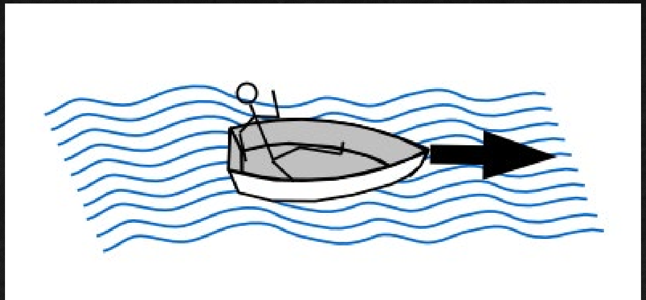
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v})$$



- Lagrangian: move with the fluid
  - Fluid quantities are functions of initial position and time

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{v}$$

  - Convective derivative: $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla$



Lagrangian form of hydro equations

- Continuity equation

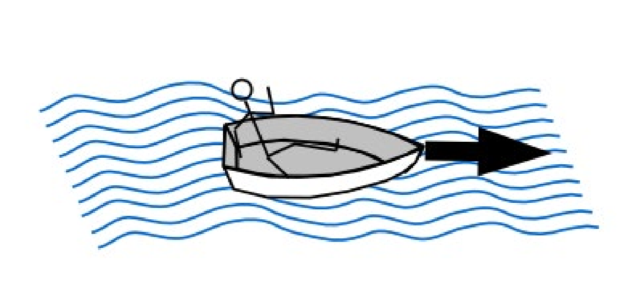
$$\frac{D\rho}{Dt} = -\rho\nabla \cdot \vec{v}$$

- Euler's equation

$$\rho\frac{D\vec{v}}{Dt} = -\nabla P$$

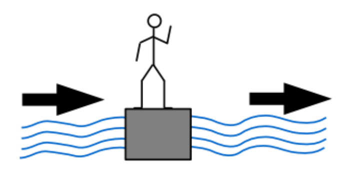
- Energy equation

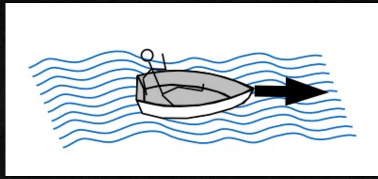
$$\rho\frac{D\epsilon}{Dt} = -P\nabla \cdot \vec{v}$$

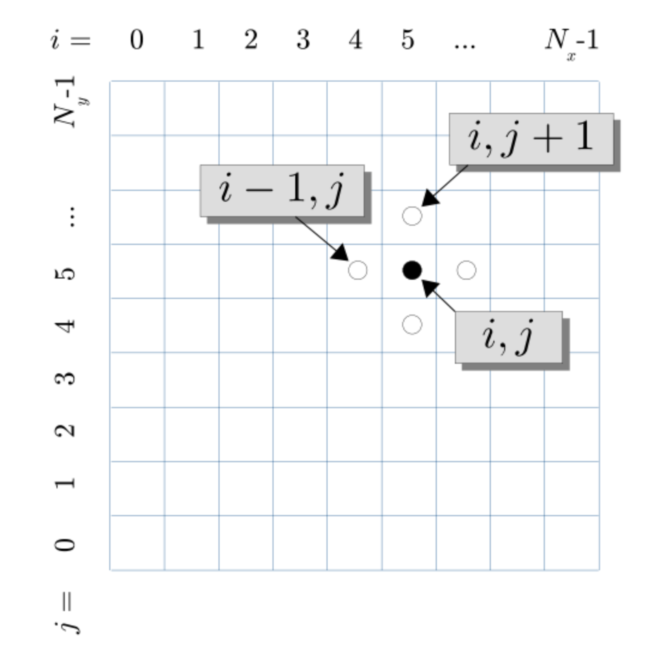


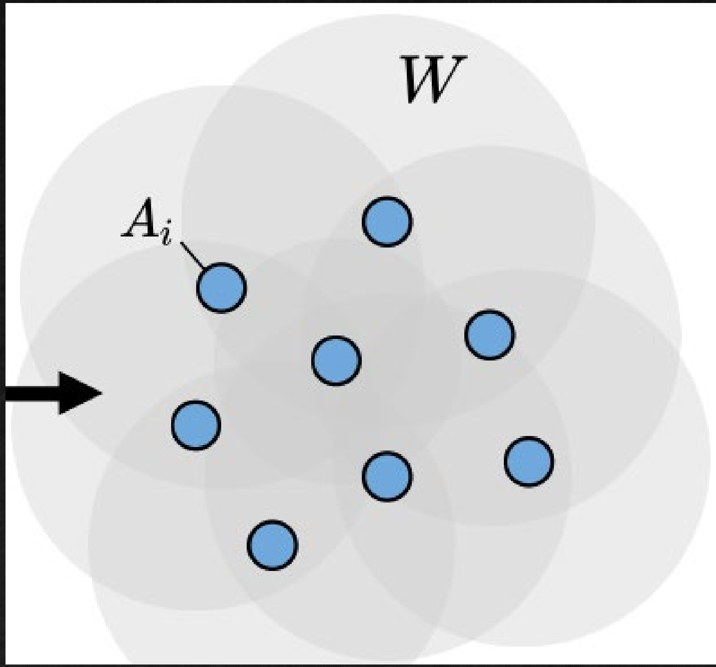
Eulerian vs Lagrangian

- To numerically solve a partial differential equation, we must discretize the system

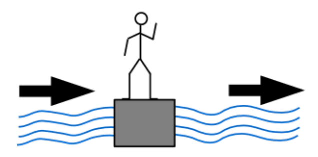








Eulerian (grid) description

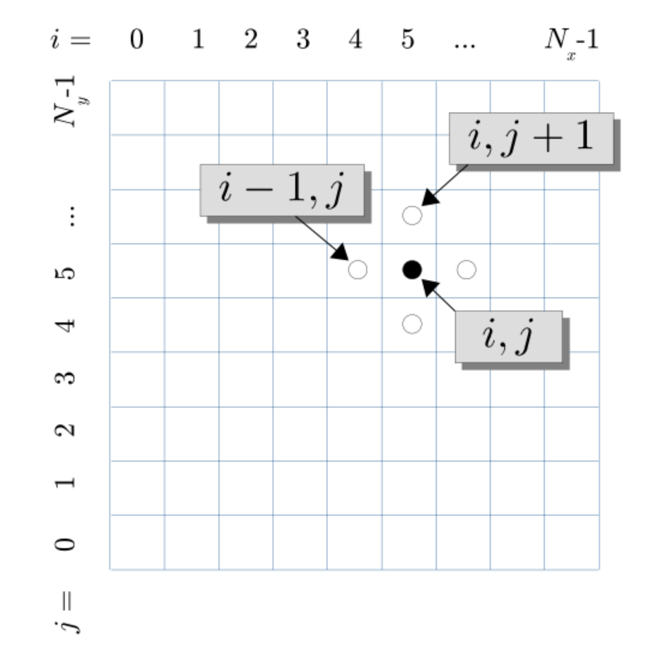


- Finite differencing: Given a fixed grid, we can estimate its derivative
- However there are many different ways with associated numerical errors and instabilities
- Take a Taylor expansion and solve for the derivative

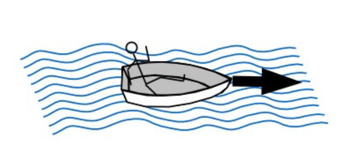
$$q(x) = q(x_i) + q'(x_i)(x - x_i) + \frac{1}{2} q''(x_i)(x - x_i)^2 + \ \ldots$$

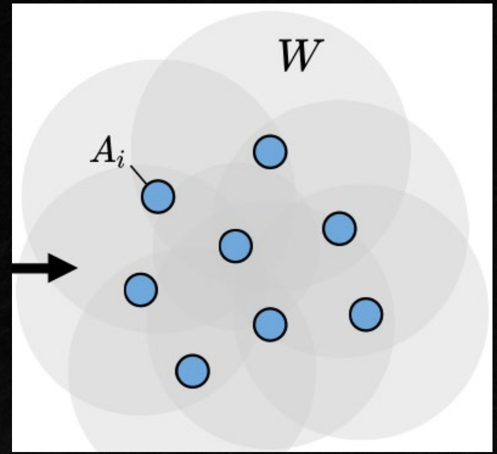
- Forward differencing (1st order accurate)

$$q'(x_i) = \frac{q(x_{i+1}) - q(x_i)}{\Delta x} + O(\Delta x)$$



Lagrangian (particle) description

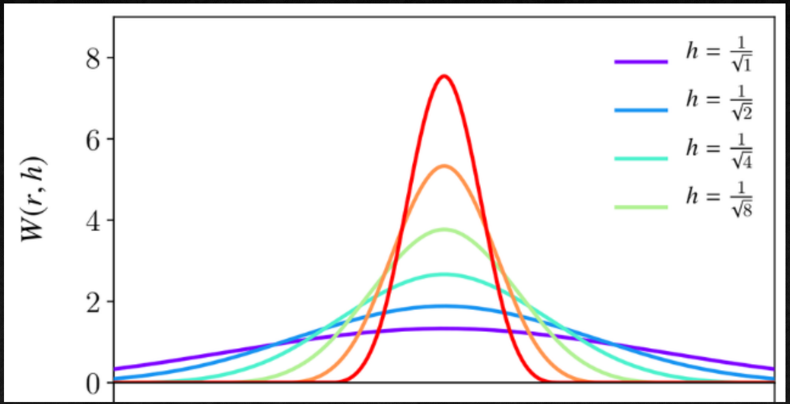


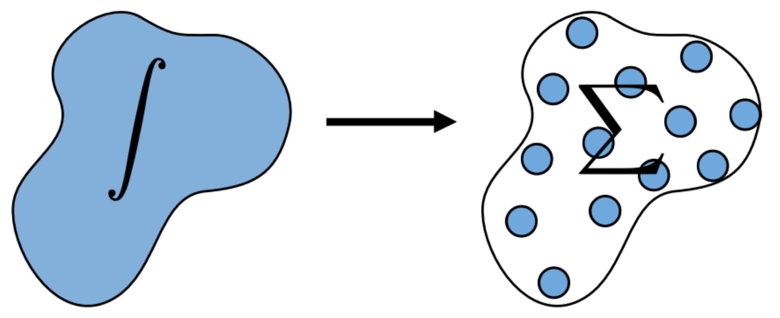


- Smoothed particle hydrodynamics (SPH)
- Kernel smoothing → continuous approximation
  - Usual choice: cubic spline
- Spread the particle's mass to its surrounding volume
- Quantities (A) are weighted averages among N nearest neighbors

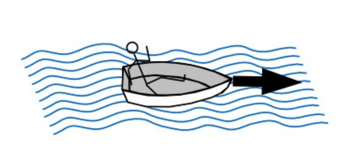
$$\langle A(x_i)\rangle = \int \frac{A(x')}{\rho(x')} W(x_i - x', h)\, \rho(x') dV'$$

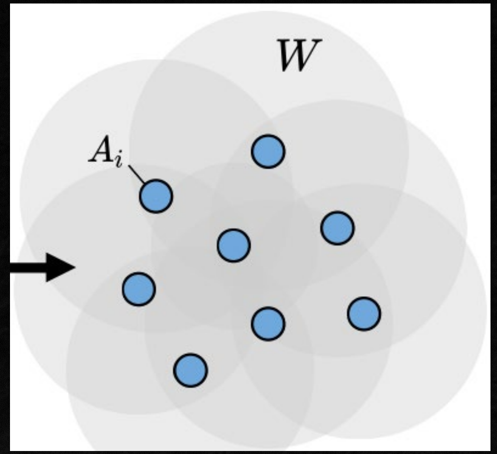
$$\approx \sum_j^N A_j \frac{m_j}{\rho_j} W(x_i - x_j, h)$$





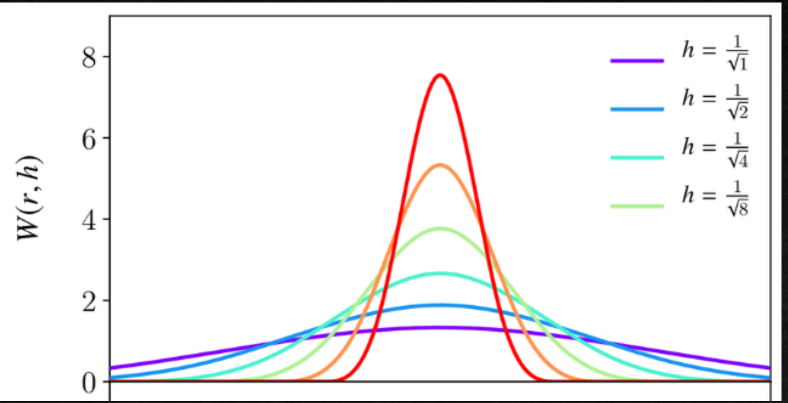
Lagrangian (particle) description



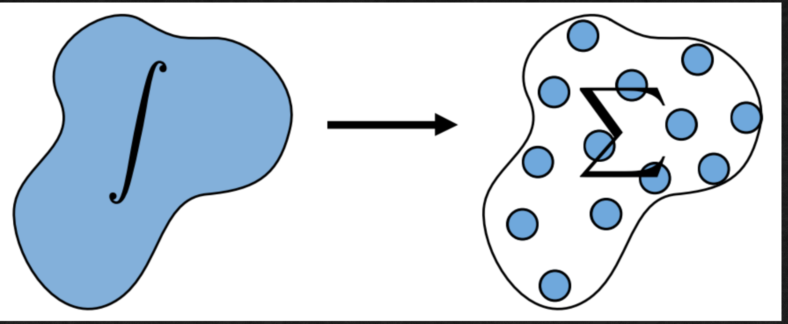


- Derivatives: most simple method is to take the direct discretization of the field (particles)

$$\nabla A_i \approx \sum_j A_j \frac{m_j}{\rho_j} \nabla W_{ij}$$



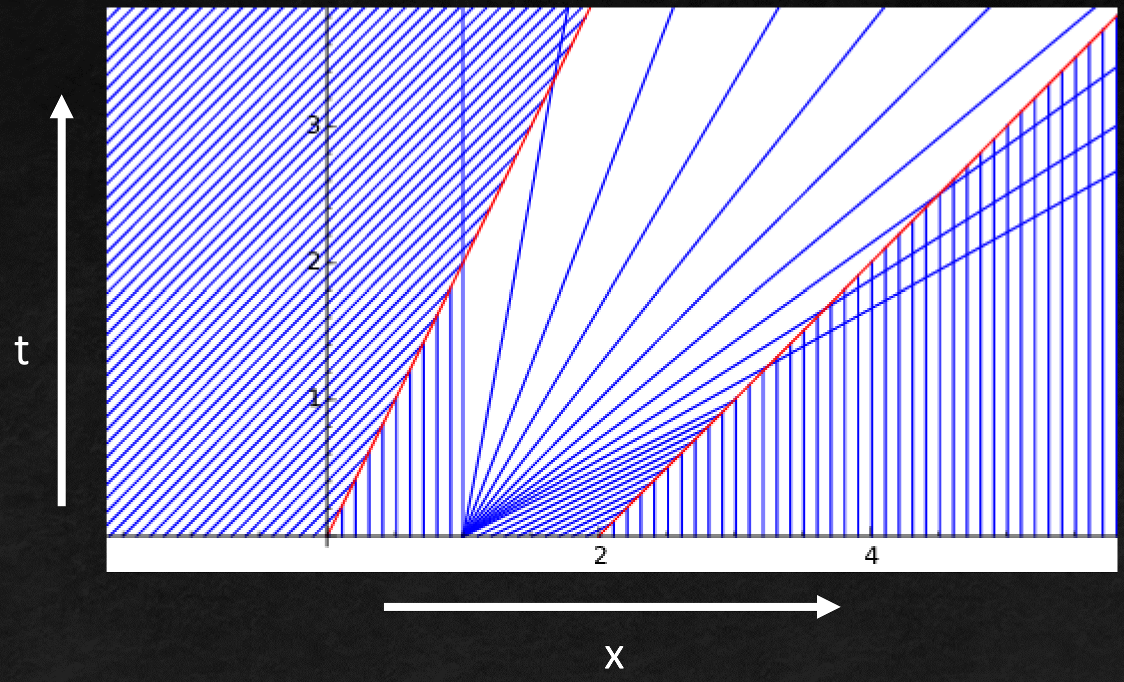
- However this leads to numerical instabilities
- Stability can be recovered from an error analysis, correcting for it (outside the scope of this class)
  - SPH Difference formula
  - Symmetric formula



Shocks: Riemann Problem

- Can solve a PDE with the method of characteristics
- This method creates a set of curves along which the PDE simplifies to an ODE

- These curves represent the path of a gas parcel, given an initial position
- In the example to the right, one sees different regions
  - Constant velocity
  - Static
  - Diverging flow

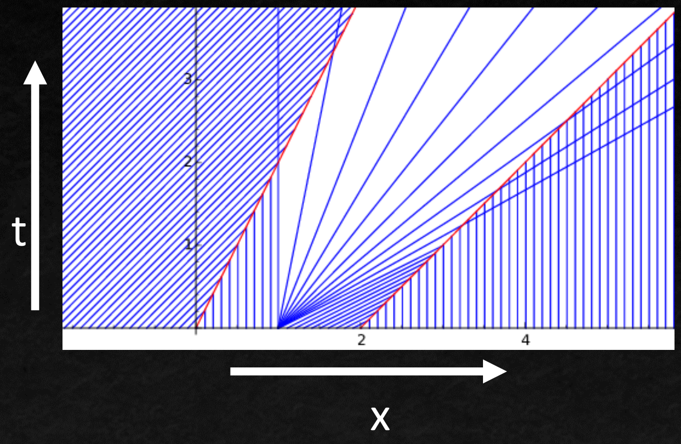


Shocks: Riemann Problem

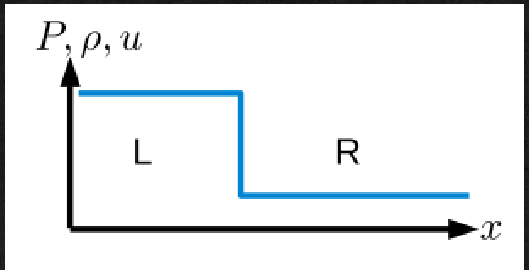
- Where the characteristics intersect, the solutions become multi-valued

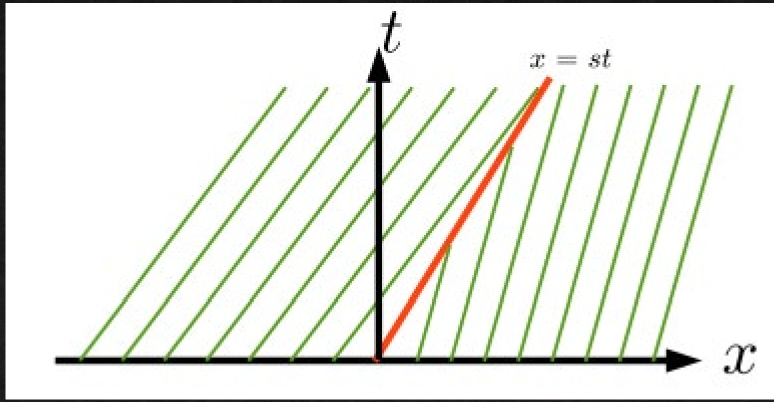
→ Shocks

- These boundaries are denoted in red



- The lower figure shows a simple system with a single shock
  - Moves at a velocity s
  - Left / right states



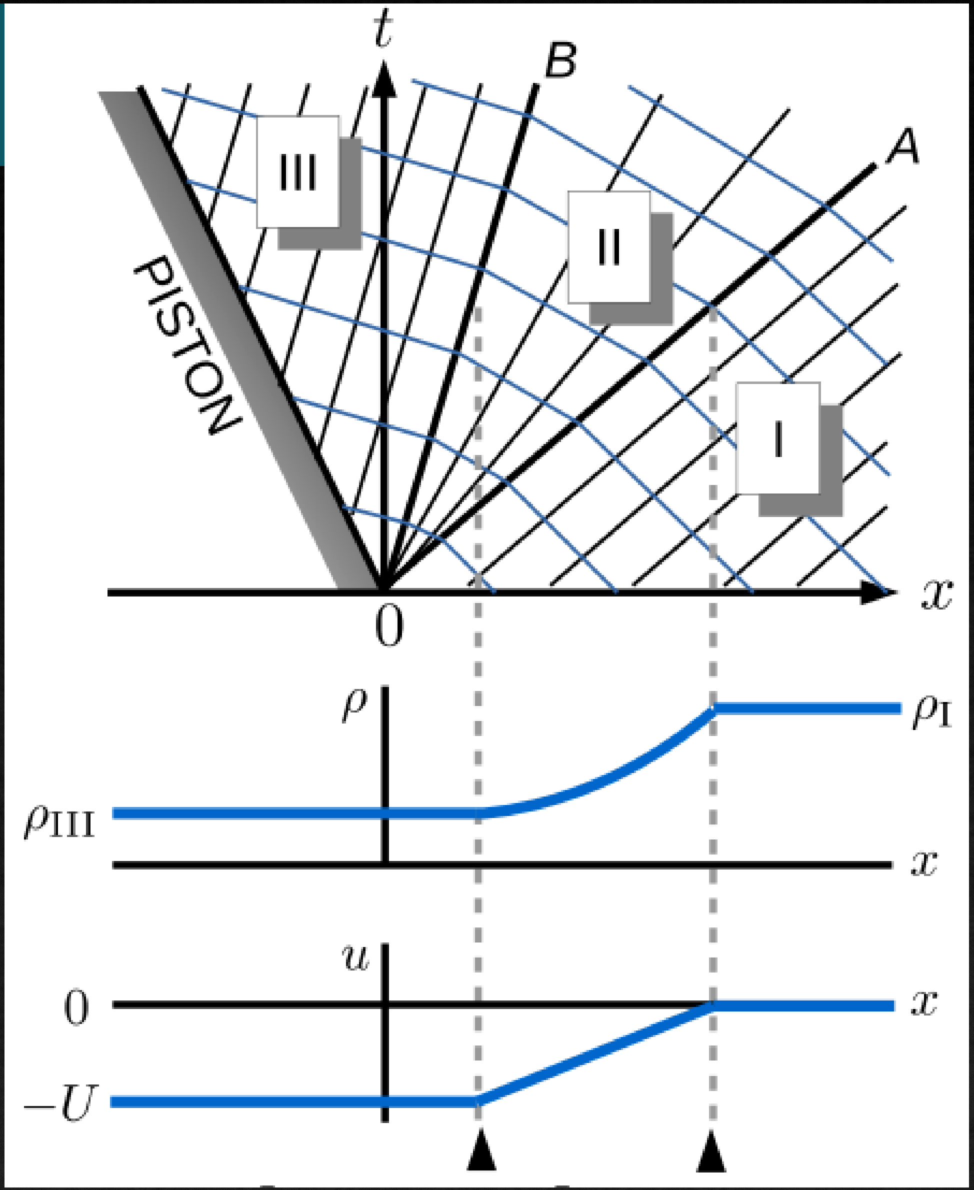


Shocks: Riemann Problem

- In addition to shocks, there are rarefaction waves
- This is a non-linear wave but with a finite width

- Imagine a 1D piston that accelerates quickly to a constant velocity –U away from the fluid to its right

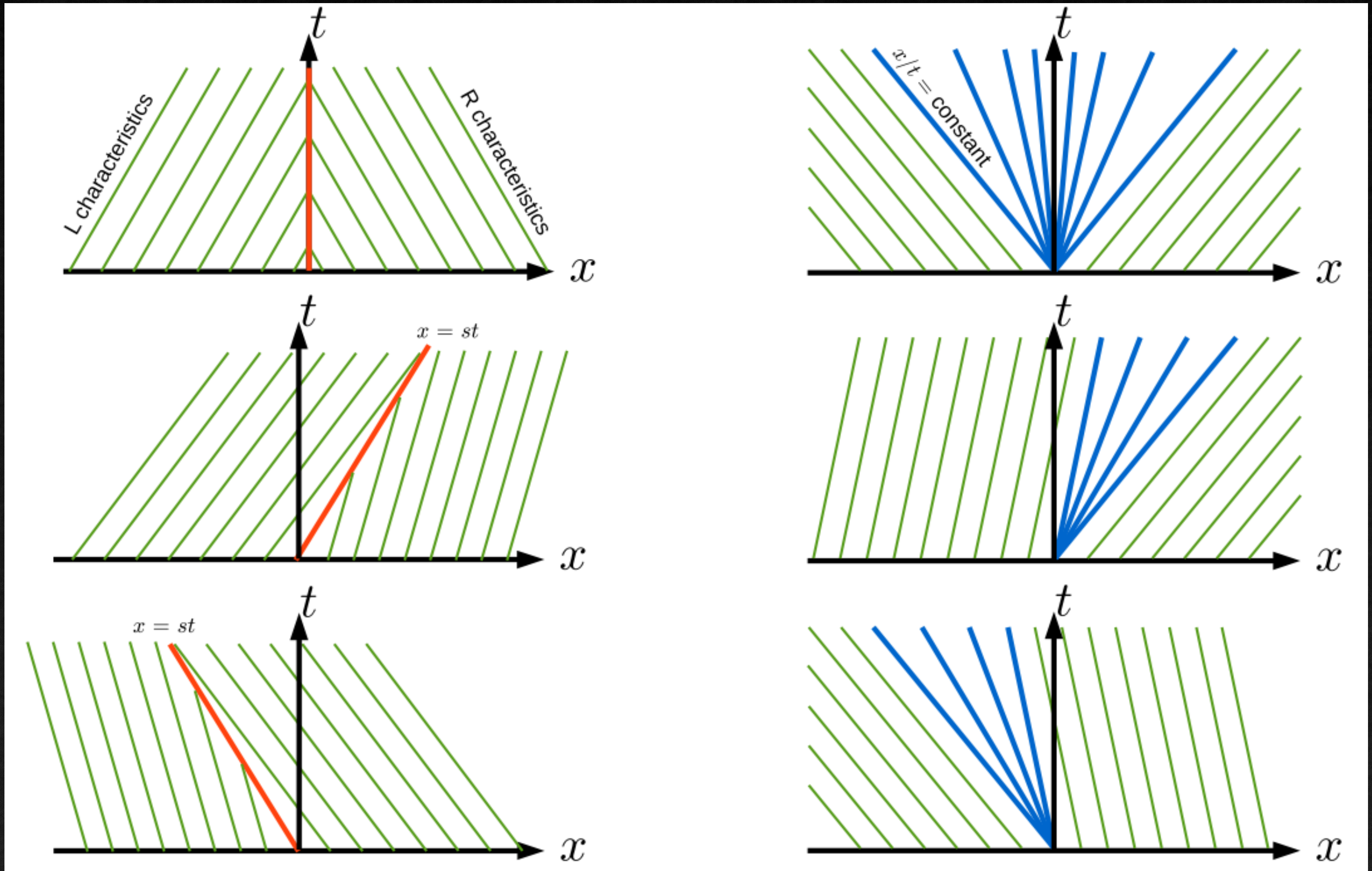
- Region I: undisturbed flow
- Region II: rarefaction fan (A = “head”, B = “tail”)



Shocks: Riemann Problem

Shocks

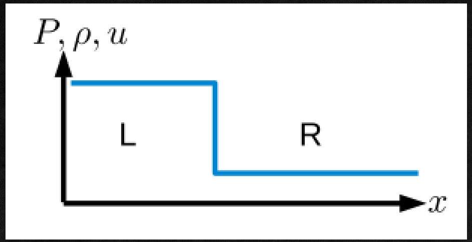
Rarefactions

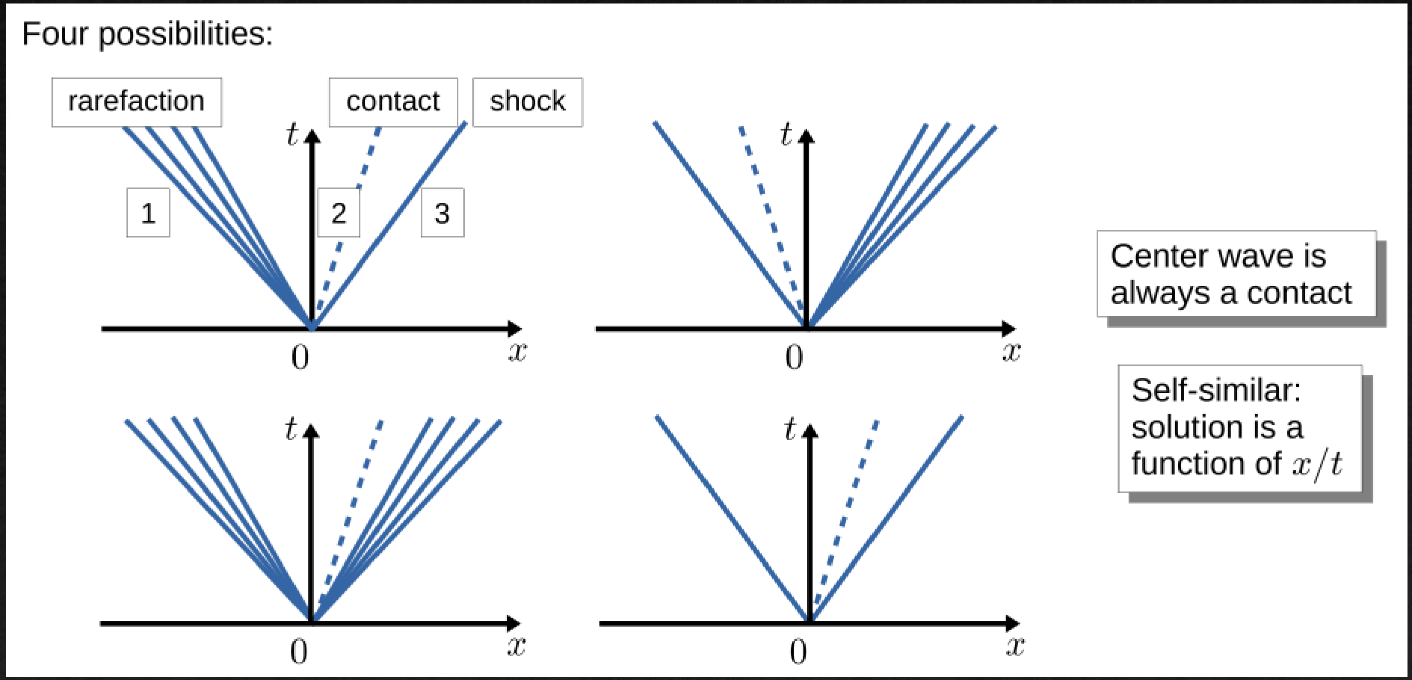


Shocks: Riemann Problem

- Riemann problem: arbitrary finite 1D jump in density, pressure, and velocity
- Need to solve for the Left and Right states

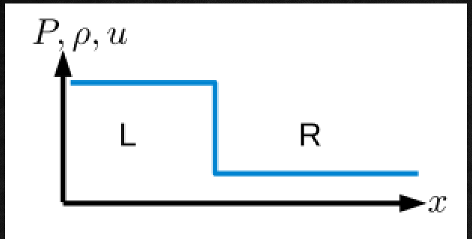
- Solution: decompose the sum of the waves from each of the three characteristic families
- Combine the time evolution of each

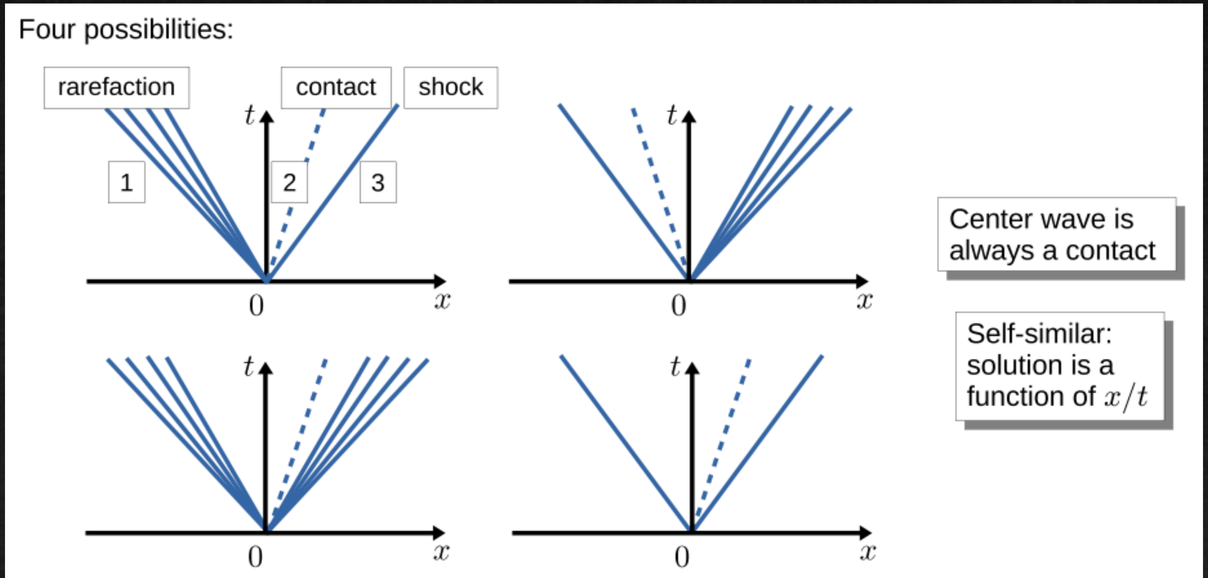




Shocks: Riemann Problem

- Contact discontinuity: associated with the "0" characteristic and move with the fluid speed
  - Density is discontinuous
  - Pressure and transverse velocities are continuous
  - Parallel velocities may be discontinuous (shear flow)





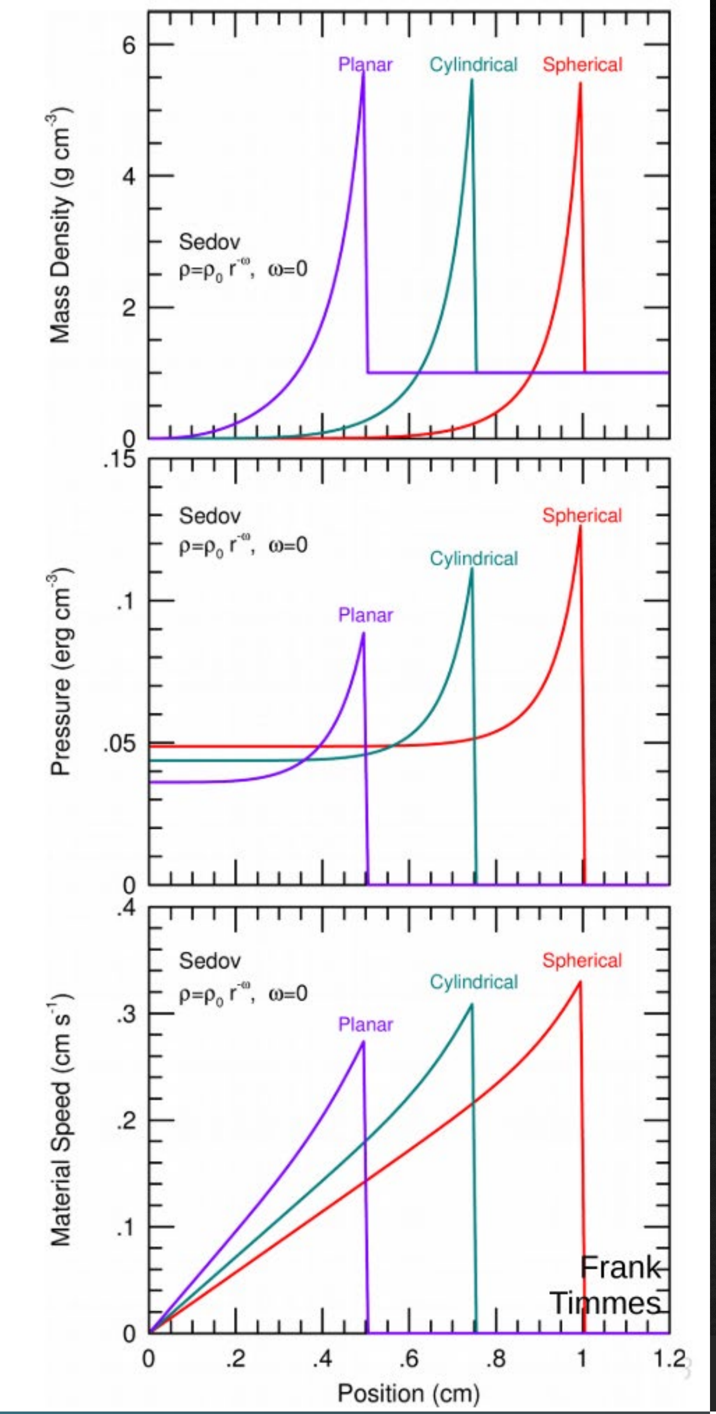
Shocks: Sedov test

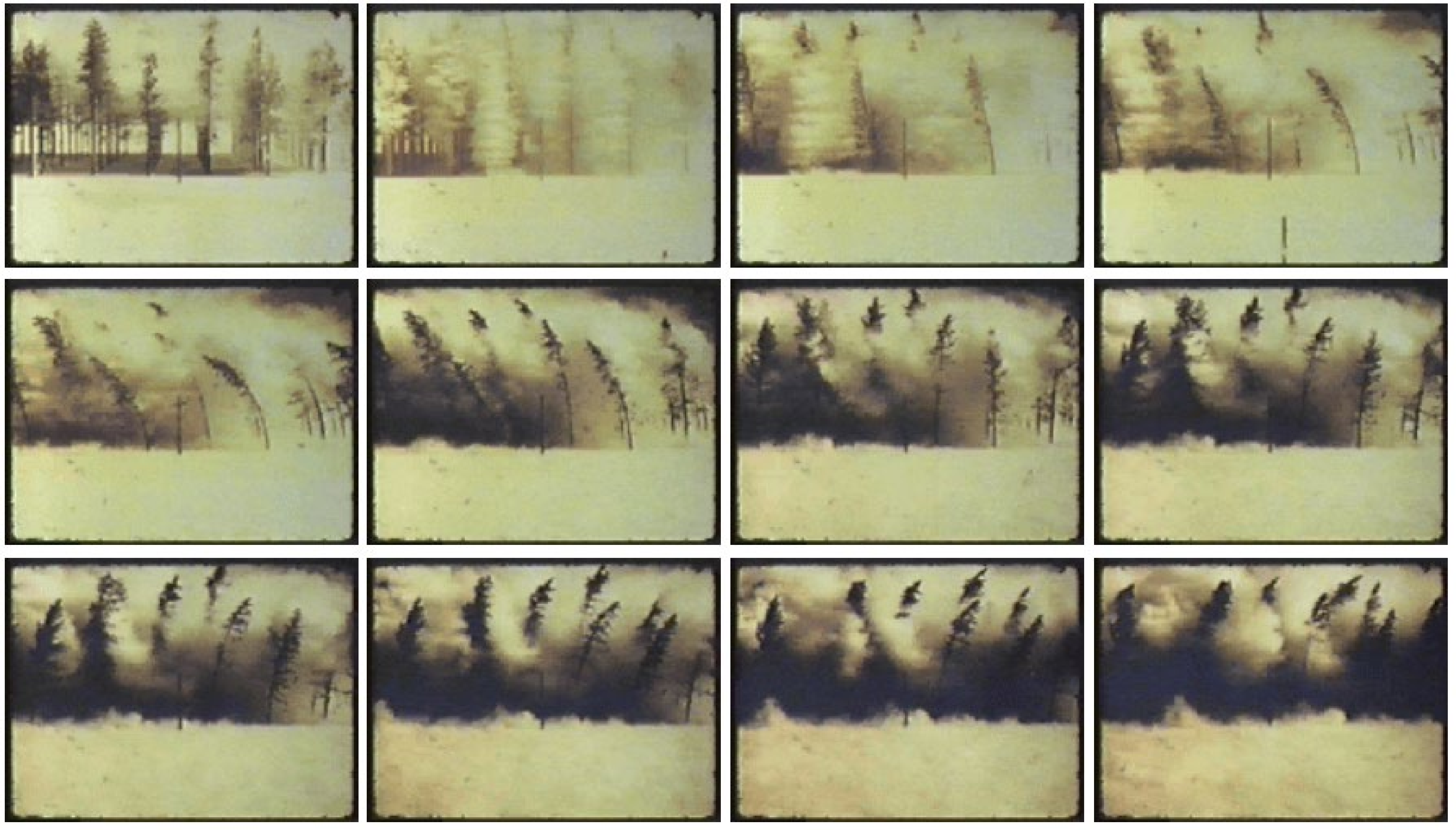
- Point explosion with energy E expands into a uniform medium with density ρ_1 and negligible pressure P_1

- Shock position solution is self-similar

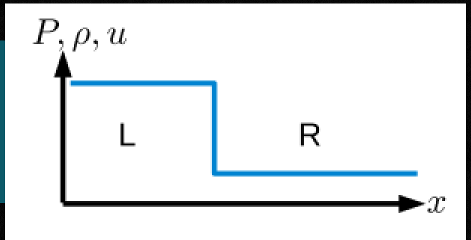
$$R(t) = \beta \left(\frac{Et^2}{\rho_1} \right)^{1/5}$$

- Shock velocity: $u_1 = dR/dt$
- Post-shock quantities
  - $\rho_2 = constant$
  - $u_2 - u_1 \propto t^{-3/5}$
  - $P_2 \propto t^{-6/5}$



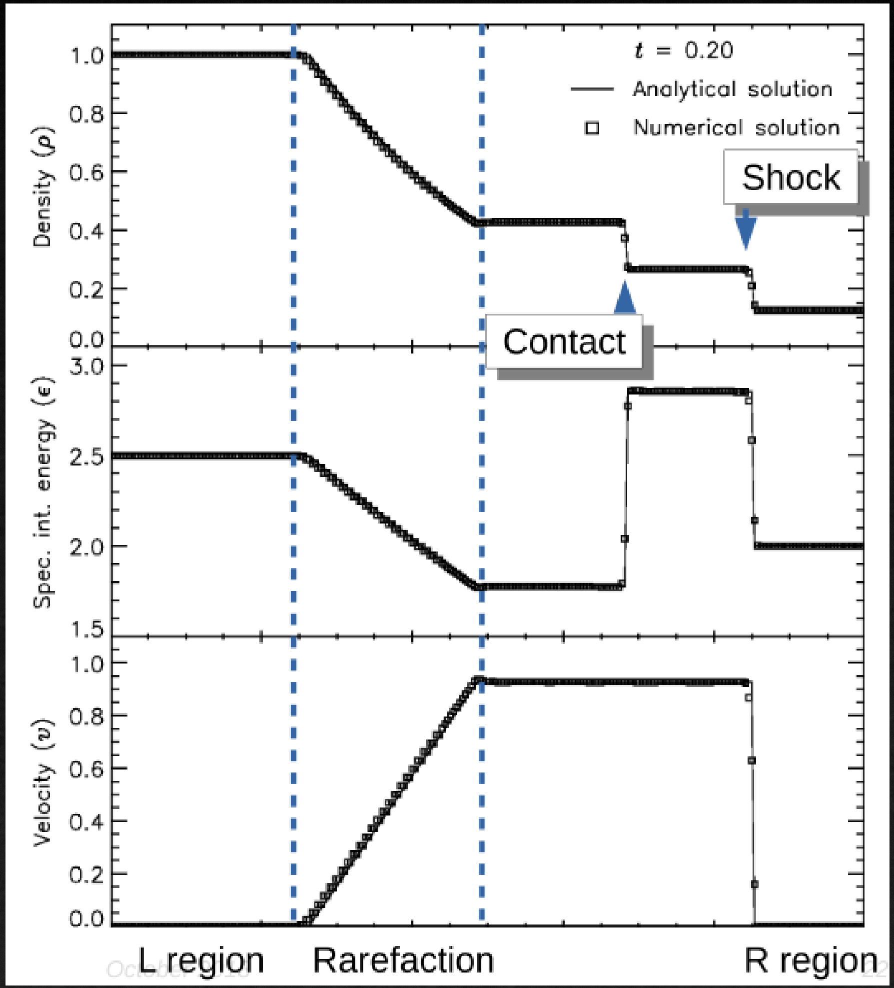


Shocks: Sod test



- Sod (1978) shock tube: standard test problem
- Fluid initially at rest
- $\gamma = 1.4$
- Left side: $\rho = 1, P = 1$
- Right side: $\rho = 0.125, P = 0.1$

- Displays all three types of non-linear waves
  - Shocks
  - Rarefaction waves
  - Contact discontinuities



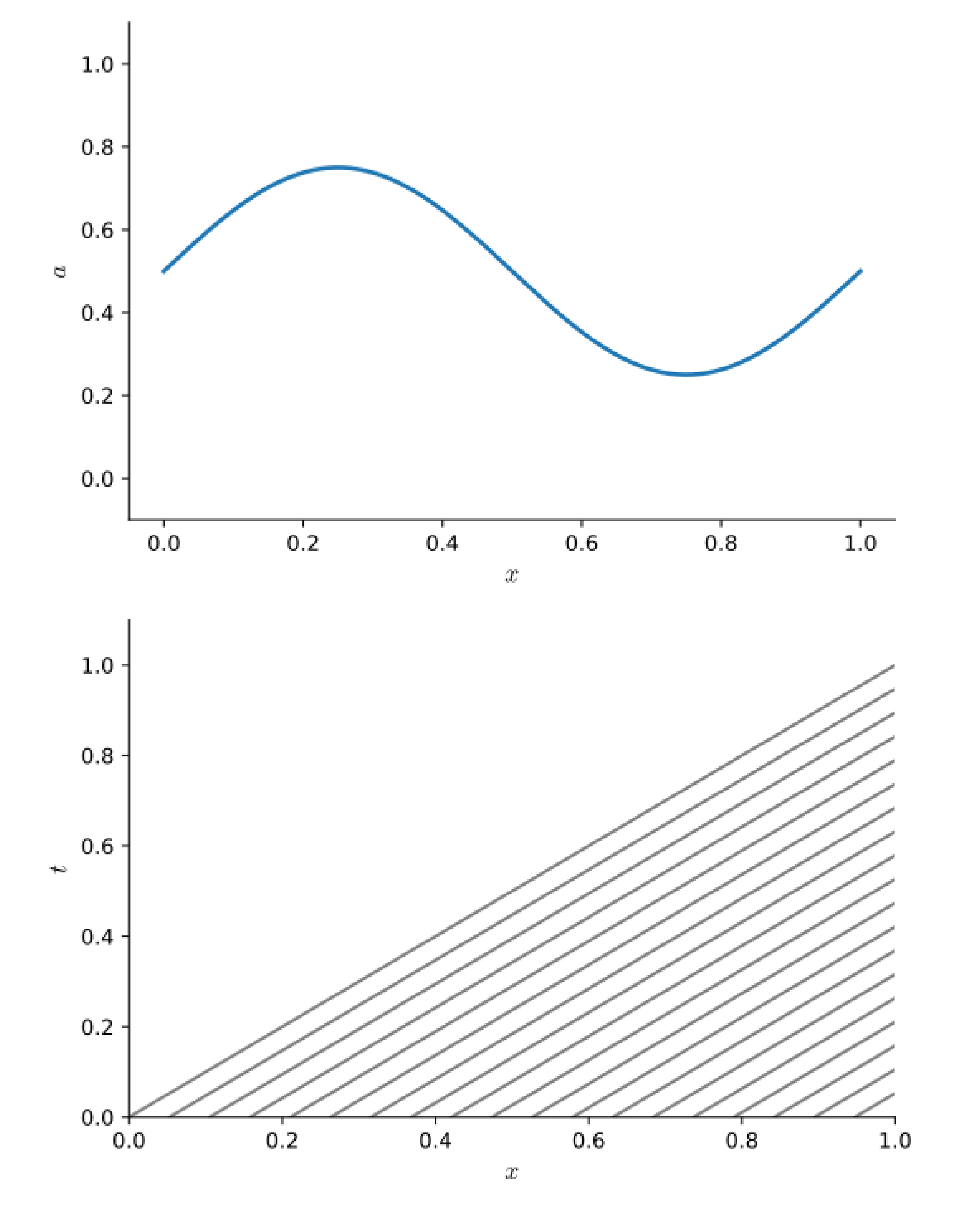
Fluid advection

- Advection equation:

$$\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0$$

$$\frac{\partial q}{\partial t} + \frac{df}{dq}\frac{\partial q}{\partial x} = 0$$

- df/dq is the wave speed
- Theoretically, any pattern should be advected without any shape change as it moves
- Numerical stability → any wave should not propagate farther than a cell width in a given timestep



Fluid advection

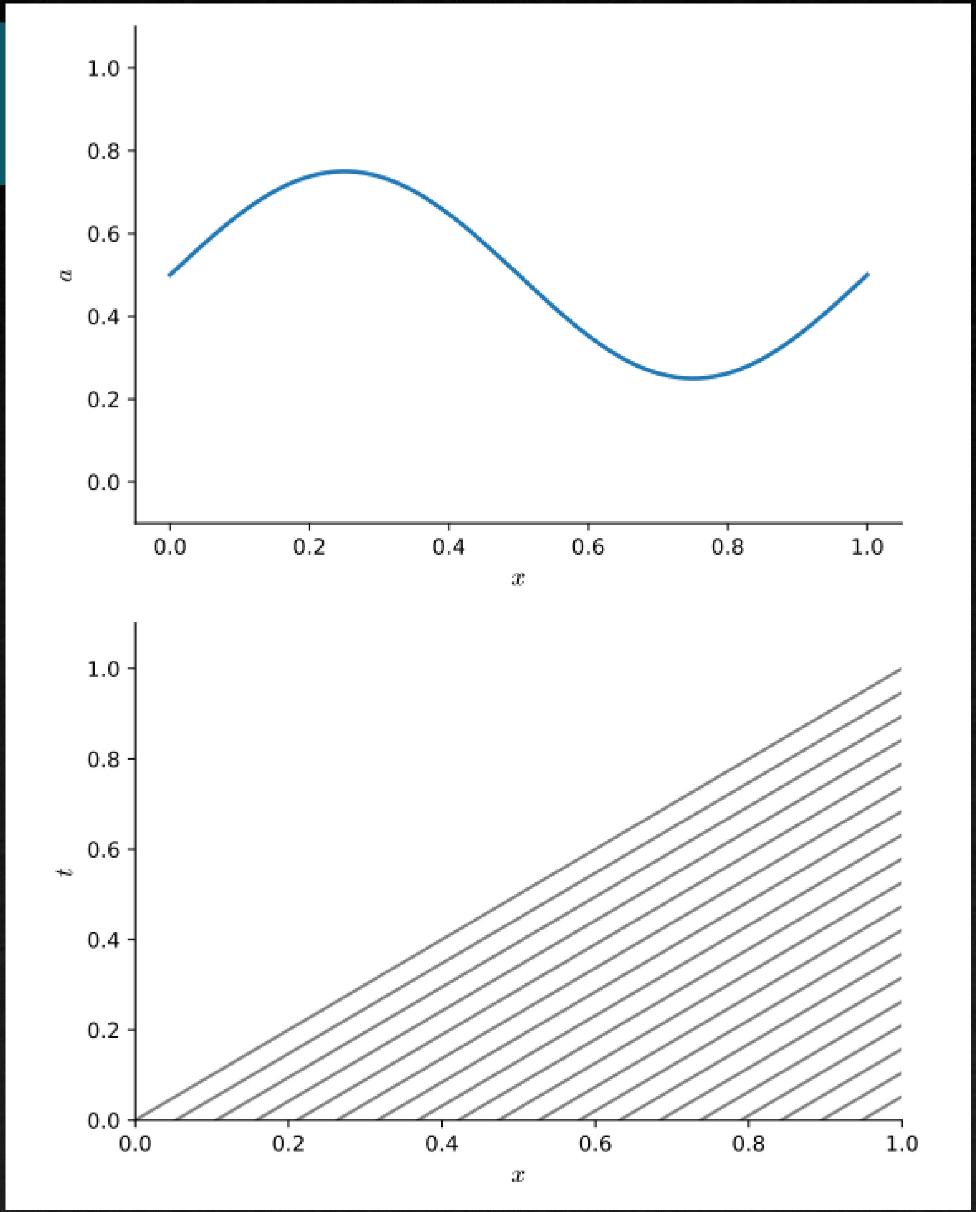
- Timestep restriction: information must not travel farther than one zone per timestep

$$\Delta t \leq \frac{\Delta x}{u}$$

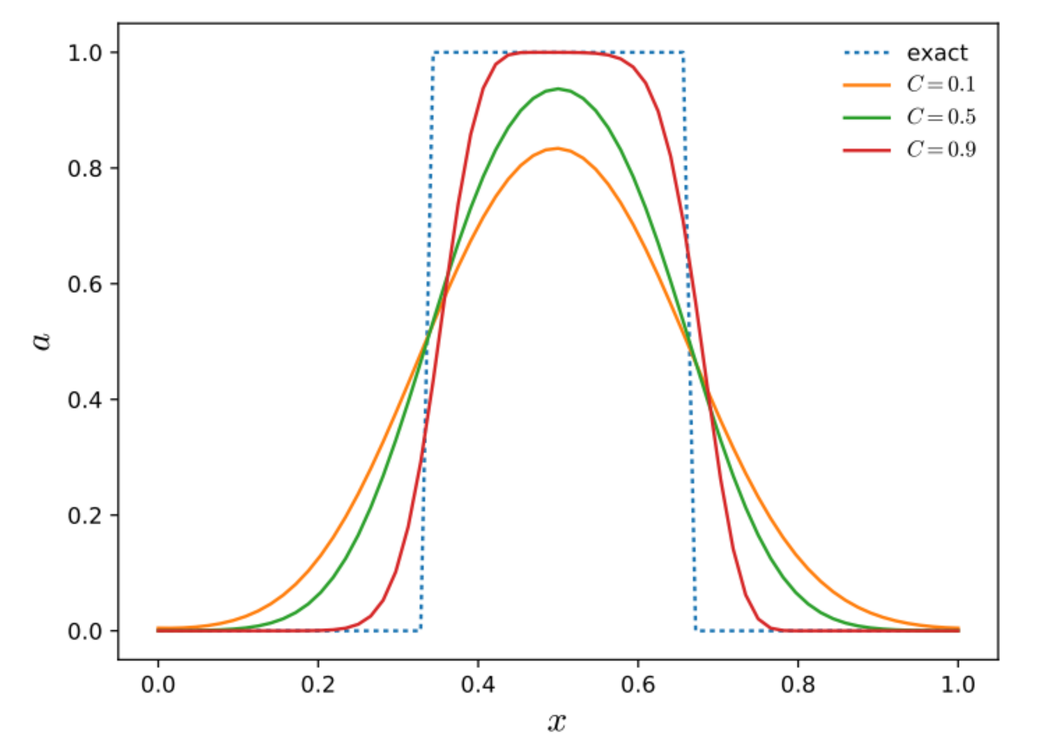
- This is known as the Courant-Friedrichs-Lewy (CFL) condition
- The CFL number is defined as

$$\mathcal{C} = \frac{u\Delta t}{\Delta x} \leq 1$$

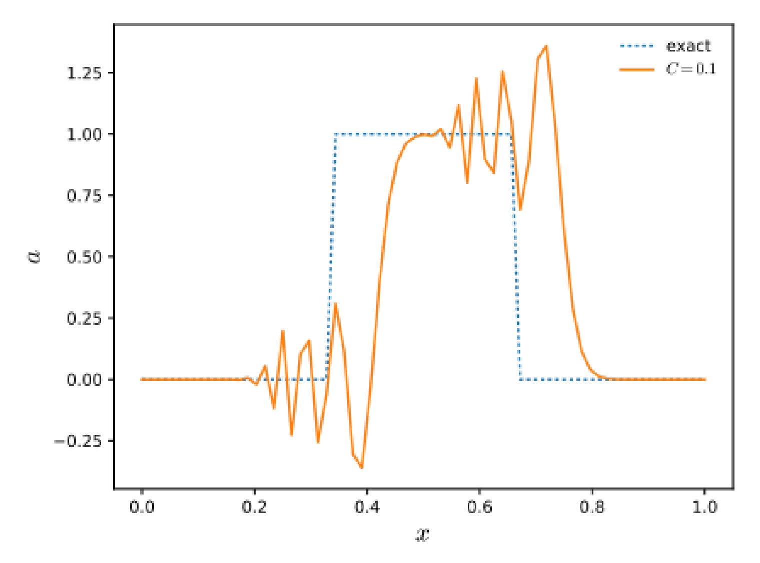
- This is a parameter in simulations and is usually set to be ≤ 0.7

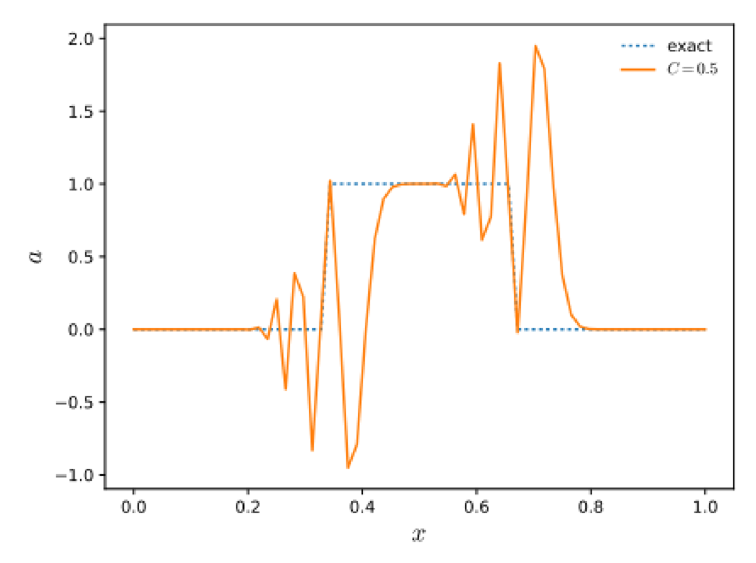


Fluid advection test



- Consider a square wave moving at velocity *u* with periodic boundary conditions
- At time t = x/u, returns to its starting position
- Basic numerical test for any numerical method
- Tests for numerical diffusion and errors

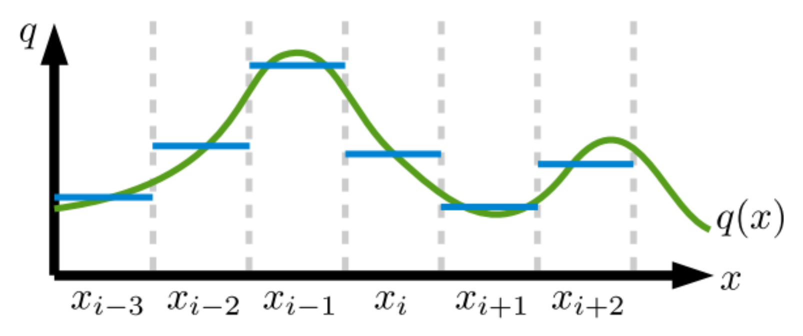




Methods

- Recall that we can approximate the derivatives with finite differencing. For example, forward differencing

$$\frac{dq}{dx} \approx \frac{q_{i+1} - q_i}{\Delta x}$$

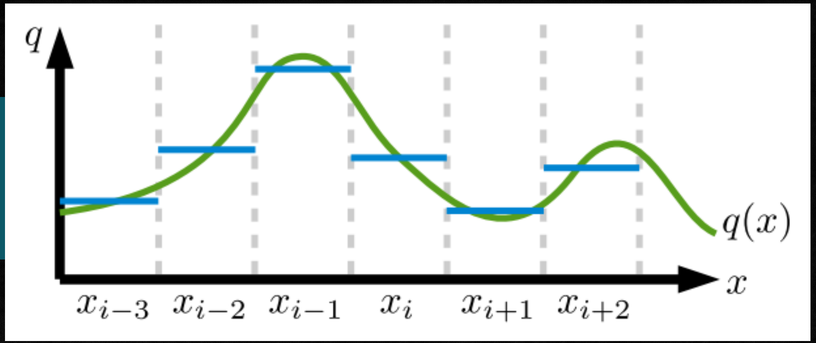


- For the advection equation, we have

$$\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0 \quad \rightarrow \quad q_i^{n+1} = q_i^n - \frac{\Delta t}{\Delta x}\left(f_{i+1/2}^{n+1/2} - f_{i-1/2}^{n+1/2}\right)$$

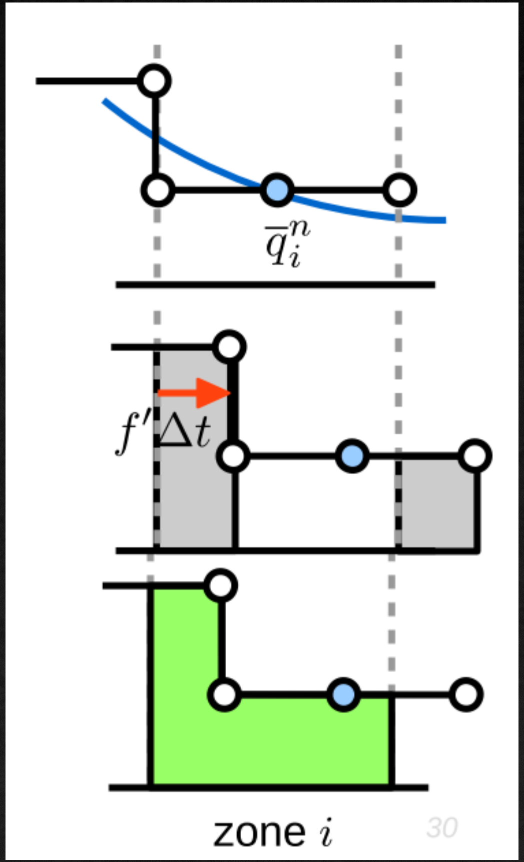
- Here the ½ steps are for better numerical stability → L/R states of a zone

Methods

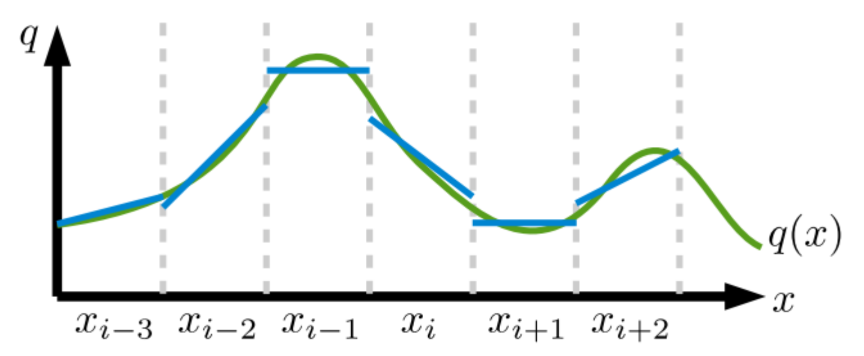


- How to represent a continuous function in a discrete fashion?
- Most simple: piecewise constant
- How to calculate the L/R edges of the zones?

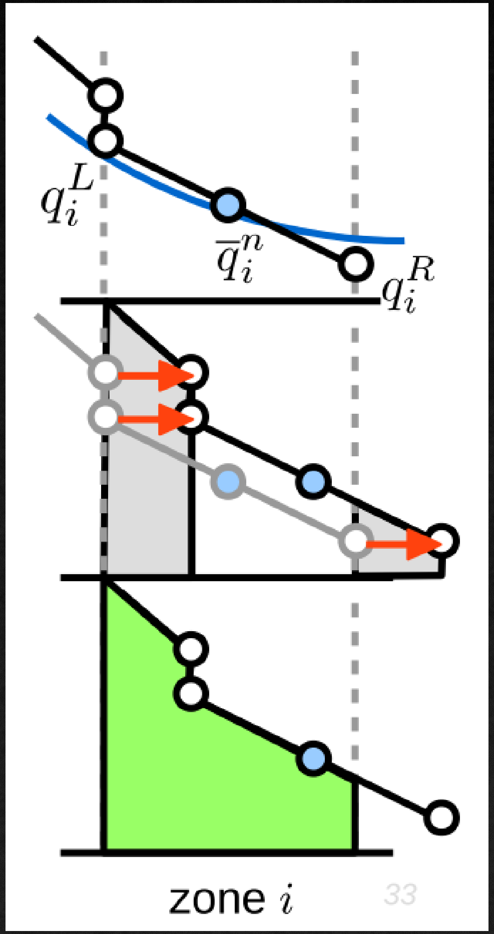
- Reconstruction: approximate solution at the edges
- Evolution: advect the constants forward through Δt
- Averaging: average the new solution over the zones



Methods

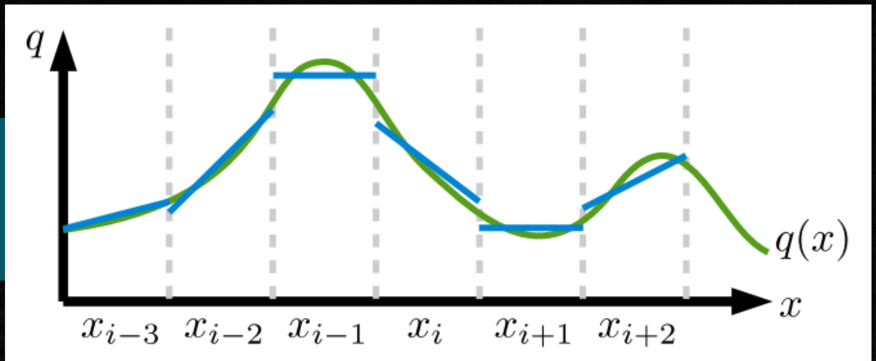


- To the next order, we can approximate the function with a piecewise linear representation

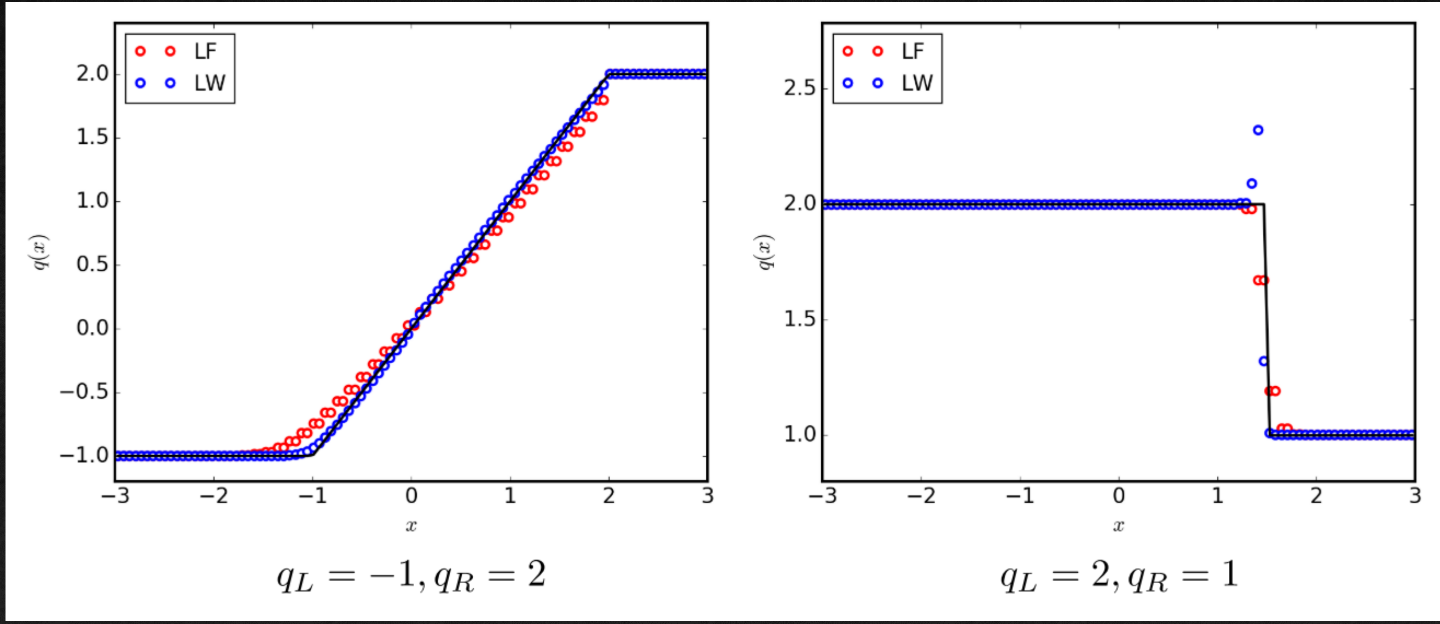


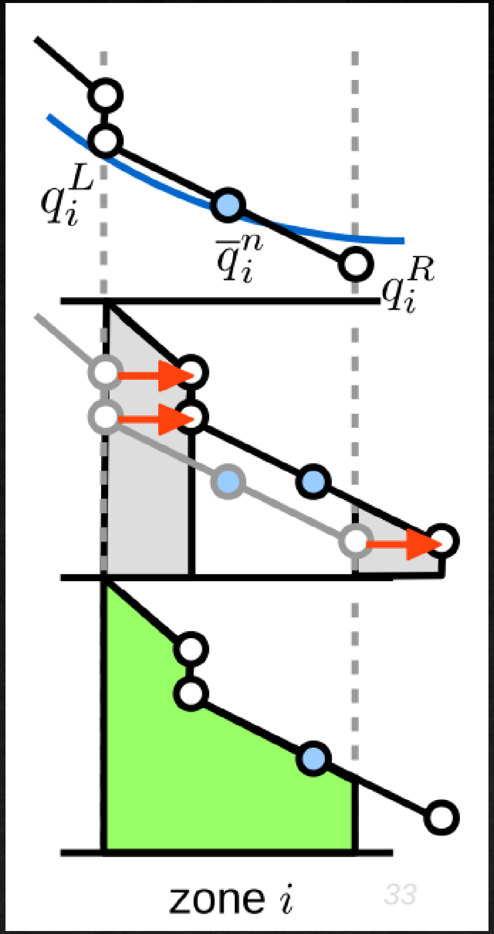
- Reconstruction: compute interpolant slopes
- Evolution: advect the constants forward through Δt
- Averaging: average the new solution over the zones
- Freedom in slope choices
  - Centered difference (Fromm's method)
  - Upwind difference (Beam-Warming method)
  - Downwind difference (Lax-Wendroff method)

Methods

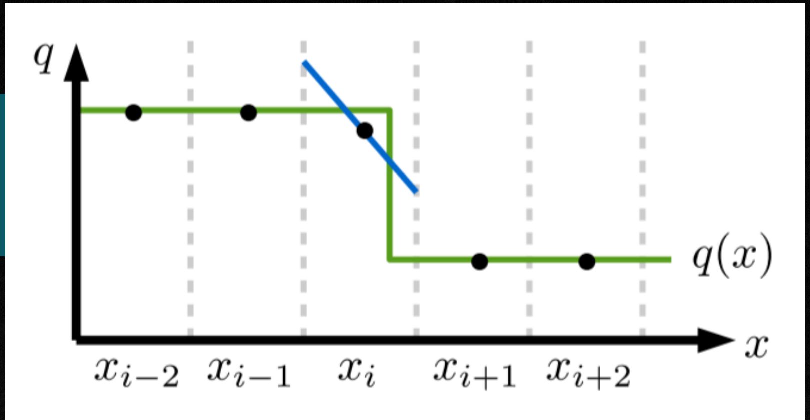


- Example: inviscid Burger's equation $f(q) = q^2/2$
- Lax-Friedrichs (1st order): diffusive, "stair-stepping"
- Lax-Wendroff (2nd order): oscillation at shocks
- Can we do better?





Methods



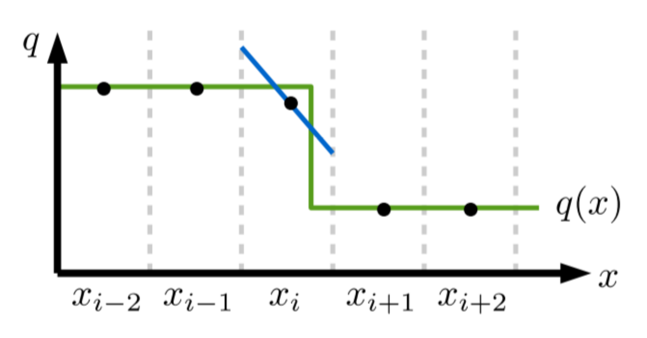
- The slope can be anything as long as

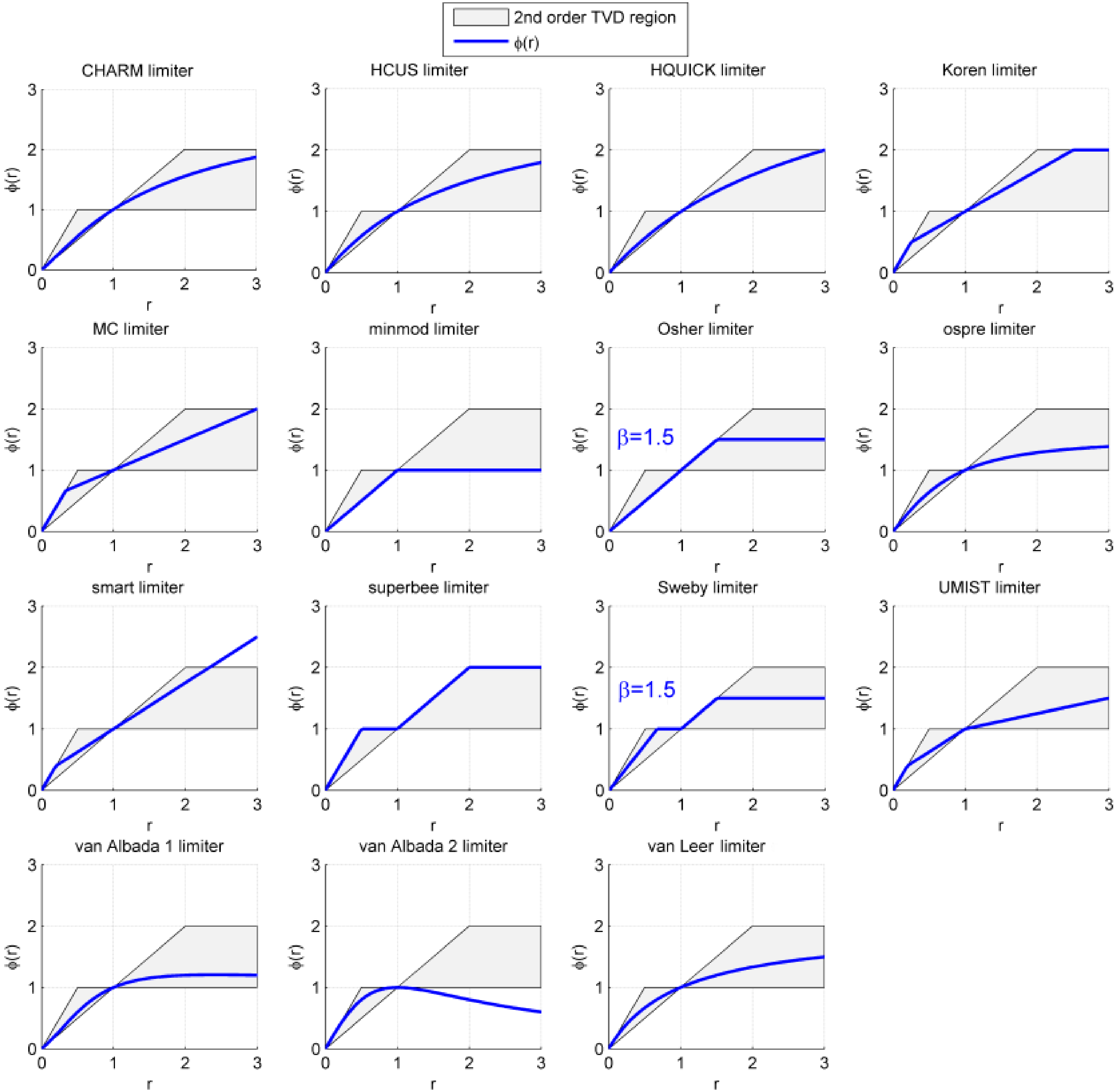
$$\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x,t^n)dx = \bar{q}_i^n$$

- At discontinuities, we should flatten the interpolants to avoid introducing spurious oscillations
- Goal: prevent numerical method from introducing oscillations → maintain monotonicity
- Define total variation: $TV(q) \equiv \sum_i^N |q_i - q_{i-1}|$
- This quantity should never increase → Total variation diminishing (TVD) method

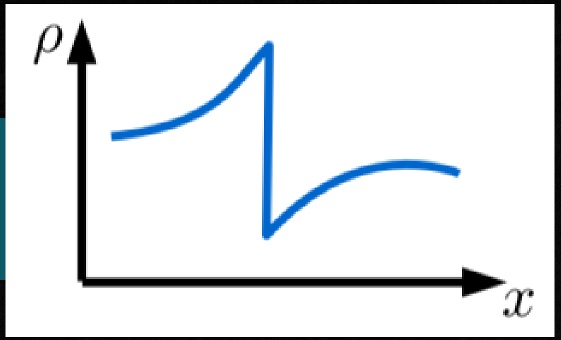
Methods

- We need to modify the slopes σ near discontinuities. Based them on the solution
- Solution: Use a slope limiter function to maintain TVD
- r is the ratio of the forward and backwards slopes



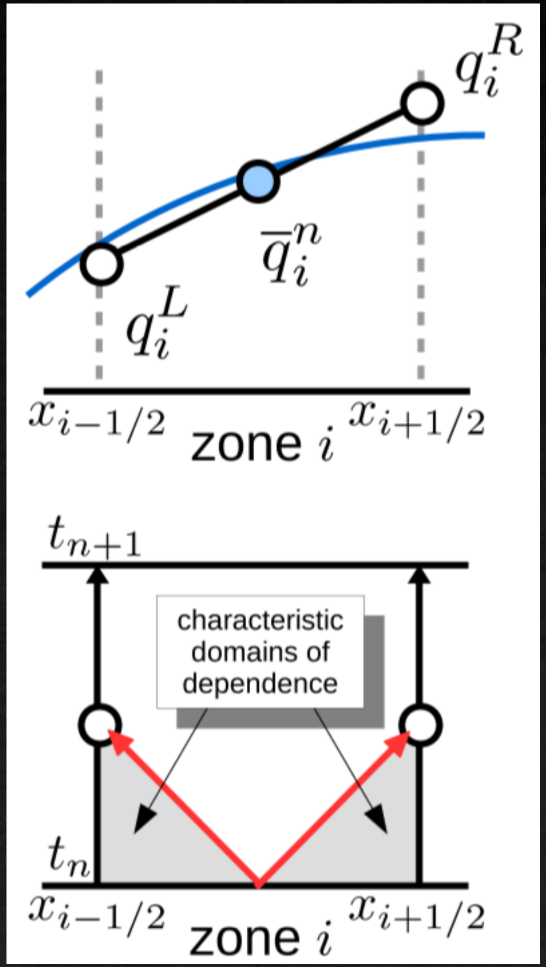


Methods

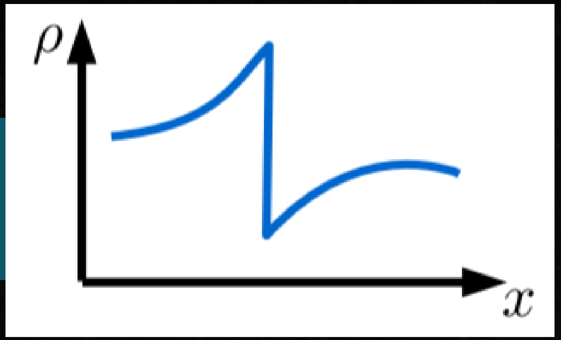


- Godunov's method: solve the Riemann problem at every zone interface
- MUSCL (Monotone Upwind Scheme for Conservation Laws; van Leer 1979): solve ordinary Riemann problem with input states modified to include characteristic information

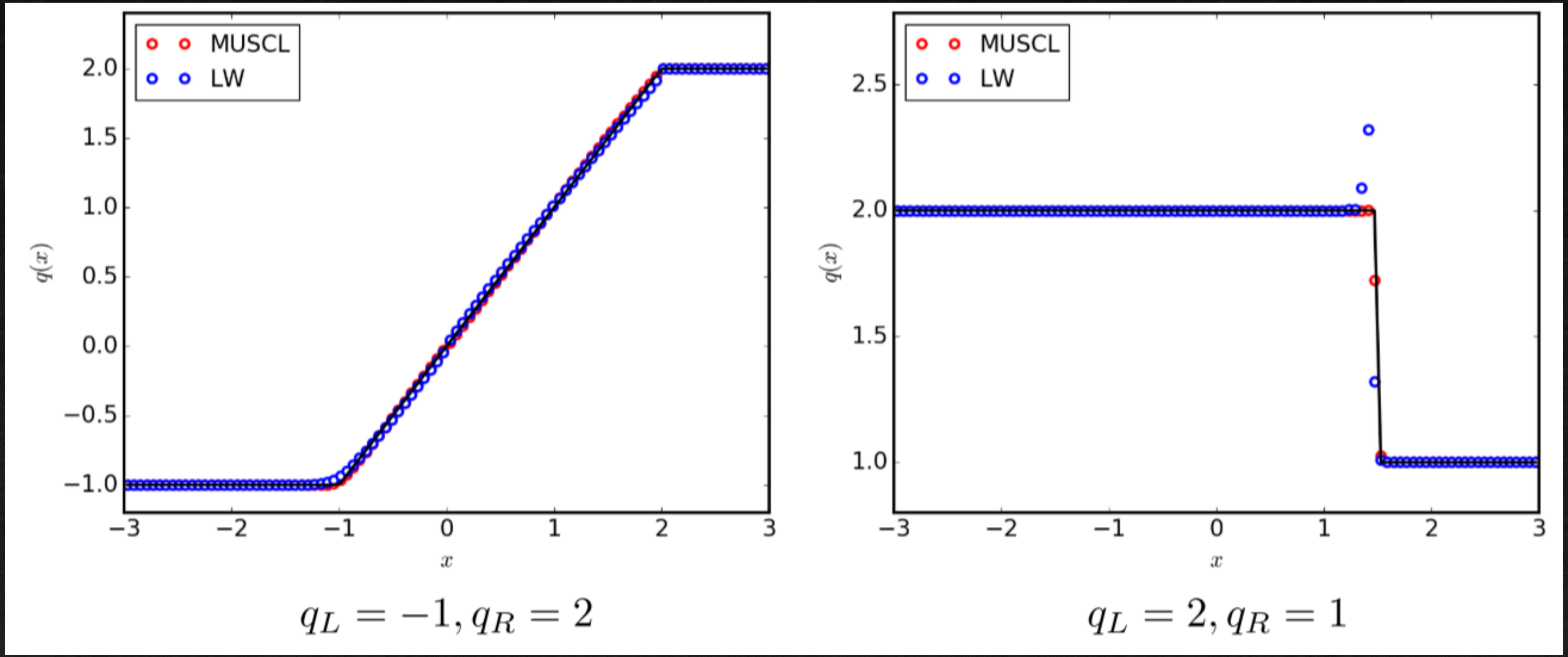
- Reconstruction: use slope limiter
- Characteristic tracing: Use limiter and wave speeds
- Evolution: Solve the Riemann problem given L/R states

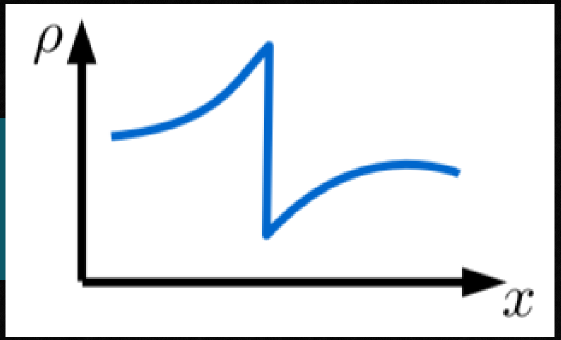


Methods



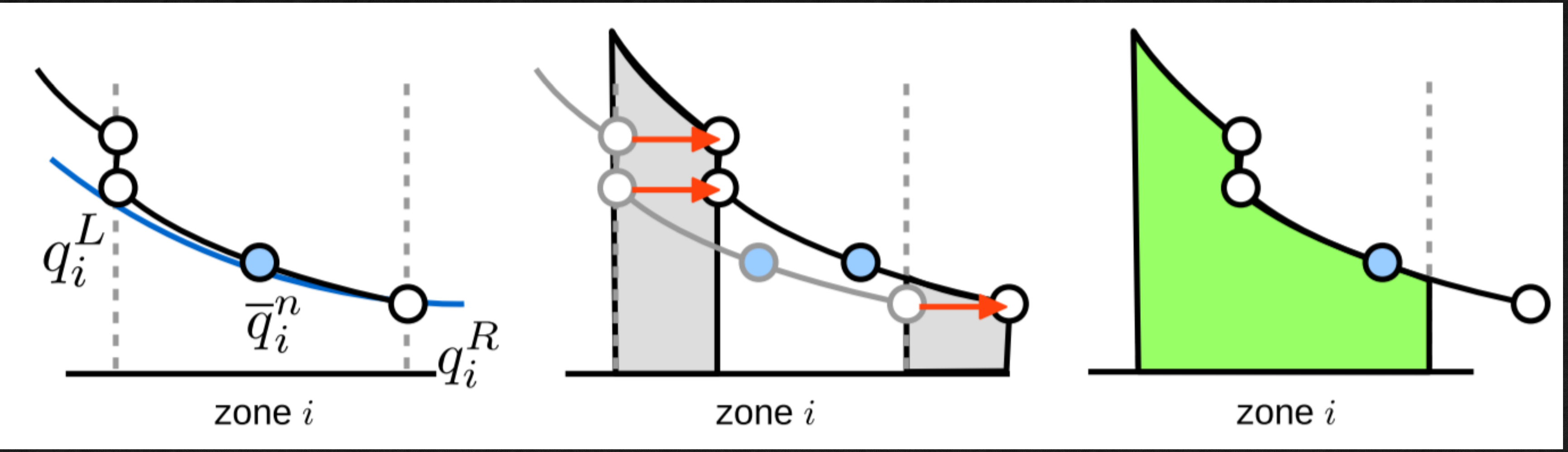
- Example: inviscid Burger's equation, $f(q) = q^2/2$
- Shock oscillation eliminated, 2nd order accurate





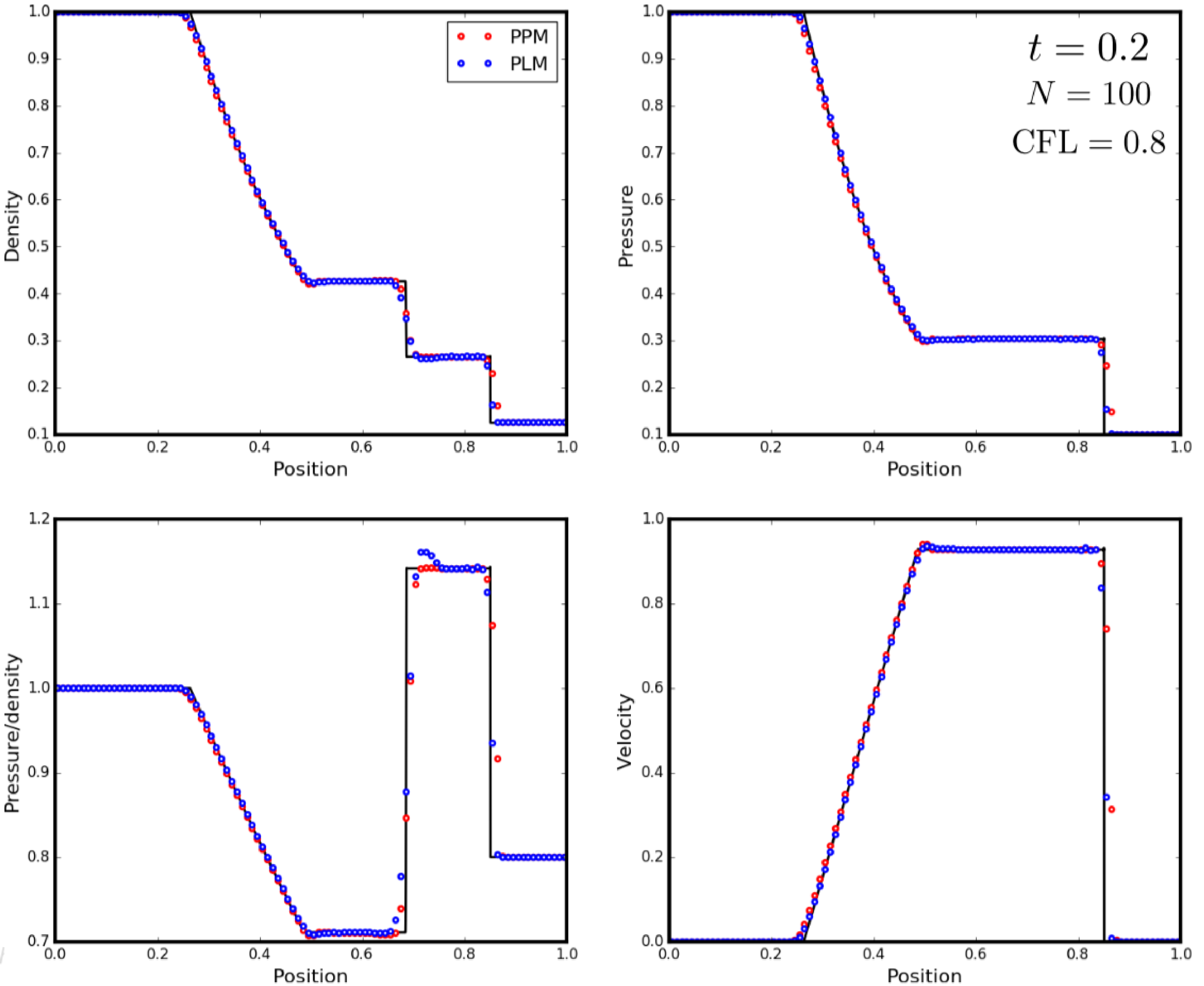
Methods

- Extensions to MUSCL to make third order accurate
  - Piecewise parabolic reconstruction
  - Extrema removal
  - 2nd order time integration
  - Artificial dissipation for strong shocks



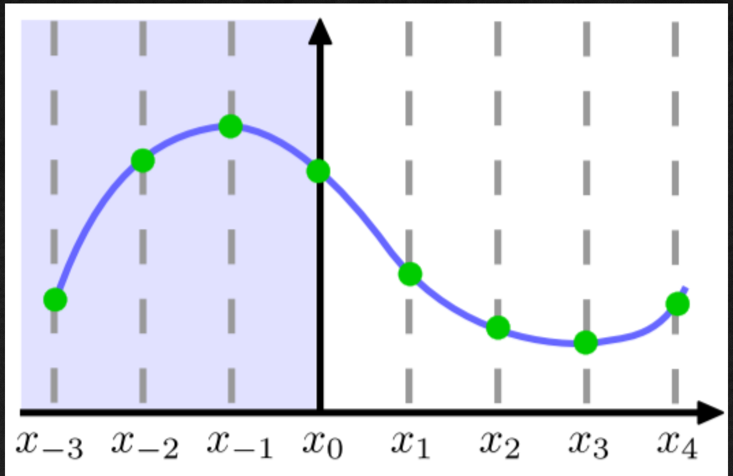
Methods

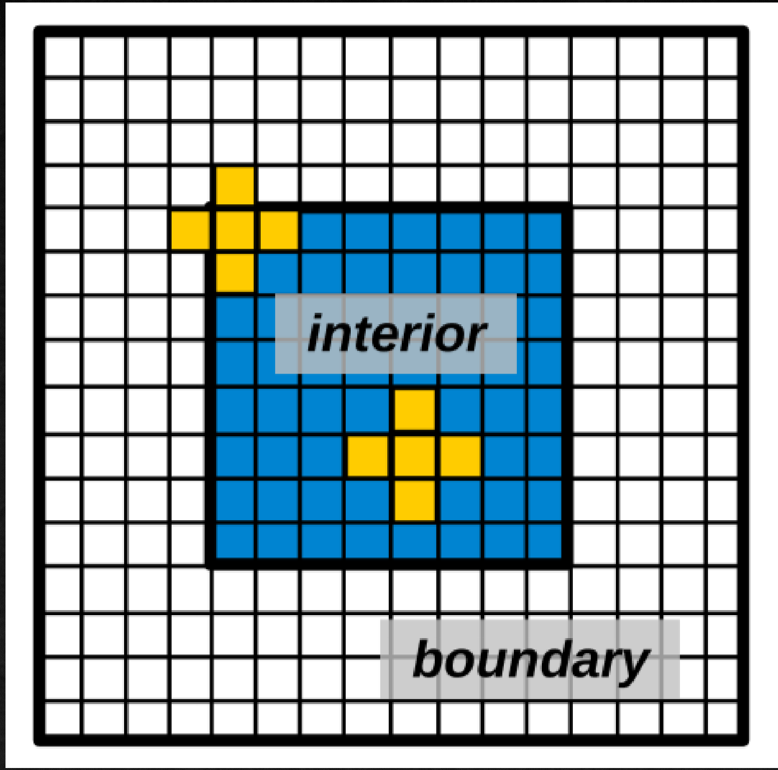
- PLM vs PPM



Boundary conditions

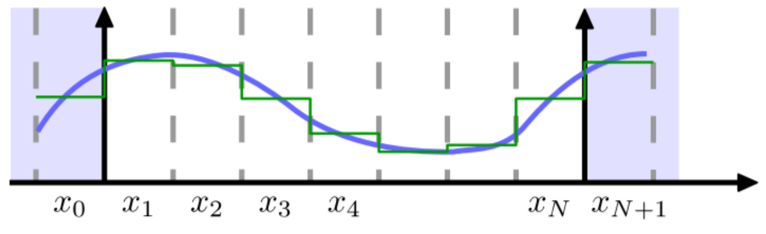
- Boundary conditions are handled with ghost zones
- Need neighboring cells for finite differencing
- The more accurate the method, the more cells are needed





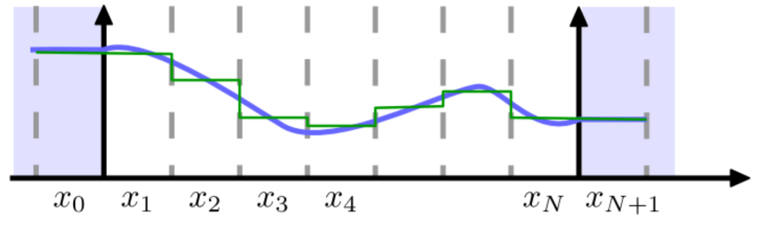
Boundary conditions

- Periodic boundaries



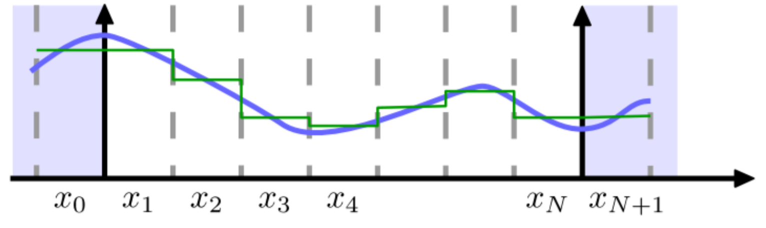
$$\begin{aligned} \overline{q}_0 &:= \overline{q}_N & \overline{q}_{N+1} &:= \overline{q}_1 \\ \overline{q}_{-1} &:= \overline{q}_{N-1} & \overline{q}_{N+2} &:= \overline{q}_2 \end{aligned}$$

- Outflow boundaries (supersonic)



$$\begin{aligned} \overline{q}_0 &:= \overline{q}_1 & \overline{q}_{N+1} &:= \overline{q}_N \\ \overline{q}_{-1} &:= \overline{q}_1 & \overline{q}_{N+2} &:= \overline{q}_N \end{aligned}$$

- Reflecting boundaries



$$\begin{aligned} \overline{q}_0 &:= \overline{q}_1 & \overline{q}_{N+1} &:= \overline{q}_N \\ \overline{q}_{-1} &:= \overline{q}_2 & \overline{q}_{N+2} &:= \overline{q}_{N-1} \end{aligned}$$

More rigor: Euler's Equations

- Now that we have a general overview of hydro solvers, let's look at the details
- In 1-dimension, we have the conservation of mass, momentum, and energy through their fluxes (subscripts denote partials)

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u u + p)_x = 0$$

$$(\rho E)_t + (\rho u E + u p)_x = 0$$

More rigor: Euler's Equations

$$\rho_t + (\rho u)_x = 0$$
$$(\rho u)_t + (\rho u u + p)_x = 0$$
$$(\rho E)_t + (\rho u E + u p)_x = 0$$

- We can write this in a conservation law form: $U_t + [F(U)]_x = 0$

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \qquad \mathrm{F(U)} = \begin{pmatrix} \rho u \\ \rho u u + p \\ \rho u E + u p \end{pmatrix}$$

- We close this system with an equation of state. Let's use a polytrope (ideal gas)

$$p = \rho e(\gamma - 1)$$
$$\rho e = \rho E \; - \rho u^2/2$$

Conservative system

$$\mathrm{F(U)} = \begin{pmatrix} \rho u \\ \rho u u + p \\ \rho u E + u p \end{pmatrix}$$

- We want to express this system like advection, which has a quasi-linear form: $U_t + A(U)U_x = 0$
- Define the flux vectors: $m \equiv \rho u, \mathcal{E} \equiv \rho E$

$$p = \rho e(\gamma - 1) = \left(\mathcal{E} - \frac{m^2}{2\rho}\right)(\gamma - 1)$$

$$F(U) = \begin{pmatrix} m \\ \frac{m^2}{2\rho}(3-\gamma) + \mathcal{E}(\gamma - 1) \\ \frac{m\mathcal{E}\gamma}{\rho} - \frac{m^3}{2\rho^2}(\gamma - 1) \end{pmatrix}$$

Conservative system

$$F(U) = \begin{pmatrix} m \\ \frac{m^2}{2\rho}(3-\gamma) + \mathcal{E}(\gamma-1) \\ \frac{m\mathcal{E}\gamma}{\rho} - \frac{m^3}{2\rho^2}(\gamma-1) \end{pmatrix}$$

- Compute the Jacobian

$$A(U) = \frac{\partial F}{\partial U} = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{1}{2}u^2(3-\gamma) & u(3-\gamma) & \gamma-1 \\ \frac{1}{2}(\gamma-2)u^3 - \frac{uc^2}{\gamma-1} & \frac{3-2\gamma}{2}u^2 + \frac{c^2}{\gamma-1} & u\gamma \end{pmatrix}$$

- Here $c \equiv \sqrt{\frac{\gamma p}{\rho}}$ is the sound speed
- Now we can write the system as desired: $U_t + A(U)U_x = 0$

Simpler alternative: primitive variable formulation

- Alternatively we can cast the system in terms of density, velocity, and pressure
- These are known as primitive variables q
- Keep the same quasi-linear form: $q_t + A(q)q_x = 0$, where

$$q = \begin{pmatrix} \rho \\ u \\ p \end{pmatrix}, \qquad A(q) = \begin{pmatrix} u & \rho & 0 \\ 0 & u & \dfrac{1}{\rho} \\ 0 & \gamma p & u \end{pmatrix}$$

Eigensystem

$$A(q) = \begin{pmatrix} u & \rho & 0 \\ 0 & u & \frac{1}{\rho} \\ 0 & \gamma p & u \end{pmatrix}, c \equiv \sqrt{\frac{\gamma p}{\rho}}$$

- For this system, the eigenvalues are

$$\lambda^{-} = u - c, \qquad \lambda^{0} = u, \qquad \lambda^{+} = u + c$$

- These are the speeds at which information travels in the system
- Three distinct wave speeds for 3 equations
- Same eigenvalues for the conservative Jacobian

Eigensystem

$$\lambda^- = u - c, \qquad \lambda^0 = u, \qquad \lambda^+ = u + c$$

- The eigenvectors (normalized: $l^i \cdot r^j = \delta_{ij}$) are

$$Ar^i = \lambda^i r^i, \qquad l^i A = \lambda^i l^i$$

$$r^- = \begin{pmatrix} 1 \\ -\frac{c}{\rho} \\ c^2 \end{pmatrix}, \qquad r^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad r^+ = \begin{pmatrix} 1 \\ \frac{c}{\rho} \\ c^2 \end{pmatrix}$$

$$l^- = \begin{pmatrix} 0 & -\frac{\rho}{2c} & \frac{1}{2c^2} \end{pmatrix}, l^0 = \begin{pmatrix} 1 & 0 & -\frac{1}{c^2} \end{pmatrix}, l^+ = \begin{pmatrix} 0 & \frac{\rho}{2c} & \frac{1}{2c^2} \end{pmatrix}$$

Characteristic variables

$$r^- = \begin{pmatrix} 1 \\ -\frac{c}{\rho} \\ c^2 \end{pmatrix}, \quad r^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad r^+ = \begin{pmatrix} 1 \\ \frac{c}{\rho} \\ c^2 \end{pmatrix}$$

$$l^- = \begin{pmatrix} 0 & -\frac{\rho}{2c} & \frac{1}{2c^2} \end{pmatrix}, l^0 = \begin{pmatrix} 1 & 0 & -\frac{1}{c^2} \end{pmatrix}, l^+ = \begin{pmatrix} 0 & \frac{\rho}{2c} & \frac{1}{2c^2} \end{pmatrix}$$

- The final form of the system is in terms of the characteristic variables
- Construct matrices of the left and right eigenvectors

$$R = (r^- | r^0 | r^+), \qquad L = \begin{pmatrix} l^- \\ l^0 \\ l^+ \end{pmatrix}$$

- These satisfy $LR = RL = \mathbb{I}$
- If we define $dw = Ldq$, our system can be written as

$$w_t + \Lambda w_x = 0$$

Characteristic variables

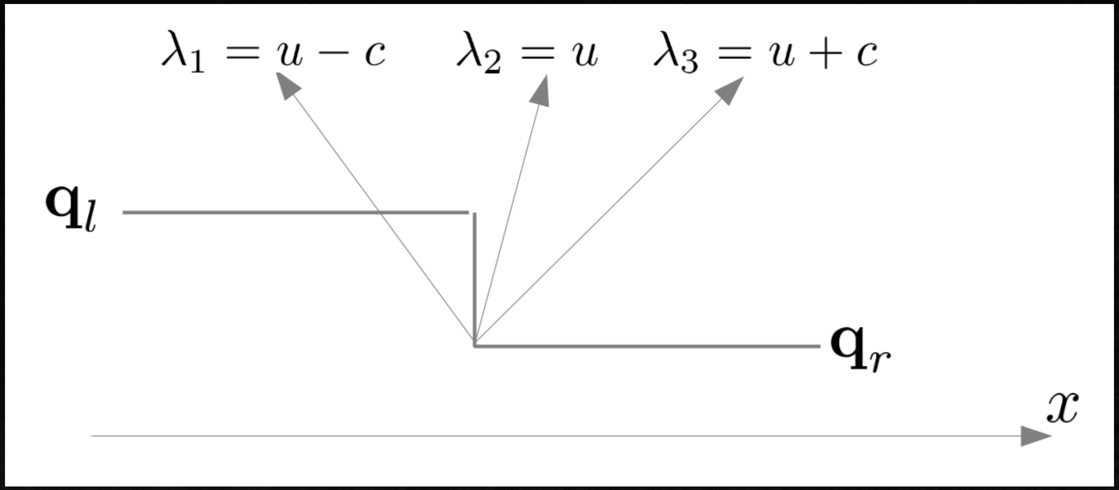
$$w_t + \Lambda w_x = 0$$

- Here w are the characteristic variables
- The three equations are now decoupled

$$\Lambda = LAR = \begin{pmatrix} \lambda^- & & \\ & \lambda^0 & \\ & & \lambda^+ \end{pmatrix}$$

- This characteristic system is telling us about the waves
- Each wave will carry a jump in their associated characteristic quantity away from the discontinuity at their speed
- The corresponding jump in the primitive variable is $dq = L^{-1}dw = R$

Jumps across waves



- Recall that there are three waves in a Riemann problem
- The eigenvectors r^i tell us the jumps in the primitive quantities

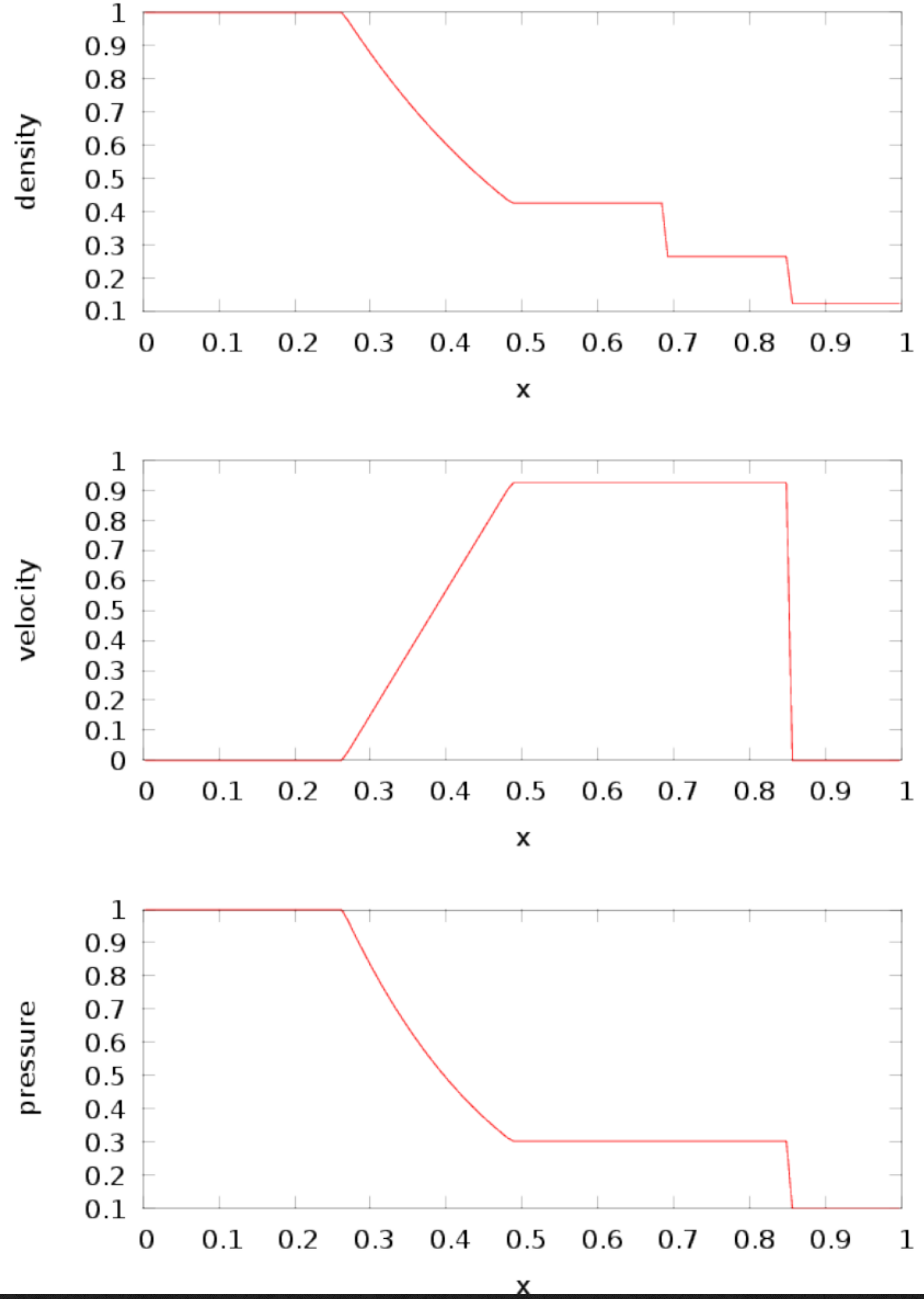
$$r^- = \begin{pmatrix} 1 \\ -\dfrac{c}{\rho} \\ c^2 \end{pmatrix}, \qquad r^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad r^+ = \begin{pmatrix} 1 \\ \dfrac{c}{\rho} \\ c^2 \end{pmatrix}$$

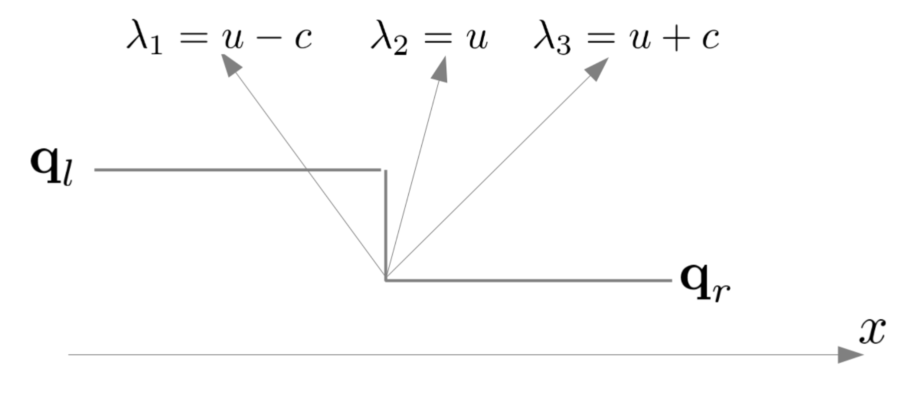
Sod shock tube

$$\rho_L = 1.0$$
$$\rho_R = 1/8$$

$$u_L = 0$$
$$u_R = 0$$

$$p_L = 1.0$$
$$p_R = 1/10$$





$$r^- = \begin{pmatrix} 1 \\ -\frac{c}{\rho} \\ c^2 \end{pmatrix}$$

$$r^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$r^+ = \begin{pmatrix} 1 \\ \frac{c}{\rho} \\ c^2 \end{pmatrix}$$