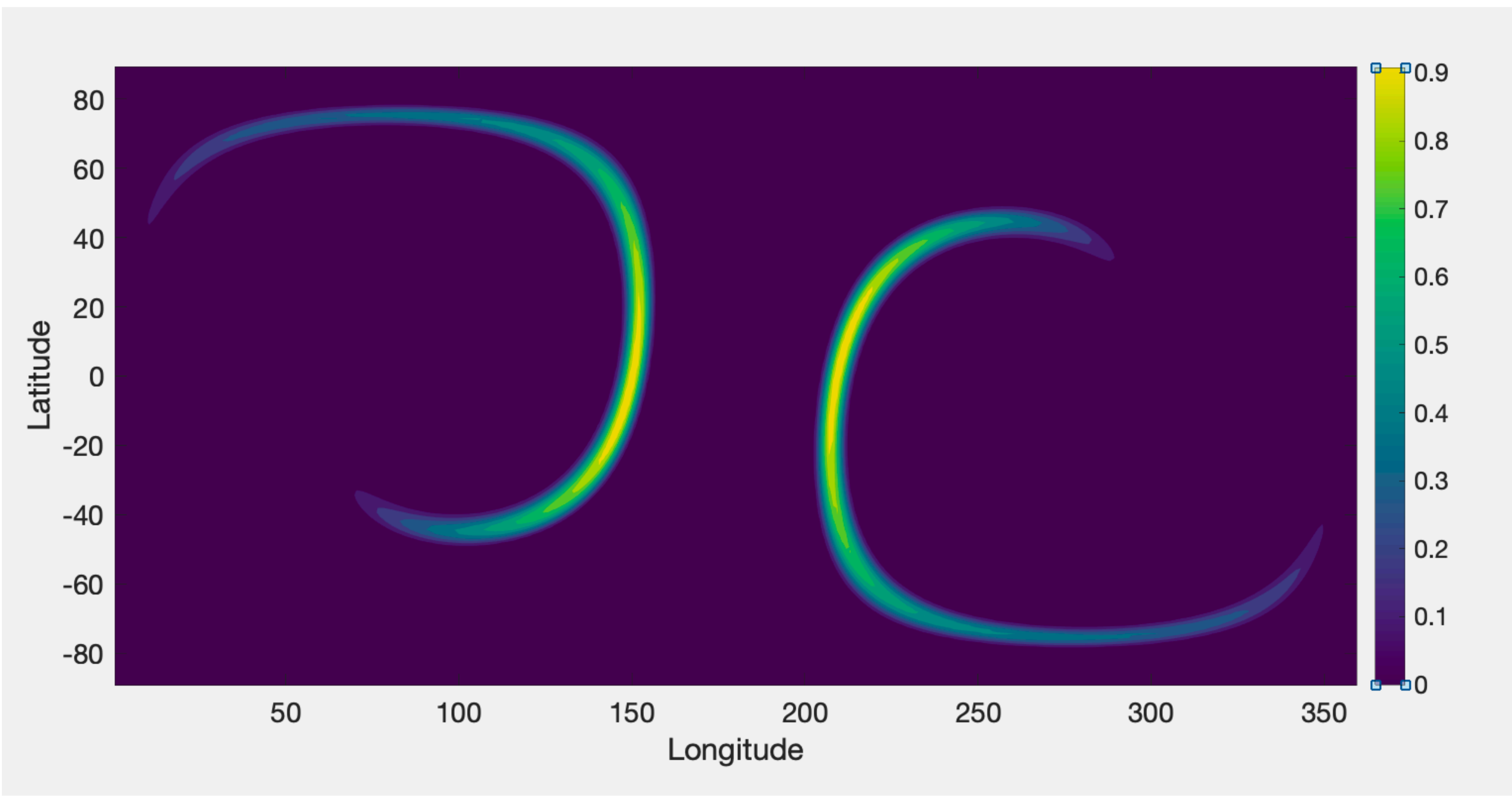
Topic 3

Numerical Solutions to the Advection-Diffusion Equations

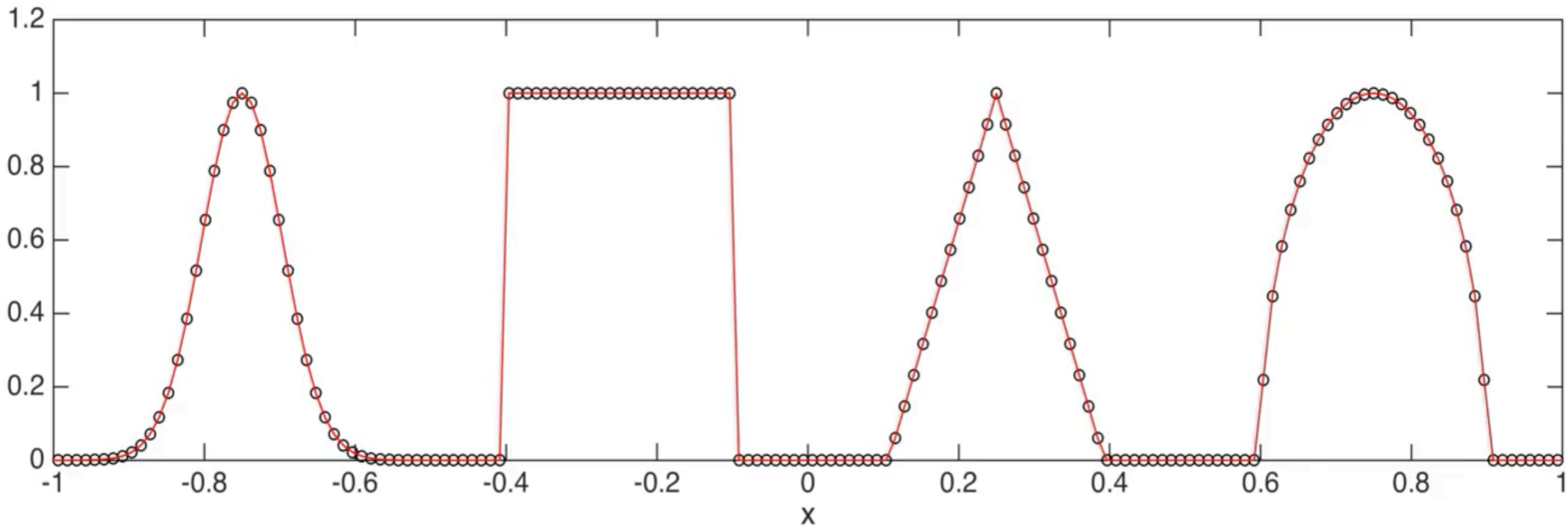


Outline

- The linear advection equation
- Why simple Finite difference methods do not work
- Introduction to Finite volume methods
- Upwind and central flux
- Reconstruction, introduction slope limiting

Advection of four shapes in 1D

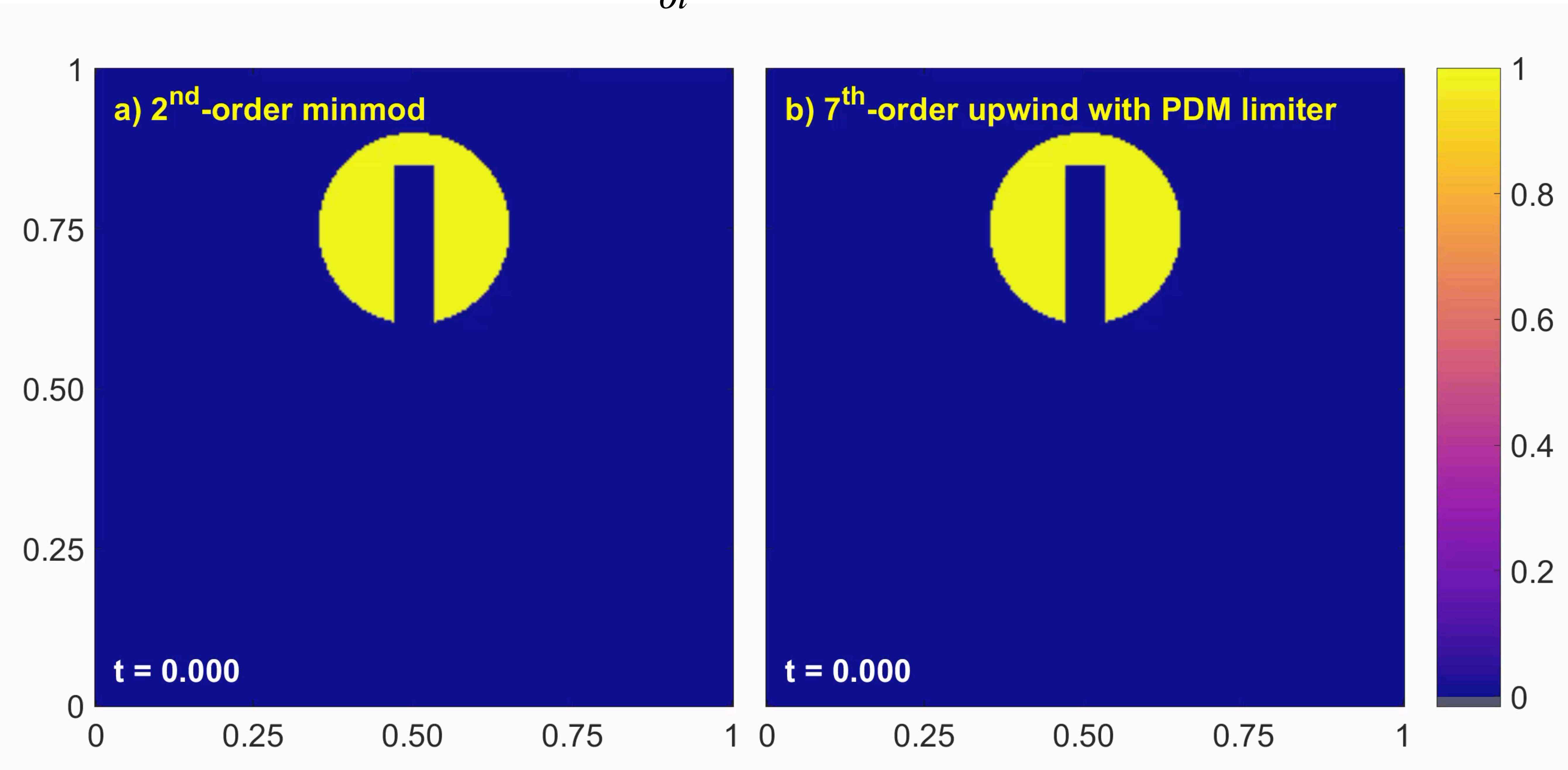
$$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$$



Gaussian	**Square**	**Triangle**	**Half-circle**
Smooth	Discontinuity	Discontinuity in 1st derivative	Steep changes in derivatives

Advection of a slotterd cylinder in 2D

$$\frac{\partial Q}{\partial t} + \mathbf{u}_0 \cdot \nabla Q = 0$$



A simple Central-Difference Method

$$\left(\frac{\partial u}{\partial t}\right)_i \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Central difference

Linear Advection Equation

$$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$$

Forward difference

Central difference

Euler Time-Stepping

$$\left.\frac{\partial Q}{\partial t}\right|_{t=t_n} = \frac{Q_i^{n+1} - Q_i^n}{\Delta t} + \mathcal{O}(\Delta t)$$

$$\left.\frac{\partial Q}{\partial t}\right|_{x=x_i} = \frac{Q_{i+1}^n - Q_{i-1}^n}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Combine the two numerical derivatives

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} = -u_0 \frac{Q_{i+1}^n - Q_{i-1}^n}{2\Delta x} + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t) \longrightarrow$$

Forward Euler method

$$\boxed{Q_i^{n+1} \approx \underbrace{Q_i^n - \frac{u_0 \Delta t}{2\Delta x}(Q_{i+1}^n - Q_{i-1}^n)}_{\text{Values on step n (known)}}}$$

We know this scheme is unstable, the question is why

Recall - Finite Difference for 1D MHD

1-D MHD equations

$$\frac{\partial}{\partial t}\rho = -\frac{\partial}{\partial x}(\rho u_x)$$

$$\frac{\partial u_x}{\partial t} = -u_x\frac{\partial u_x}{\partial x} + \frac{1}{\rho}\left(-\frac{\partial p}{\partial x} - J_z B_y\right)$$

$$\frac{\partial u_y}{\partial t} = -u_x\frac{\partial u_y}{\partial x} + \frac{1}{\rho}J_z B_{x0}$$

$$\frac{\partial B_y}{\partial t} = \frac{\partial E_z}{\partial x}$$

$$E_z = -u_x B_y + u_y B_{x0}$$

$$J_z = \frac{\partial B_y}{\partial x}$$

$$p = \frac{\beta_0}{2}\rho^{\gamma}$$

$$\Longrightarrow$$

Finite-Difference Approximations

$$\frac{\partial\rho}{\partial t}\Big|_i = \frac{u^n_{x,i+1}\rho^n_{i+1} - u^n_{x,i-1}\rho^n_{i-1}}{2\Delta x}$$

$$\frac{\partial u_x}{\partial t}\Big|_i = -u_{x,i}\frac{u^n_{x,i+1} - u^n_{x,i-1}}{2\Delta x} + \frac{1}{\rho^n_i}\left(\frac{p^n_{i+1} - p_{i-1}}{2\Delta x} - J^n_{z,i}B^n_{y,i}\right)$$

$$\frac{\partial u_y}{\partial t}\Big|_i = -u_{x,i}\frac{u^n_{y,i+1} - u^n_{y,i-1}}{2\Delta x} + \frac{1}{\rho^n_i}J^n_{z,i}B_{x0}$$

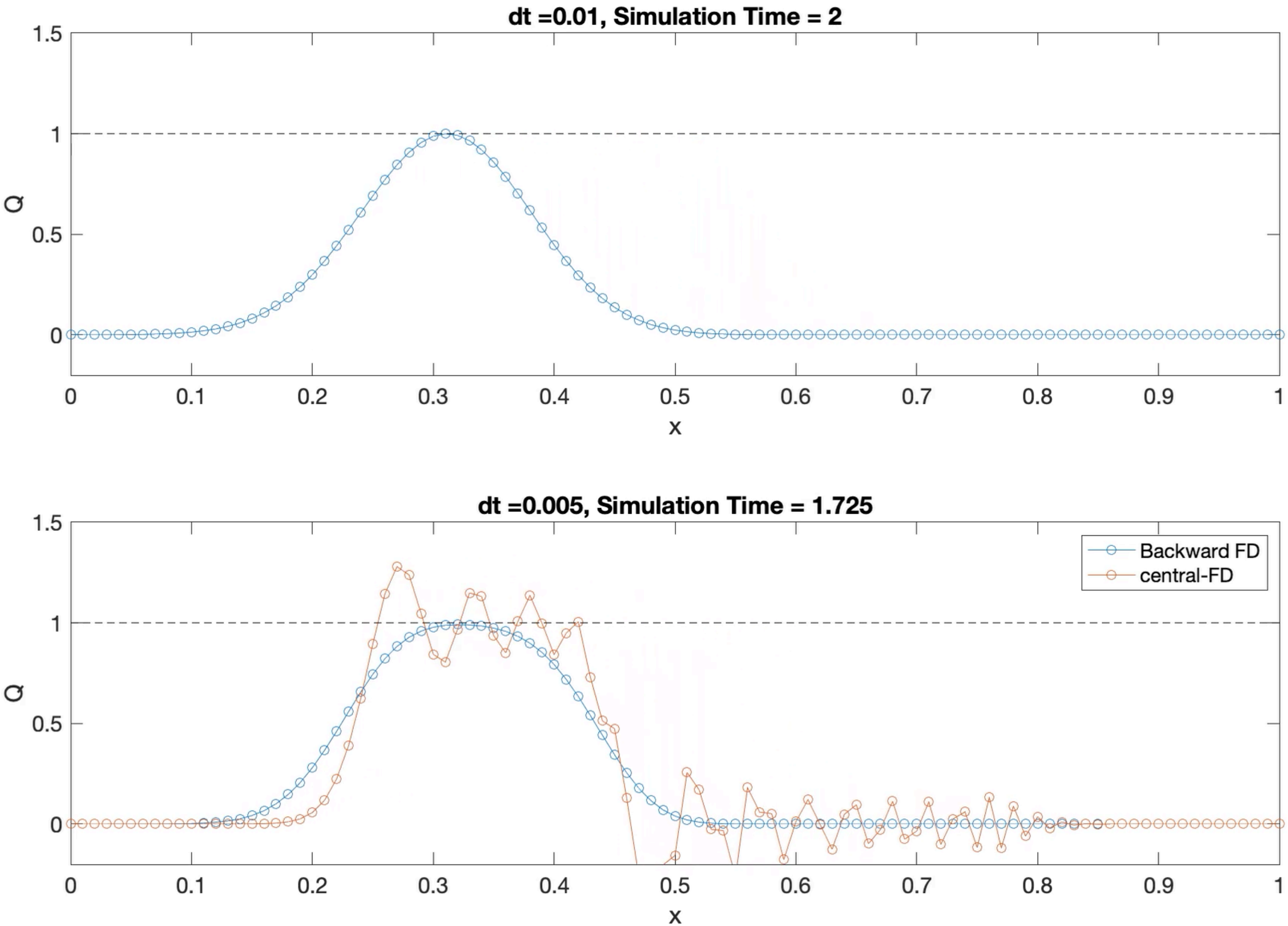
$$\frac{\partial B_y}{\partial t}\Big|_i = -\frac{E^n_{z,i+1} - E^n_{z,i-1}}{2\Delta x}$$

$$E^n_{z,i} = -u^n_{x,i}B^n_{y,i} + u^n_{y,i}B_{x0}$$

$$J^n_{z,i} = \frac{B^n_{y,i+1} - B^n_{y,i-1}}{2\Delta x}$$

$$p^n_{z,i} = \frac{\beta_0}{2}(\rho^n_i)^{\gamma}$$

Results form Central-Difference Method



Recall the Upwind Method

$$\left(\frac{\partial u}{\partial t}\right)_i \approx \frac{u_i - u_{i-1}}{\Delta x}$$

Backward difference

$$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$$

Forward difference

$$\left.\frac{\partial Q}{\partial t}\right|_{t=t_n} = \frac{Q_i^{n+1} - Q_i^n}{\Delta t} + \mathcal{O}(\Delta t)$$

Backward difference

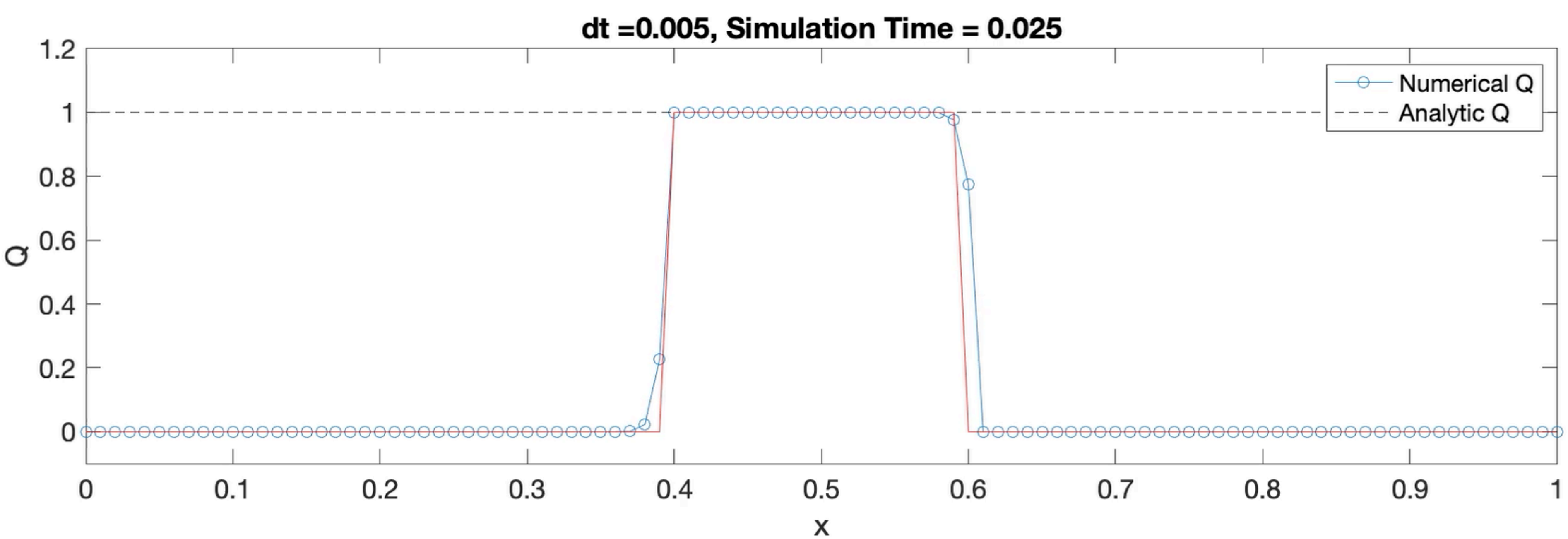
$$\left.\frac{\partial Q}{\partial t}\right|_{x=x_i} = \frac{Q_i^n - Q_{i-1}^n}{\Delta x} + \mathcal{O}(\Delta x)$$

Now use the backward spatial difference:

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} = u_0 \frac{Q_i^n - Q_{i-1}^n}{\Delta x} + \mathcal{O}(\Delta x) + \mathcal{O}(\Delta t) \longrightarrow$$

Backward Euler method

$$\boxed{Q_i^{n+1} \approx Q_i^n + \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)}$$

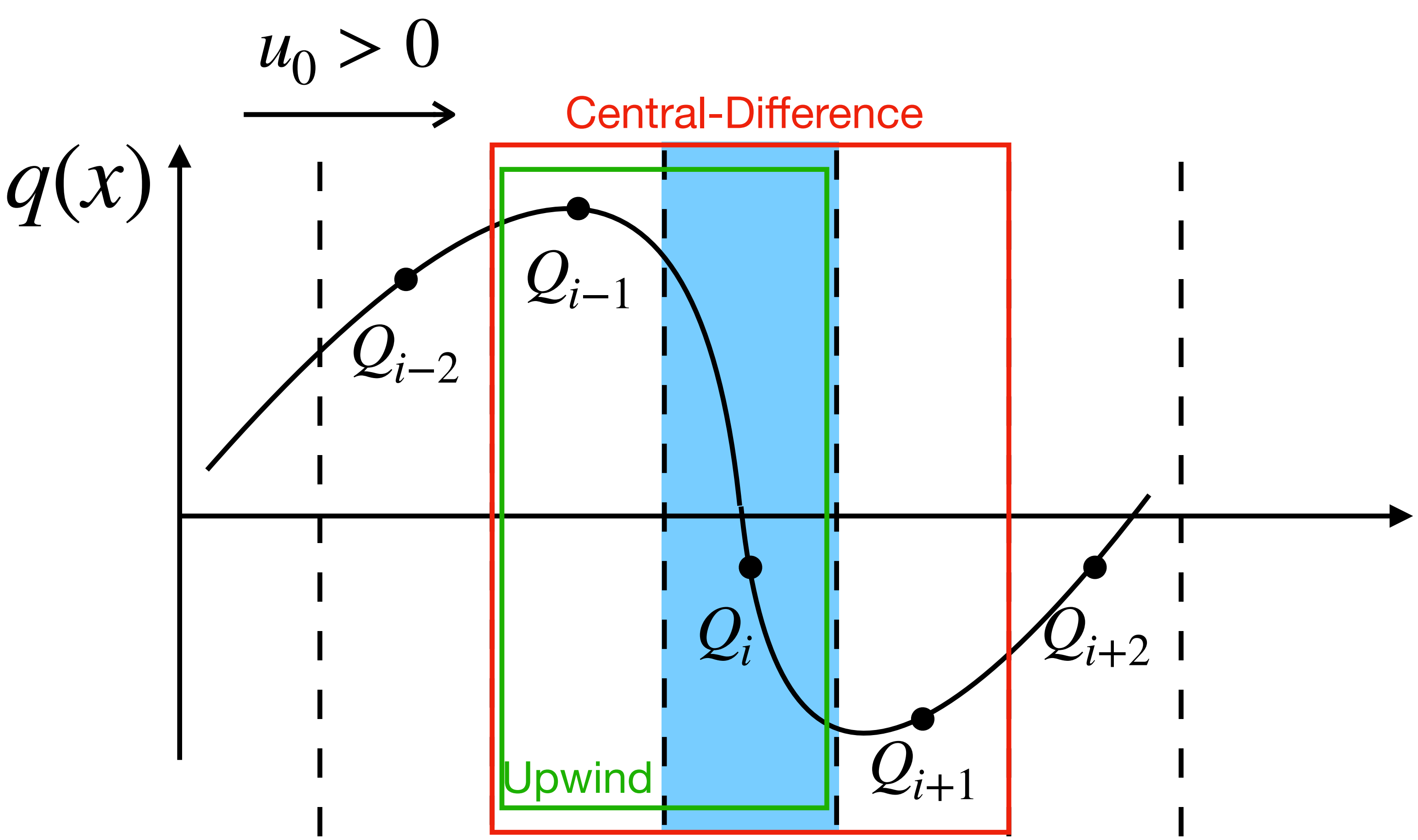


Physical Necessity of Upwinding

Wave propagation

The 1-D linear advection equation $\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$ has an analytical solution:

$$Q(x,t) \sim f(x - u_0 t)$$



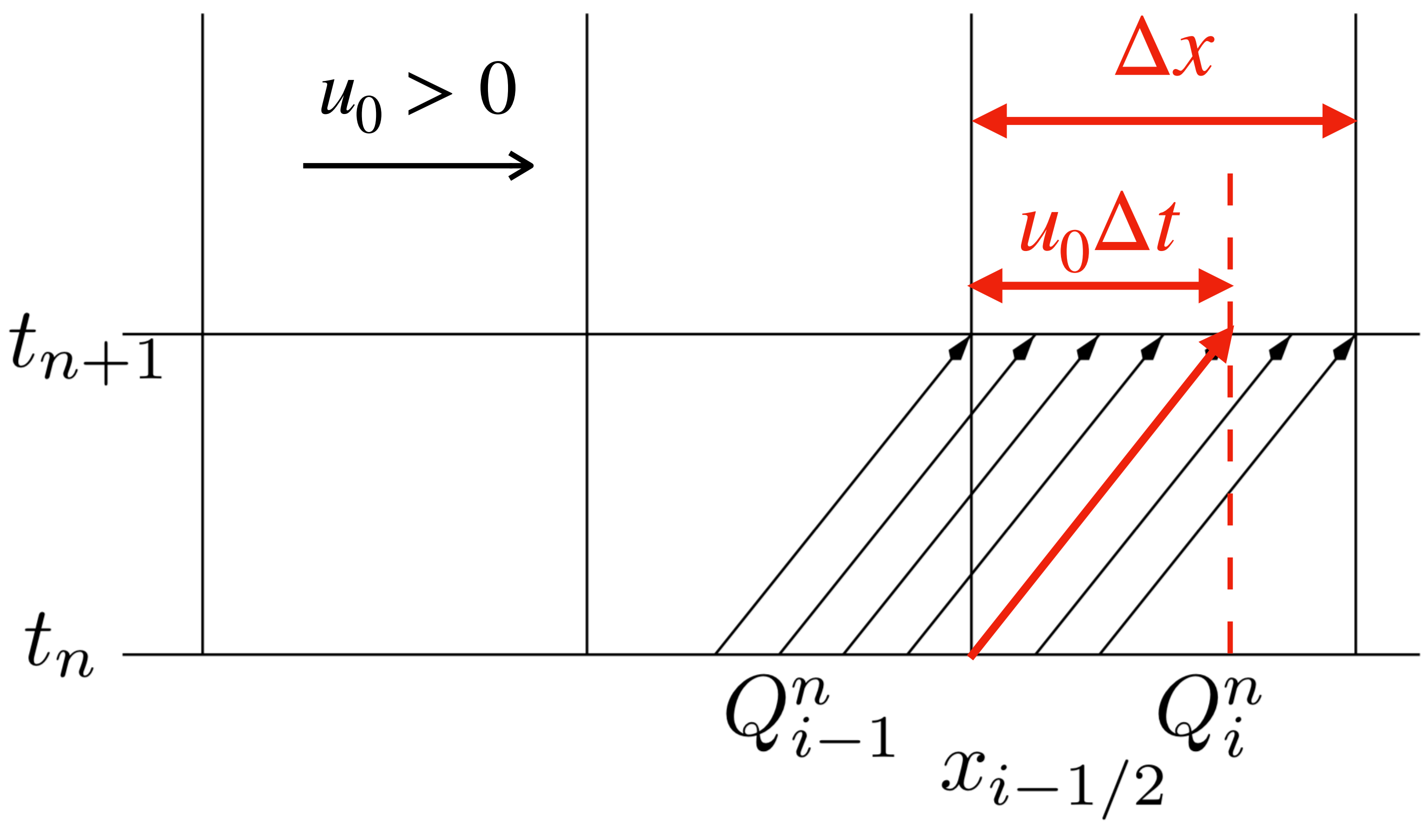
$$Q_i^{n+1} \approx Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$$

Wave propagates towards right

- Information only goes from left to right
- Solution of Q_i is only affected by Q_{i-1}
- Solution of Q_i has nothing to do with any cell on the right side of i
- The central difference uses information from cell i+1 which is non-physical
- The upwind solution is physical

The CFL Stability Condition

How the waves propagate CFL

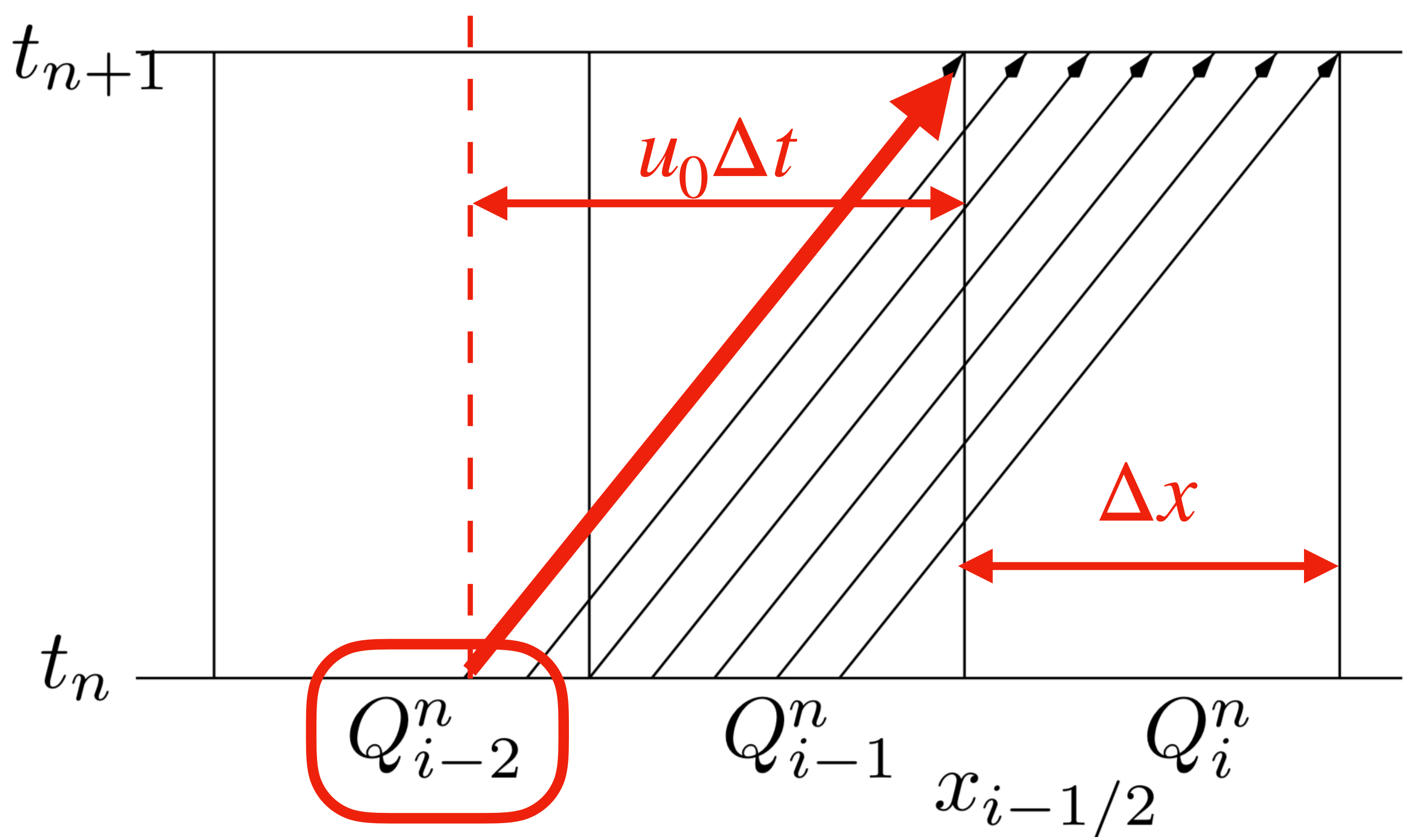


- Solution of Q_i is only affected by Q_{i-1} and Q_i

$$Q_i^{n+1} \approx Q_i^n - \frac{u_0\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$$

Requires $u_0\Delta t <= \Delta x$

What if $u_0\Delta t > \Delta x$?



- Solution of Q_i is not just affected by Q_{i-1} and Q_i, information from Q_{i-2} also affects the solution

Which means the scheme is UNSTABLE

This is the so-called CFL condition

Why simple finite difference won't work

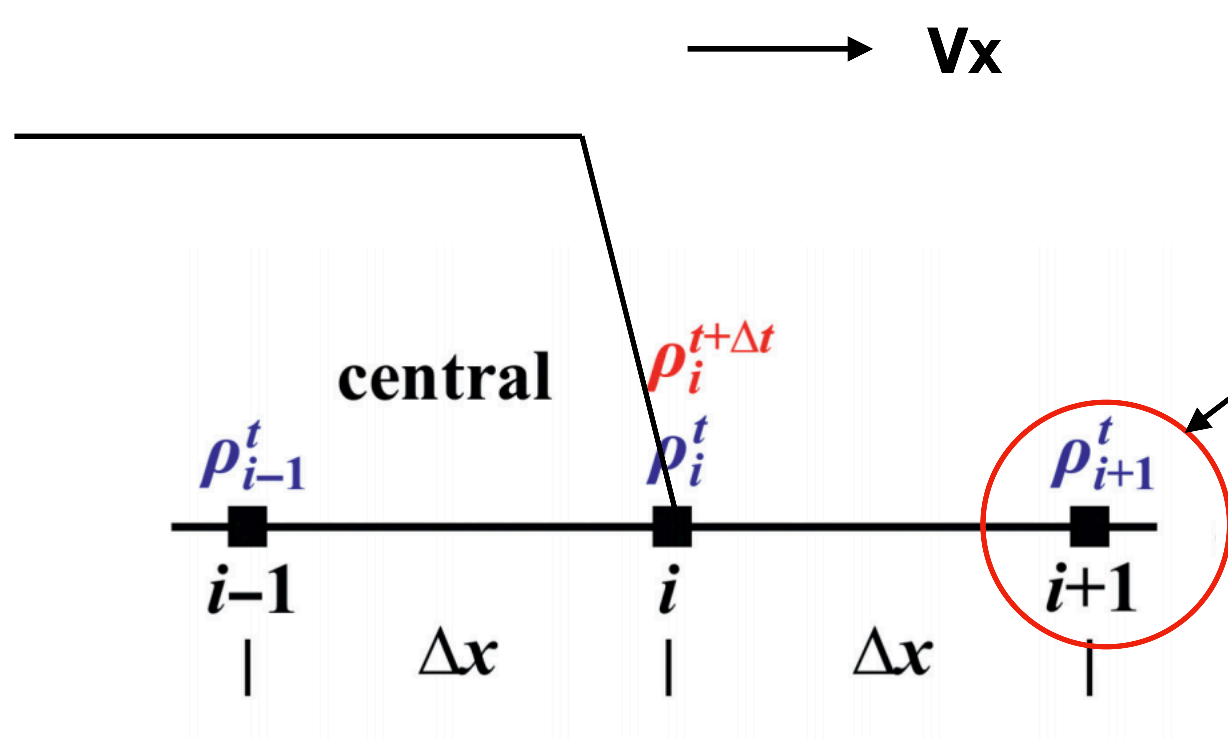
Mathematical reason:

This term is huge when u is discontinuous!

Central difference

$$\Rightarrow \left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{1}{6}\Delta x^2 \left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

Physical reason:



Information from this cell is non-physical for wave propagation

A few things about the modified equation

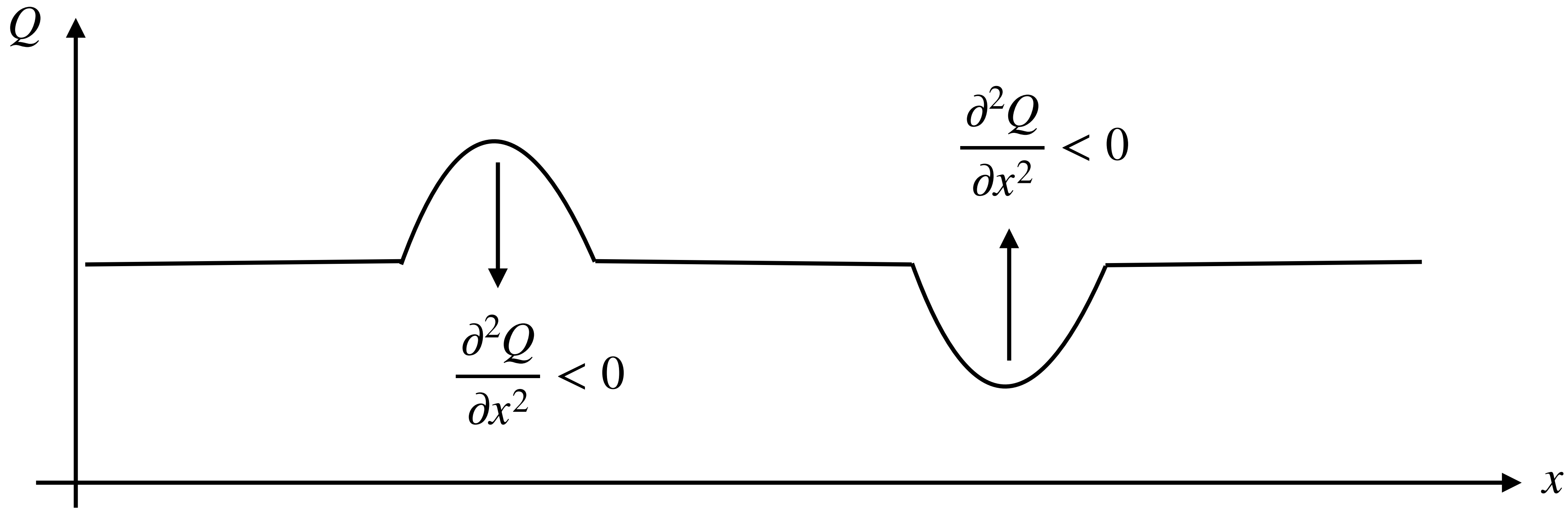
Upwind method

Original Equation	Numerical Approximation	Modified Equation
$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$	$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$	$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \beta_{xx} \frac{\partial^2 q}{\partial x^2}$

Lessons learned from the above analysis:

- The upwind scheme is an approximation to the advection equation
- The leading error term is delta x
- The upwind scheme is equivalent to an advection-diffusion equation
- The diffusion coefficient is beta_xx which is large:
    - If $\frac{u_0 \Delta t}{\Delta x} = 1 \longrightarrow \beta_{xx} = \frac{1}{2} u_0 \Delta x \left(1 - \frac{u_0 \Delta t}{\Delta x}\right) \equiv 0$ NO diffusion!
    - If $\Delta x \to 0 \longrightarrow \beta_{xx} \to 0$ Converged solution
    - If $0 < \frac{u_0 \Delta t}{\Delta x} < 1 \longrightarrow \beta_{xx} > 0$ Always have numerical diffusion

What is Numerical Diffusion?



$$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \beta_{xx} \frac{\partial^2 q}{\partial x^2}$$

Analytical solutions to the advection diffusion equation goes like

$$q(x,t) = \int_{-\infty}^{+\infty} f(\xi - u_0 t) e^{-\frac{(\xi - x)^2}{\beta_{xx}}} d\xi$$

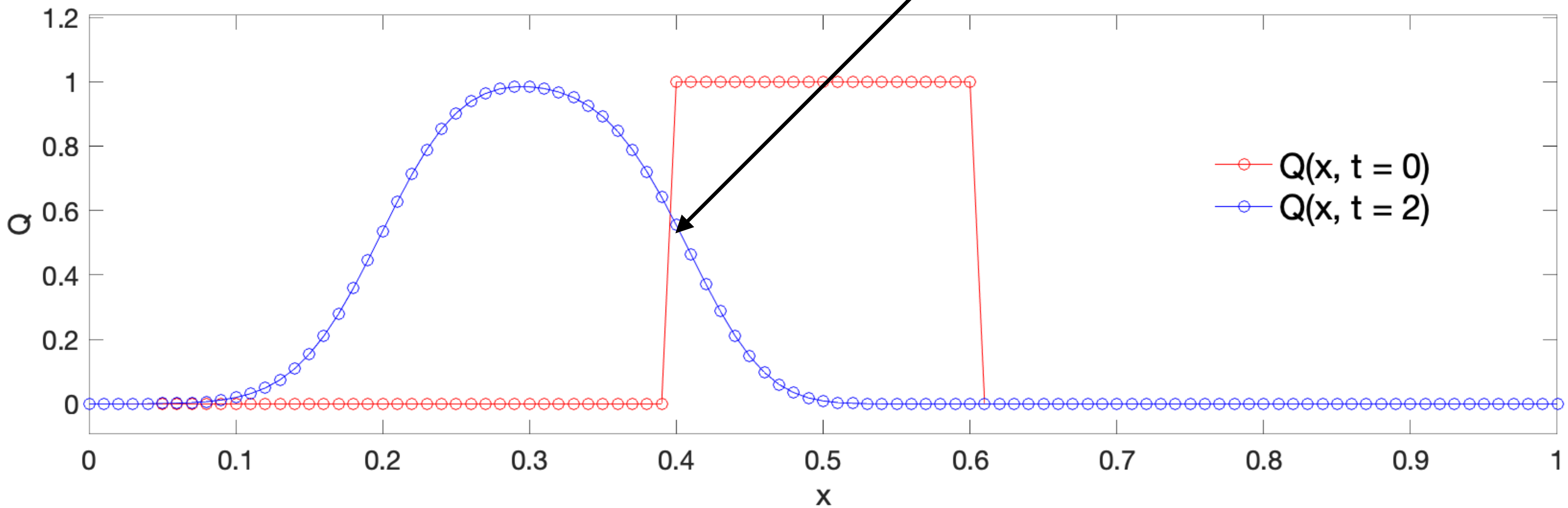
b) Run the linear_adv_lec_2.m code with a square wave as the initial profile: Q=1.0 for 0.4<x<0.6 and Q = 0.0 otherwise. Compare the final profile of Q with the initial condition and describe your result.

To setup a square wave for the initial Q profile, simply use:

```
Q = x*0;
Q(abs(x-0.5)<0.1)=1;
Q_init = Q; % save the initial profile for the final plot
```

After the simulation, plot Q and Q_init in the same plot

Square wave "smeared" by numerical diffusion




```
% plot the initial and final profiles of Q
figure('position',[442    668    988    280]) % create a blank figure to show the advection results
plot(x,Q_init,'-ro'); hold on
plot(x,Q,'-bo')
xlabel('x')
ylabel('Q')
ylim([-0.1 1.2])
set(gca,'fontsize',14)
```

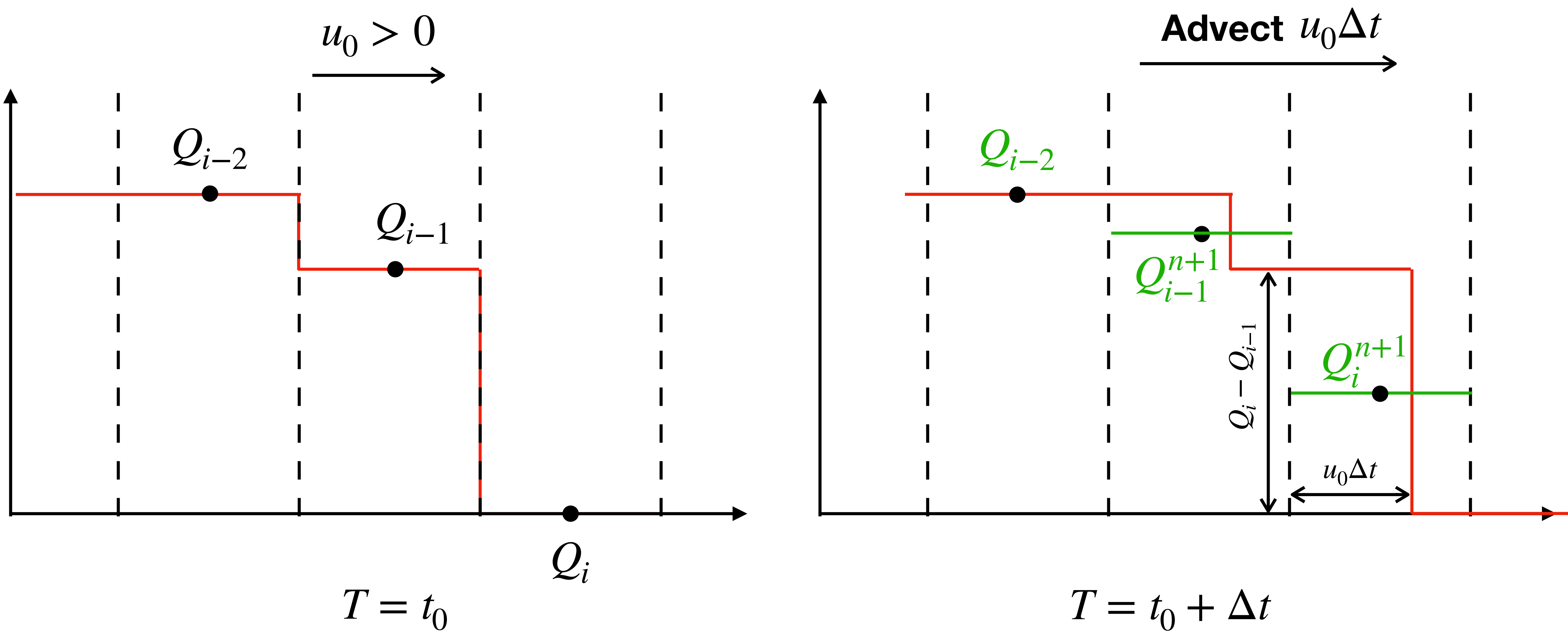
So the numerical solution of Q "spreads" in the x-direction - it deforms from a square function into something like a Gaussian function (mathematically it's the error function"

The Advection Nature of the equation

The REA framework

The upwind scheme can be written as $Q_i^{n+1} = Q_i^n - \boxed{\dfrac{u_0 \Delta t (Q_i^n - Q_{i-1}^n)}{\Delta x}}$ Density change within one step

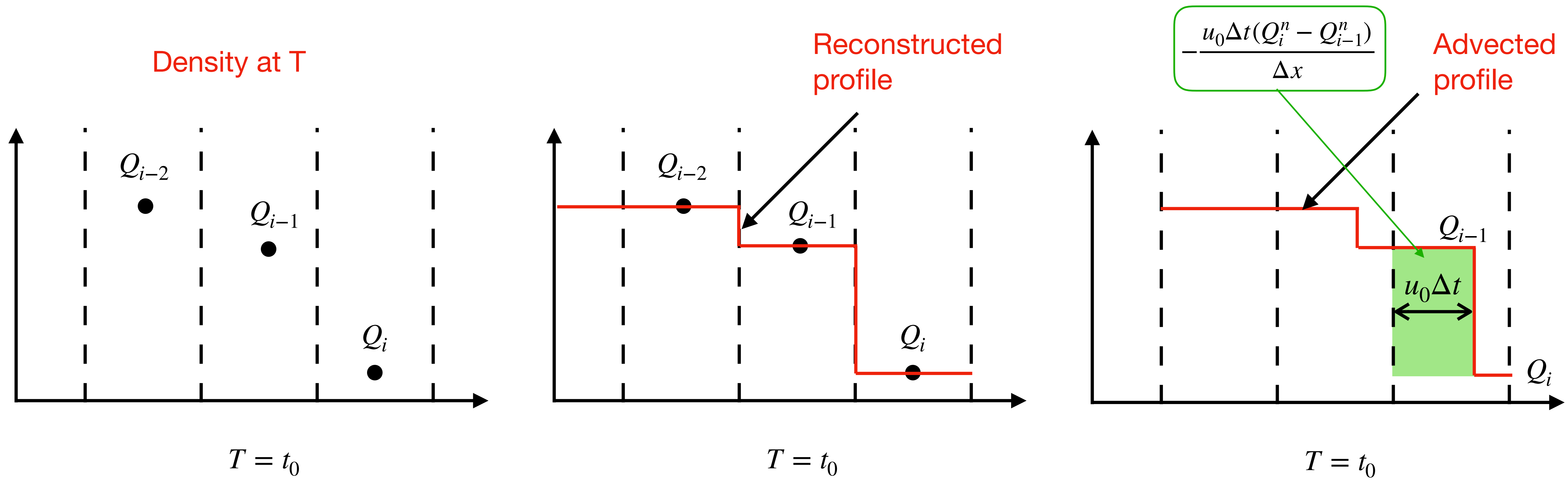
$u_0 \Delta t$ is the distance advected, $(Q_i^n - Q_{i-1}^n)$ is the density difference between the cells



The Advection Nature of the equation

The REA framework

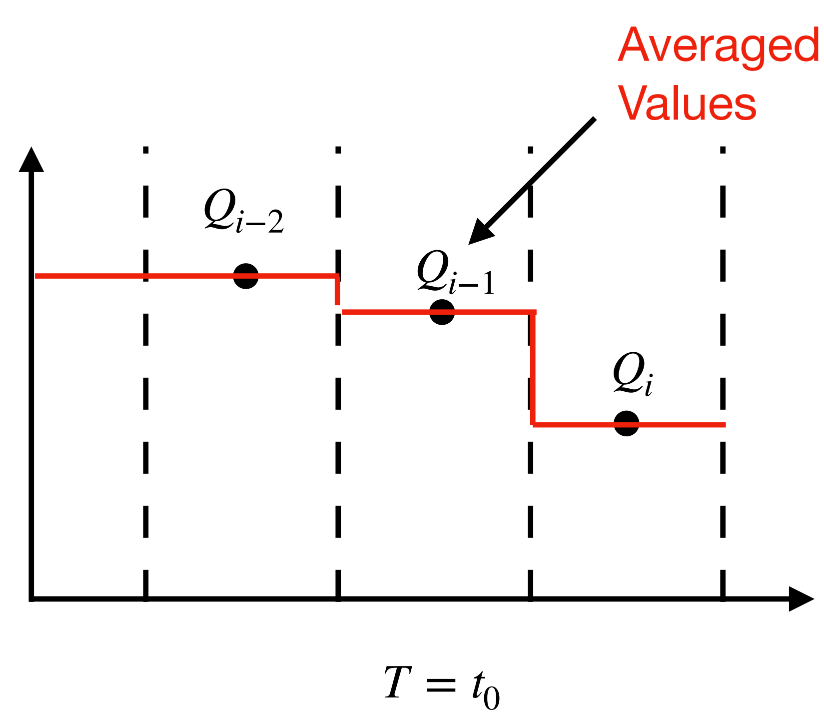
So the upwind scheme is basically an advection



Here's what happened in the upwind method:

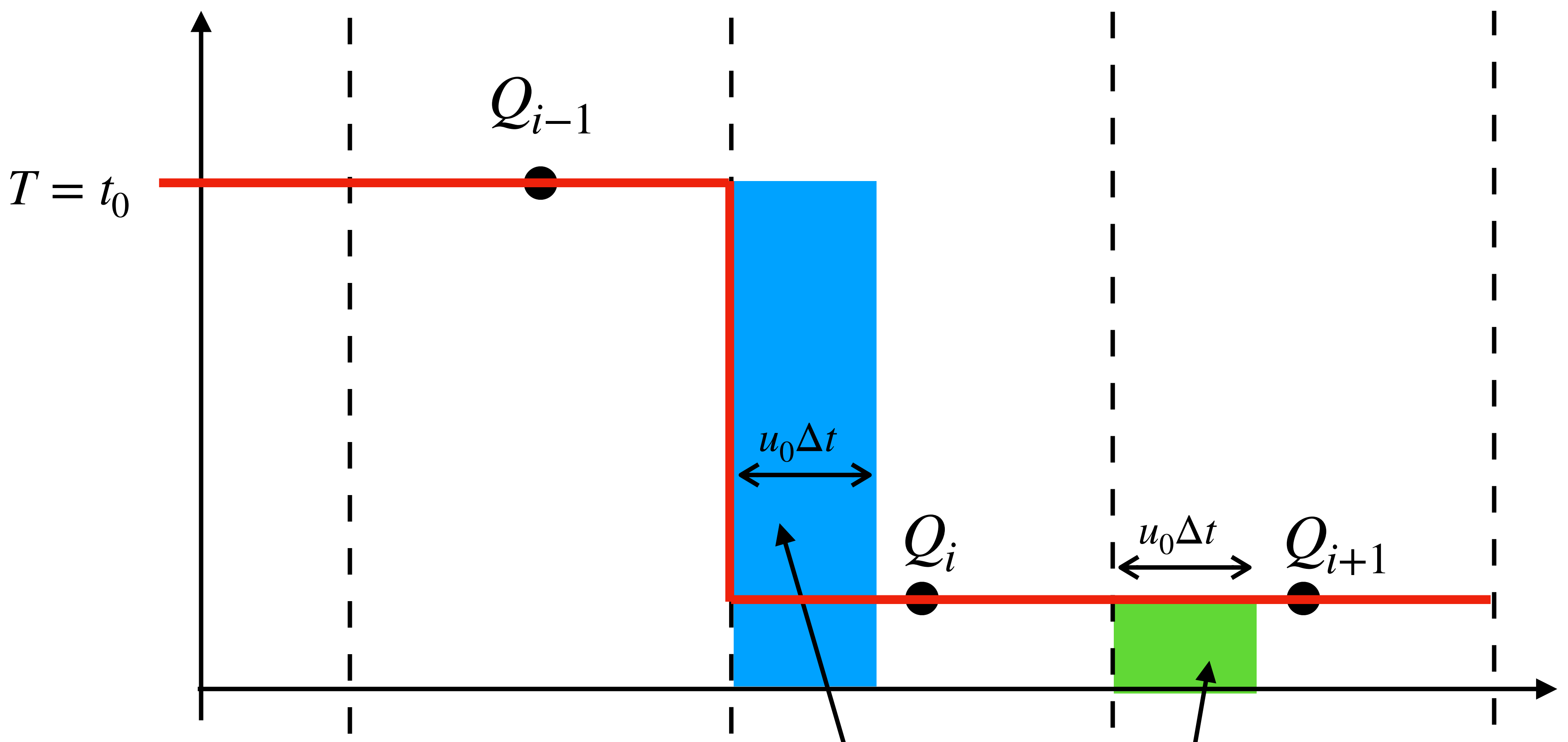
1. From Q_i, do a piecewise-constant reconstruction;
2. Move the reconstructed profile by u*delta t
3. Average the shifted profile in each cell to get new Q_i

Reconstruct - ***Evolve*** - ***Average*** (REA framework)



The Transport Nature of the equation

The flux balance interpretation



$$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t (Q_i^n - Q_{i-1}^n)}{\Delta x} = Q_i^n + \left(\boxed{\frac{u_0 \Delta t}{\Delta x} Q_{i-1}^n} - \boxed{\frac{u_0 \Delta t}{\Delta x} Q_i^n} \right) \in (Q_{i-1}, Q_i)$$

Mass entering cell i

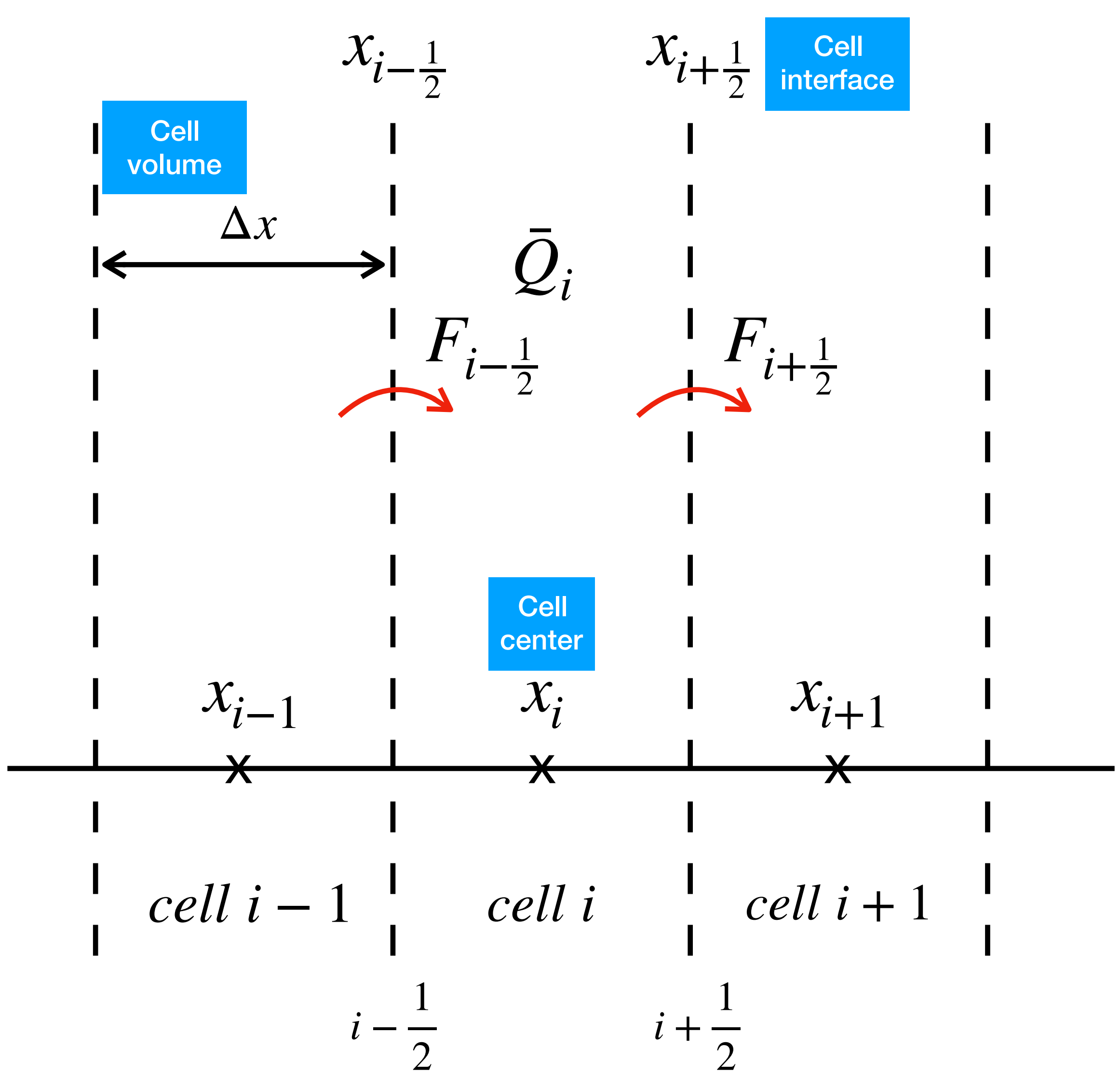
Mass leaving cell i

Finite Volume Methods

Basic form

$$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0 \xrightarrow{\text{re-write}} \frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial x} = 0 \qquad F(Q) = u_0 Q \quad \text{for linear advection}$$

Let's discretize the solution domain:



Integrate the PDE in cell i

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} dx \left(\frac{\partial Q}{\partial t} + \frac{\partial F(Q)}{\partial x} \right) = 0$$

$$\longrightarrow \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial Q}{\partial t} dx = - \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial F(Q)}{\partial x} dx$$

$$\longrightarrow \frac{\partial}{\partial t} \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} Q dx = - F(Q) \Big|_{i-\frac{1}{2}}^{i+\frac{1}{2}}$$

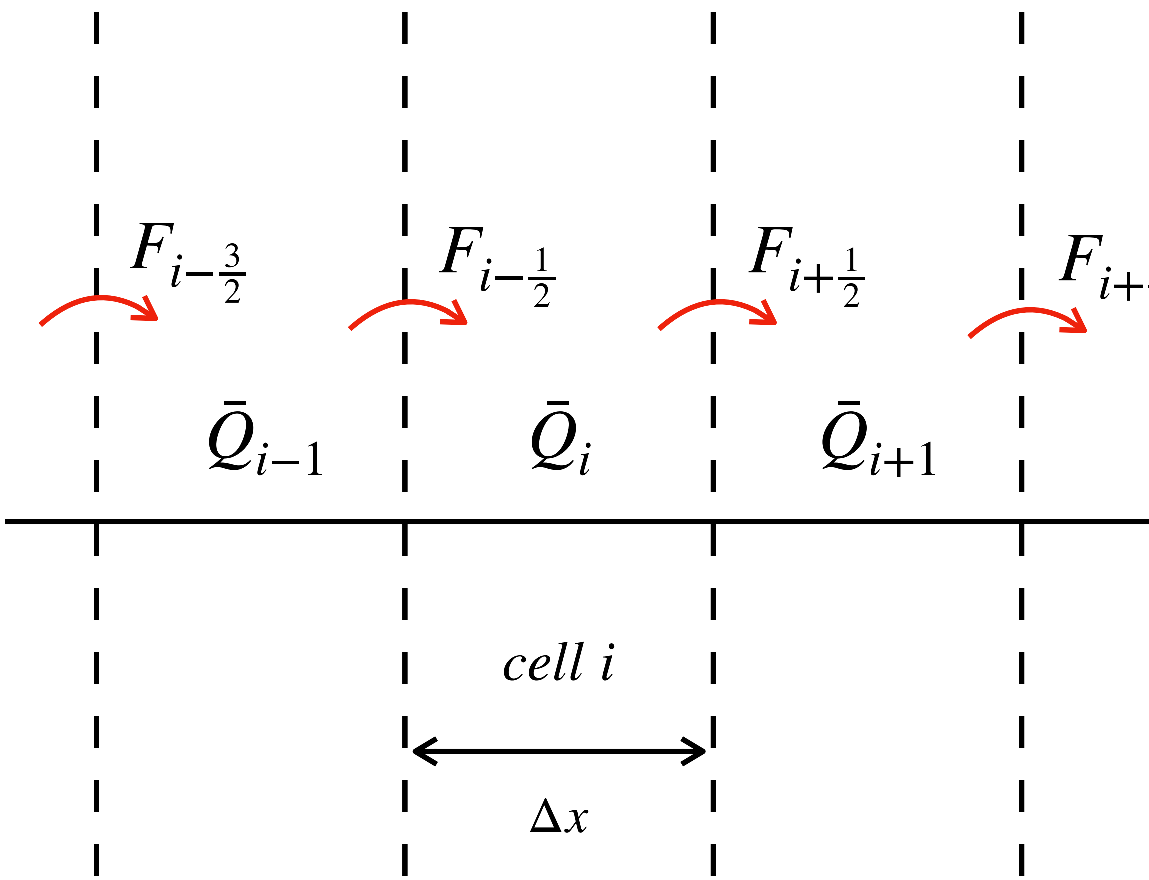
$$\longrightarrow \frac{\partial}{\partial t} \bar{Q} \Delta x = - F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}$$

Rate of mass change

Flux in & out of cell i

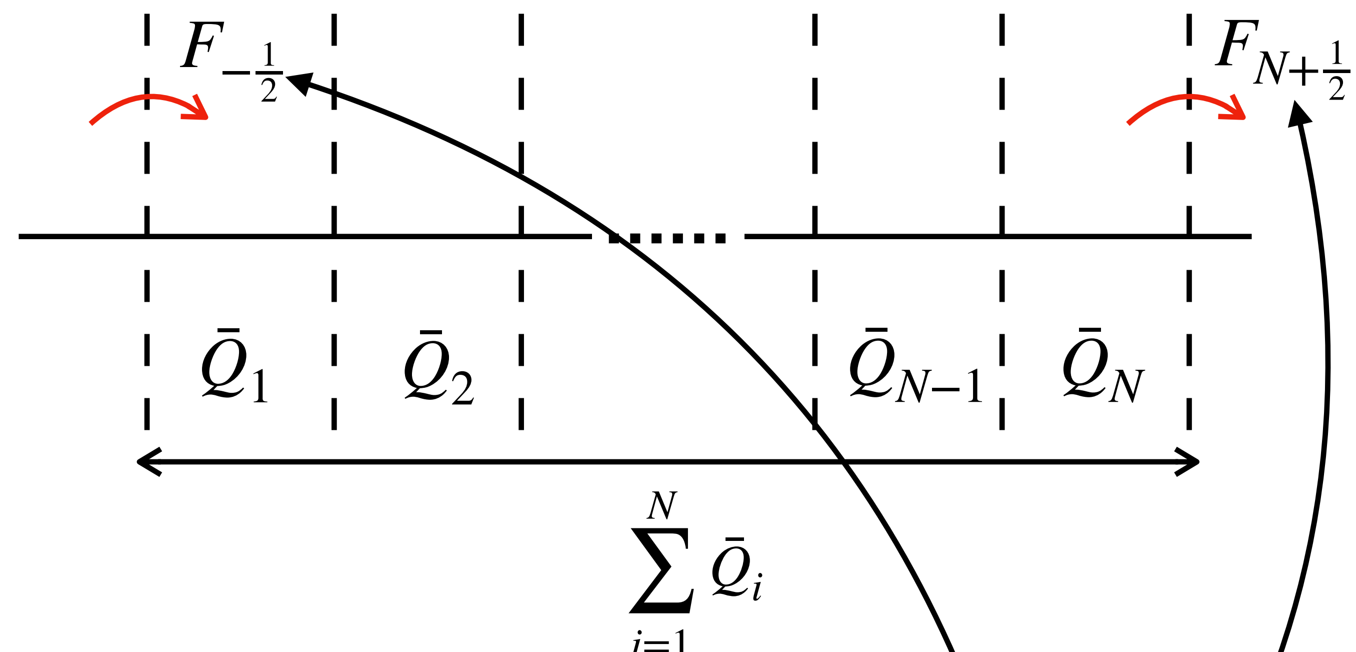
Finite Volume Methods

Conservation nature



$$\frac{\partial}{\partial t}\bar{Q}_i = -\frac{1}{\Delta x}(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})$$

Sum over all the cells:



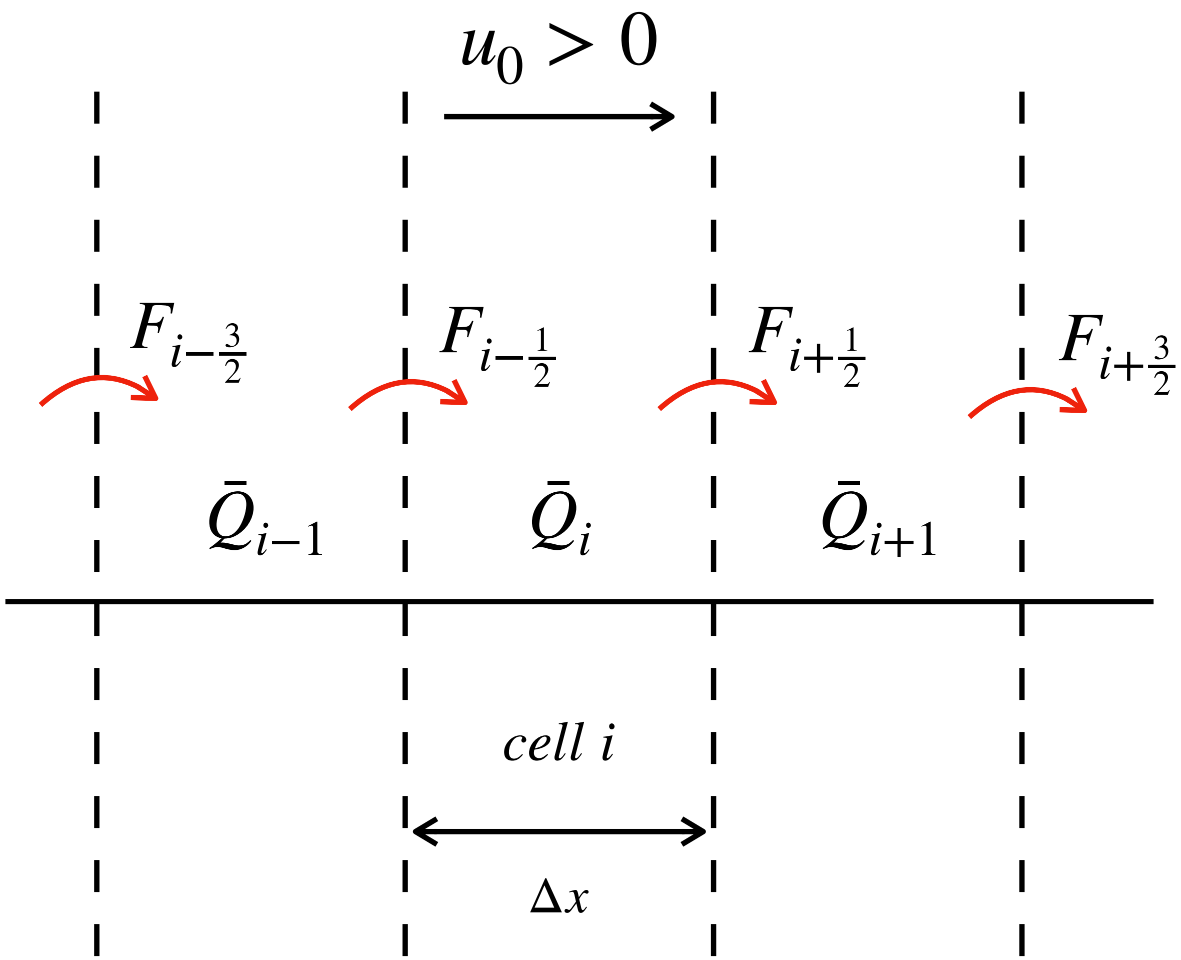
$$\sum_{i=1}^{N}\frac{\partial}{\partial t}\bar{Q}_i = \frac{\partial}{\partial t}\sum_{i=1}^{N}\bar{Q}_i = \frac{1}{\Delta x}\sum_{i=1}^{N}(F_{i-\frac{1}{2}} - F_{i+\frac{1}{2}})$$

$$= \frac{1}{\Delta x}\left[(F_{-\frac{1}{2}} - \cancel{F_{\frac{1}{2}}}) + (\cancel{F_{\frac{1}{2}}} - \cancel{F_{\frac{3}{2}}}) + (\cancel{F_{\frac{3}{2}}} - \cancel{F_{\frac{5}{2}}}) + \dots (\cancel{F_{N-\frac{1}{2}}} - F_{N+\frac{1}{2}})\right] = \frac{1}{\Delta x}(\boxed{F_{-\frac{1}{2}}} - \boxed{F_{N+\frac{1}{2}}})$$

If the flux at i=-1/2 and i=N+1/2 is zero, then the total mass is not going to change

Finite Volume Methods

The upwind method in the FV framework



$$\frac{\partial}{\partial t}\bar{Q}_i = -\frac{1}{\Delta x}(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})$$

Let's drop the bar and use Q in the following

If the advection towards right (u_0 > 0), a natural choice for the flux at interface is

$$F_{i+\frac{1}{2}} = u_0 Q_i^n \quad (F_{i-\frac{1}{2}} = u_0 Q_{i-1}^n)$$

Now the updates becomes

$$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$$

Another natural choice of the interface flux is

$$F_{i+\frac{1}{2}} = \frac{1}{2}(u_0 Q_i^n + u_0 Q_{i+1}^n) \qquad F_{i-\frac{1}{2}} = \frac{1}{2}(u_0 Q_{i-1}^n + u_0 Q_i^n)$$

Which gives

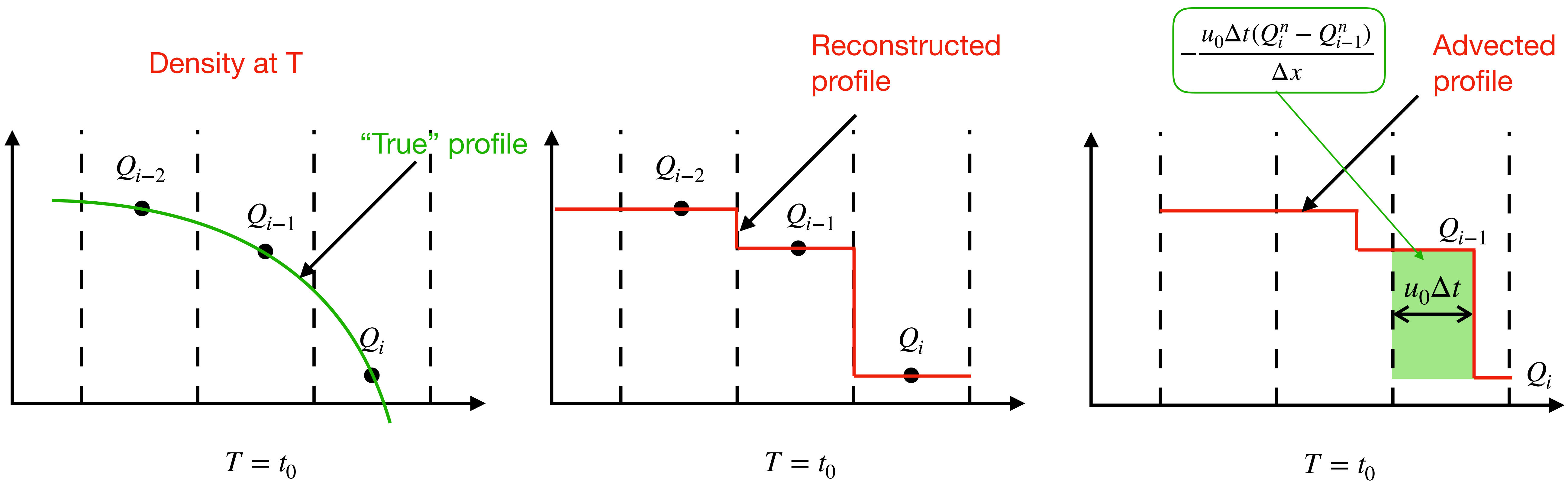
$$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{2\Delta x}(Q_{i+1}^n - Q_{i-1}^n)$$

The UNSTABLE central scheme!

Finite Volume Methods

REA w/ the 1st-order upwind method

The upwind method is basically a piecewise constant reconstruction scheme



Which means we're assuming the density profile within cell i is constant:

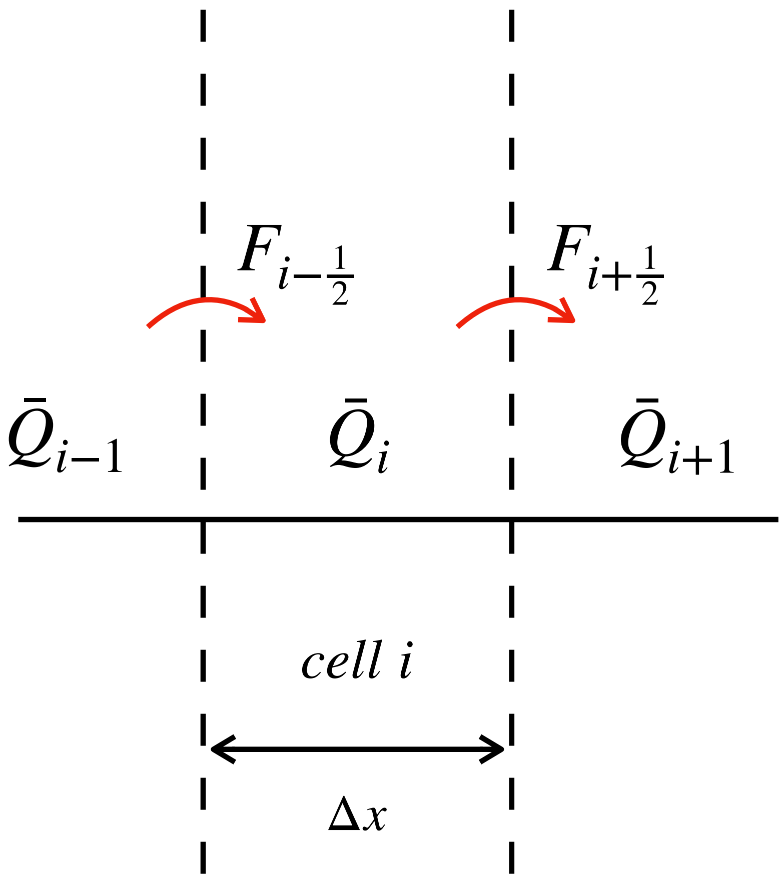
$$q(x) = Q_i, \;\; x \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$$

By doing this, the modified equation has an explicit diffusion term $\dfrac{\partial q}{\partial t} + u_0 \dfrac{\partial q}{\partial x} \approx \beta_{xx} \dfrac{\partial^2 q}{\partial x^2}$

This is because we are treating the initial profile Q(x) as step functions - possible very far away from the "true" solution unless delta x is really small.

The 1st-order upwind scheme is horrible

Flux of the 1st-order upwind method



FV form:

$$\frac{\partial}{\partial t}Q_i = -\frac{1}{\Delta x}(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})$$

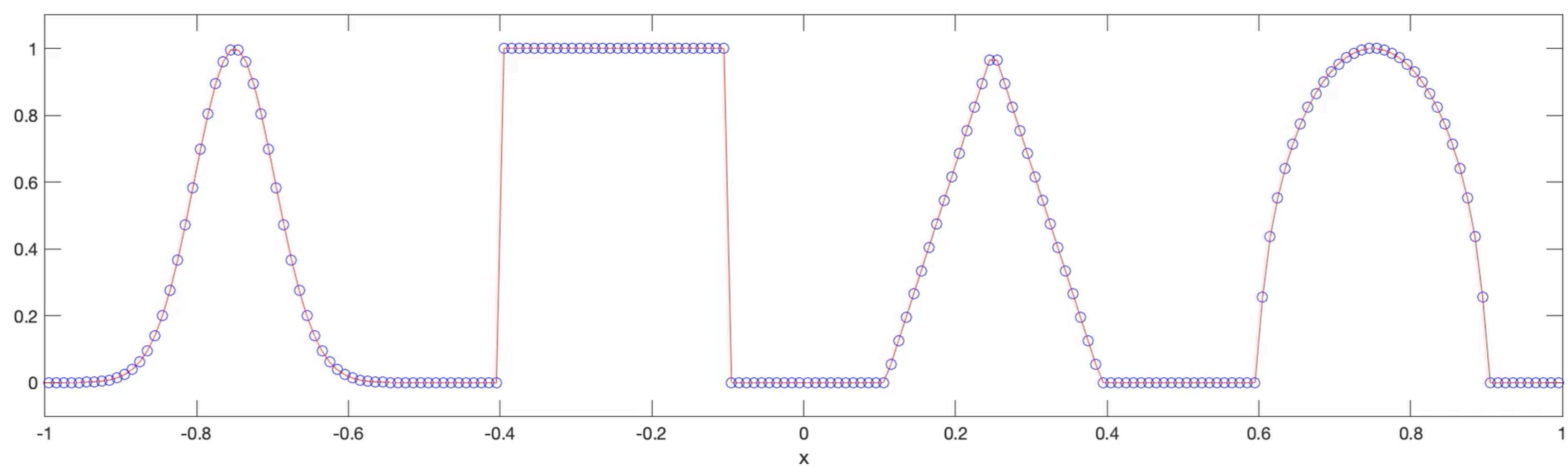
Interface Flux:

$$F_{i+\frac{1}{2}}(Q_i, Q_{i+1}) = \frac{1}{2}(u_0 Q_i + u_0 Q_{i+1}) - \frac{1}{2}|u_0|(Q_{i+1} - Q_i)$$

Alternatively:

$F(Q) = u_0 Q$

$$F_{i+\frac{1}{2}}(Q_i, Q_{i+1}) = \frac{1}{2}(F(Q_i) + F(Q_{i+1})) - \frac{1}{2}|u_0|(Q_{i+1} - Q_i)$$



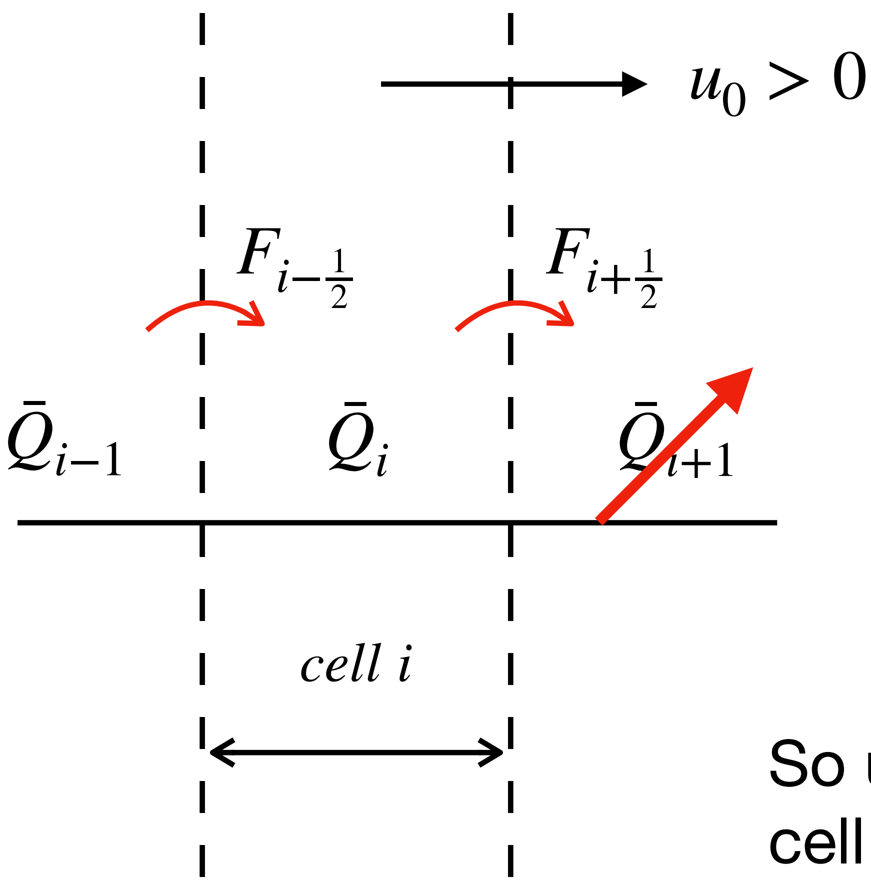
Upwind flux versus Central flux

We now know that the upwind scheme can be written as a combination of a second-order flux with a diffusion term:

$F(Q) = u_0 Q$

$$F_{i+\frac{1}{2}}(Q_i, Q_{i+1}) = \underbrace{\frac{1}{2}(F(Q_i) + F(Q_{i+1}))}_{\textbf{2nd-order flux}} - \underbrace{\frac{1}{2}|u_0|(Q_{i+1} - Q_i)}_{\textbf{Diffusion term}}$$

why?



Let’s difference the flux F_i+1/2:

$$F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} \sim -\frac{1}{2}|u_0|\underbrace{(Q_{i+1} - 2Q_i + Q_{i-1})}_{\sim \frac{\partial^2 Q}{\partial x^2}}$$

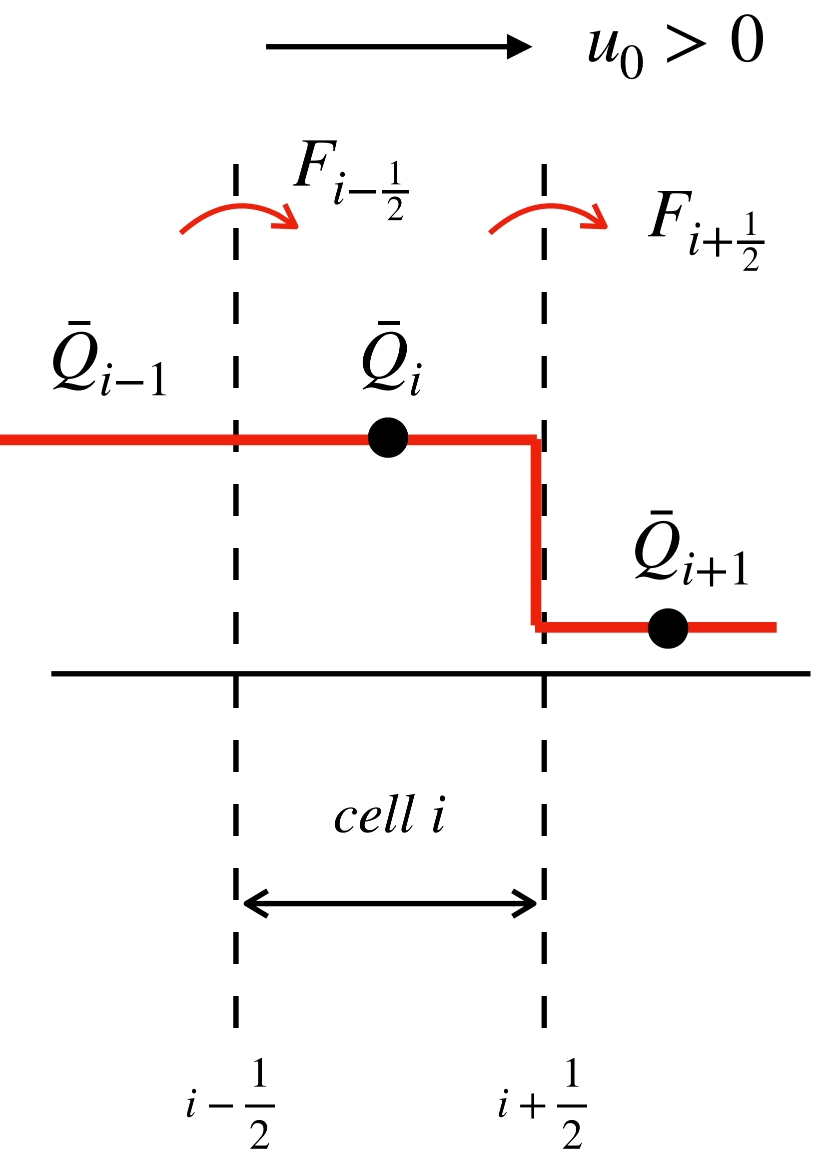
So upwind scheme basically cancels out the furthest downwind cell and make the flux one-sided

This leads to the so-called family of **central schemes**

Which means as long as we know the speed of the waves, we don’t need to care about the direction of the propagation anymore

Origin of Numerical diffusion in Upwind

Upwind: $$F_{i+\frac{1}{2}}(Q_i, Q_{i+1}) = \frac{1}{2}(F(Q_i) + F(Q_{i+1})) - \frac{1}{2}|u_0|(Q_{i+1} - Q_i)$$



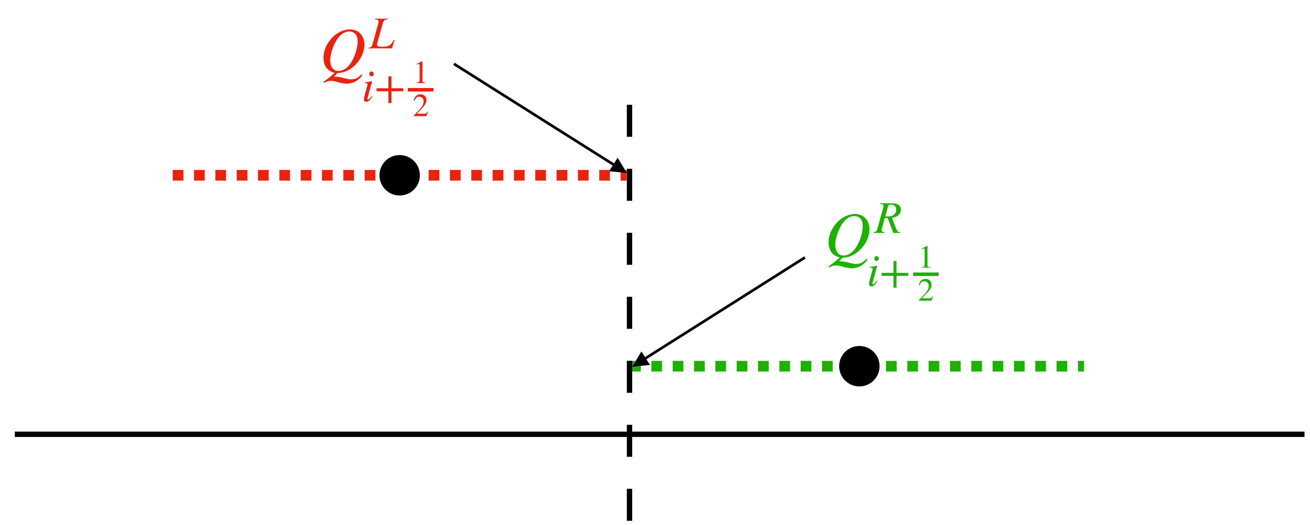
So as long as Q_i is not equal to Q_i-1, numerical diffusion is introduced, which is described by the modified equation as

$$\boxed{\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \beta_{xx} \frac{\partial^2 q}{\partial x^2}}$$

Numerical diffusion

Modified equation

If we regard Qi and Q_i+1 as zeroth-order reconstruction:

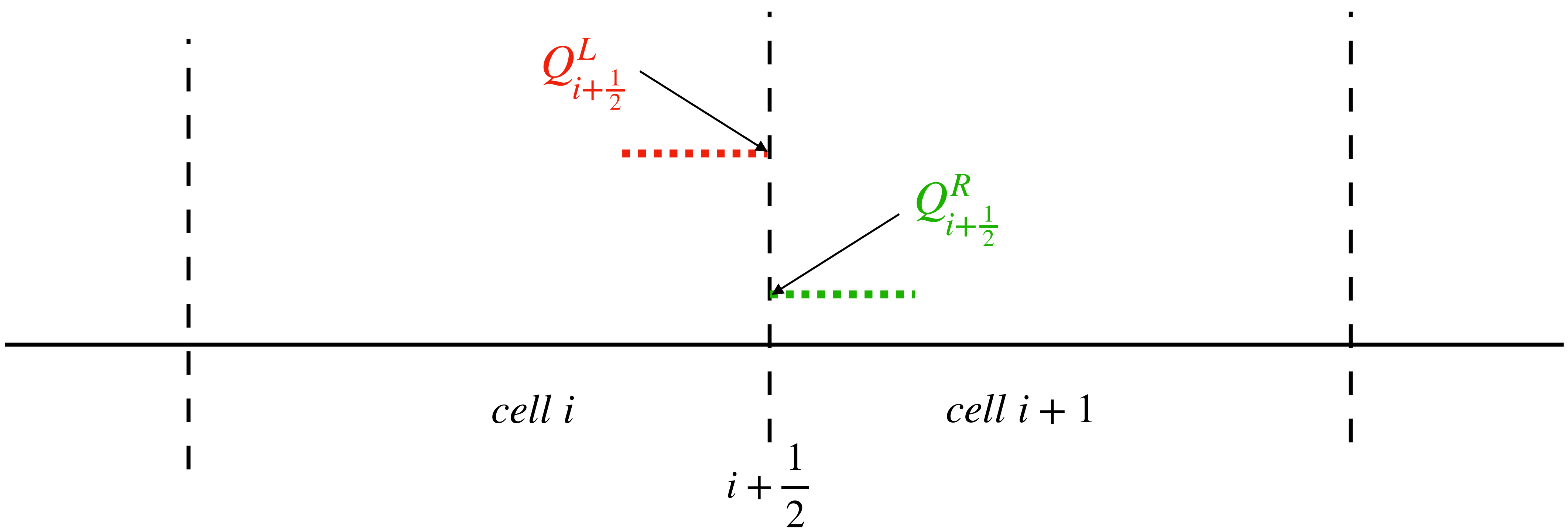


Upwind Flux is basically: $$F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \frac{1}{2}|u_0|(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})$$

Central Schemes

Interface states and wave speed

The use of upwind schemes require the knowledge of the wave speed and direction of the propagation - not always available in non-linear problems. So central schemes are convenient which does not require the information of the wave propagation:



Lax-Friedrichs $$F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \frac{\Delta x}{2\Delta t}(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})$$

Rusanov $$F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \frac{1}{2}|u_{max}|(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})$$

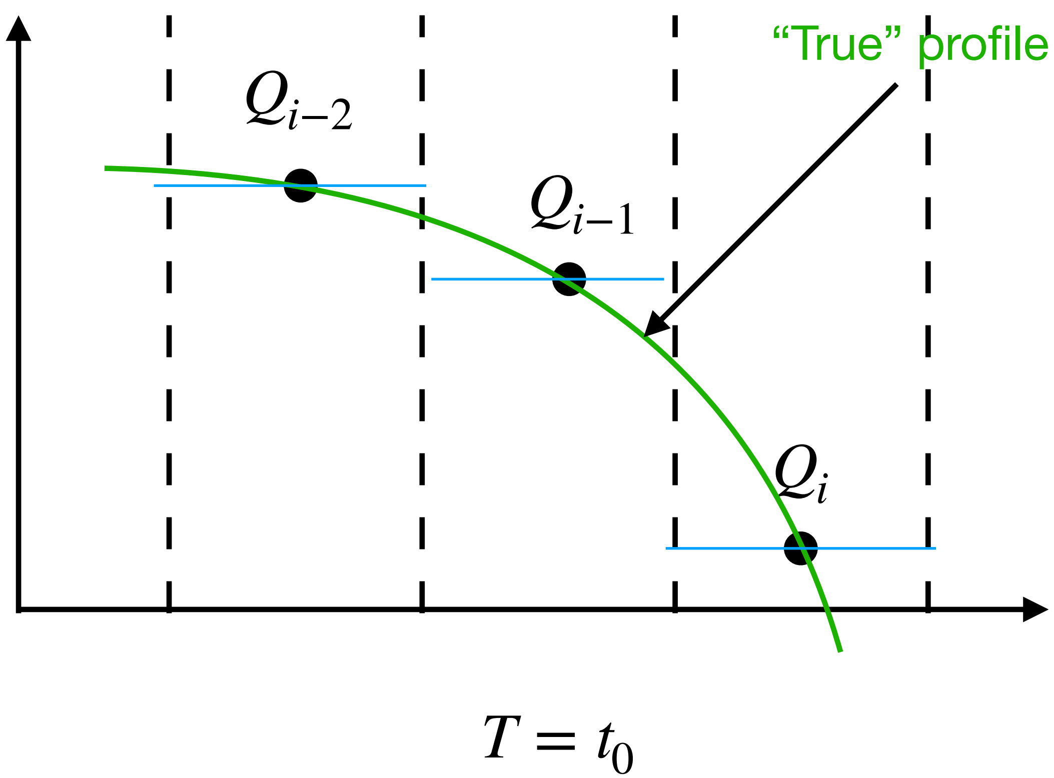
So the numerical diffusion is basically from Q_R - Q_L, how to reduce that?

Finite Volume Methods

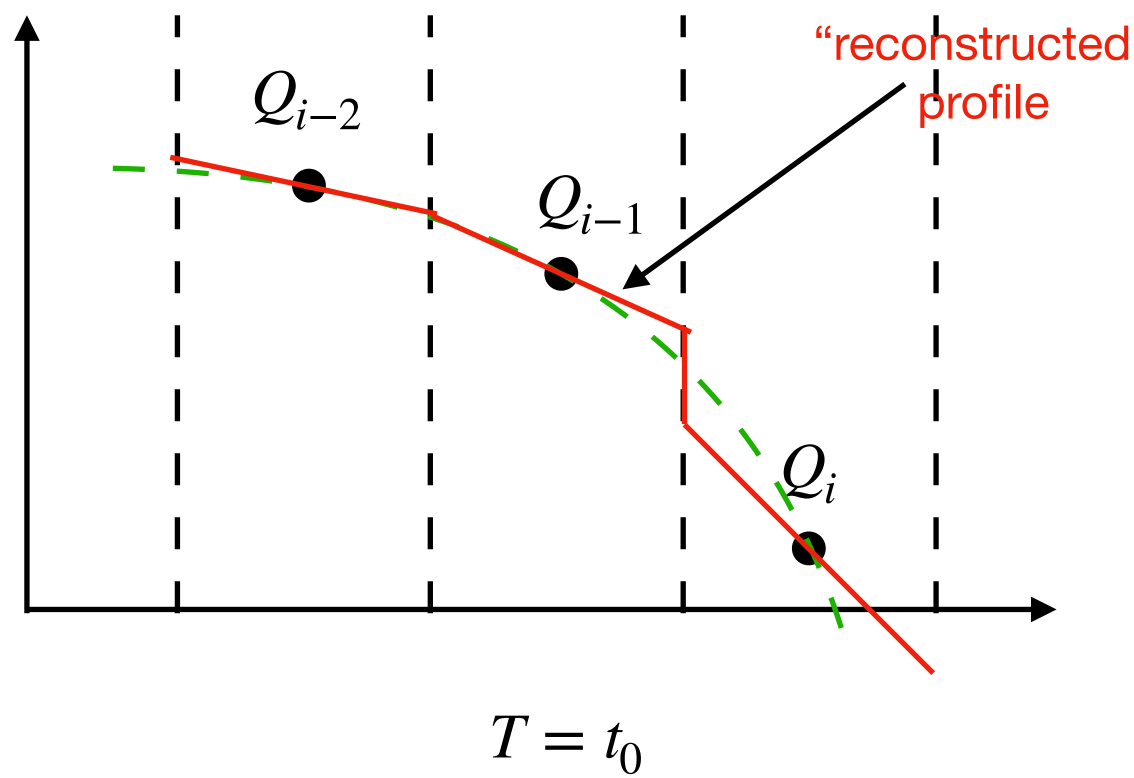
REA with Second-order methods

Now to improve the solution, using a more accurate reconstruction for the profile is needed:

Piecewise-constant



Piecewise-linear



Which means we’re assuming the density profile within cell i is linear:

$$q(x) = Q_i + \sigma_i (x - x_i), \;\; x \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$$

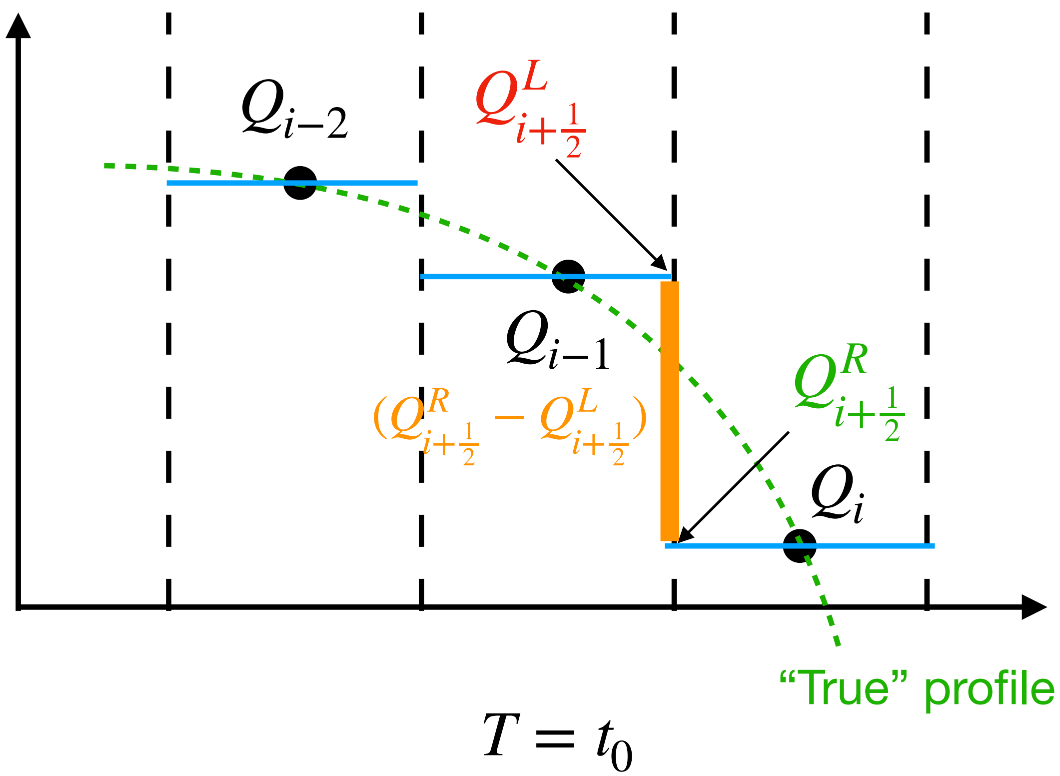
This is called *piecewise linear* reconstruction for Q, and the method is generally 2nd order

Finite Volume Methods

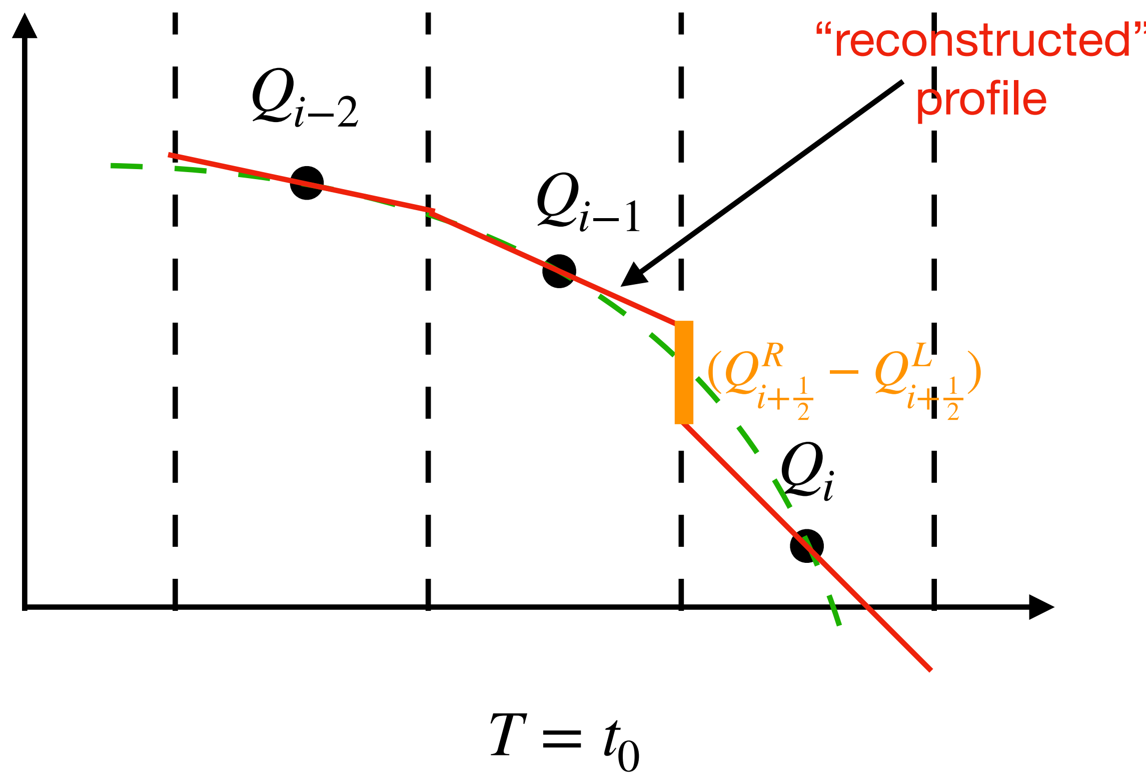
REA with Second-order methods

Now to improve the solution, using a more accurate reconstruction for the profile is needed:

Zeroth-order Reconstruction



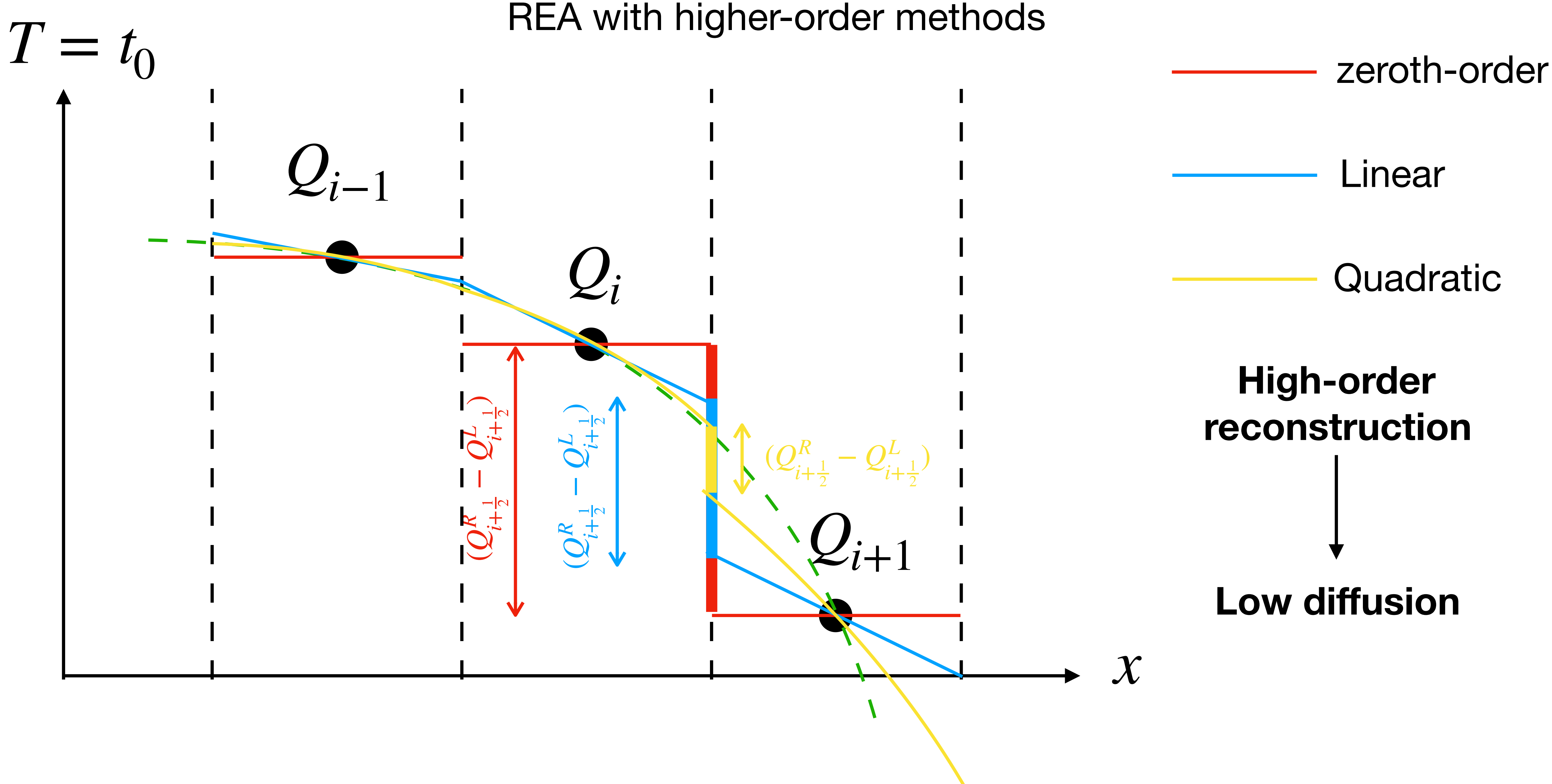
1st-order Reconstruction



Flux is basically: $F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \underbrace{\frac{1}{2}|u_0|\boxed{(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})}}_{\text{Diffusion term}}$

Finite Volume Methods

REA with higher-order methods



$$F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \frac{1}{2}|u_0| \underbrace{\boxed{(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})}}_{\text{Diffusion term}}$$

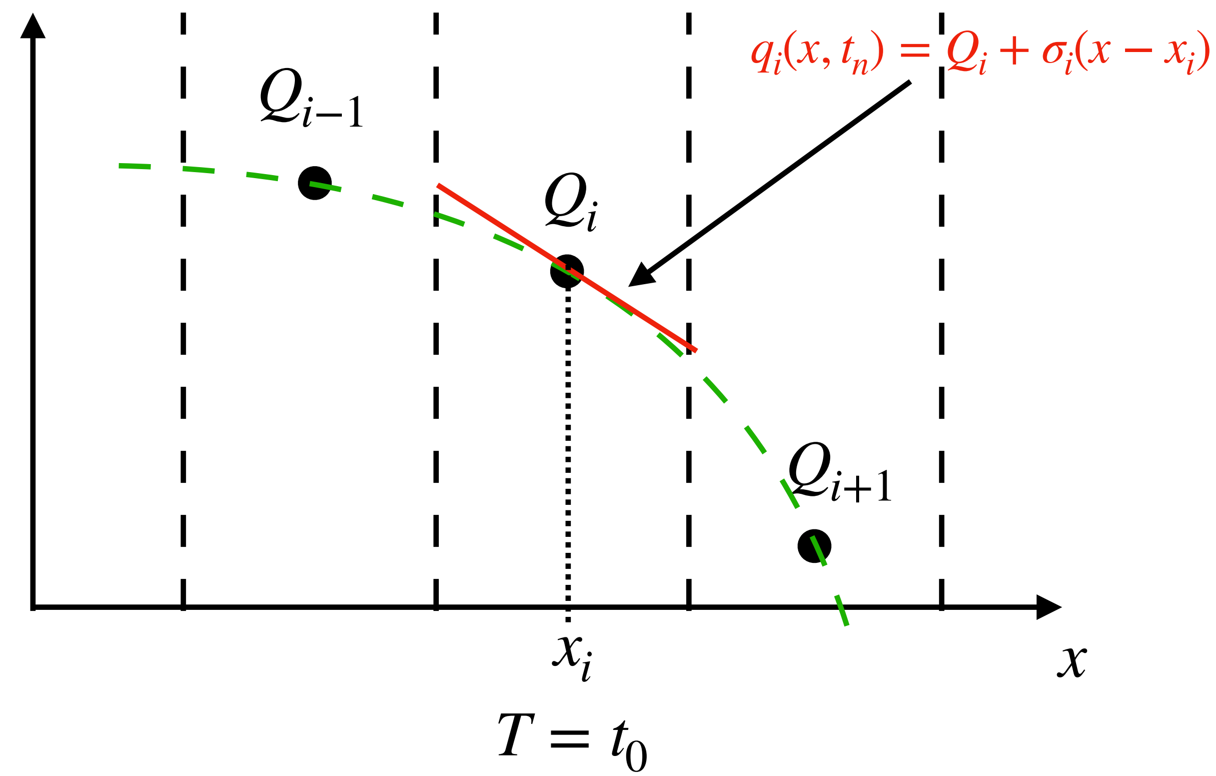
Does that mean we can go arbitrary high order reconstruction for QL and QR?

Unfortunately, It's not that simple

Slope and preview of limiters

the density profile within cell i is linear:

$$q(x,t_n) = Q_i + \sigma_i(x - x_i), \;\; x \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$$



It is straightforward to show that

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} q(x,t_n)dx = Q_i$$

Which means the reconstruction is *conservative*

After one step, the solution becomes

$q(x,t_{n+1}) = q(x - u_0\Delta t, t_n)$ which is a shift of the q(x) profile towards right

The finite volume solution is then

$$Q_i^{n+1} = -\frac{1}{\Delta x}\left(\int_{x_{i-\frac{1}{2}}}^{x_{i-\frac{1}{2}}+u_0\Delta t} q_{i-1}(x - u_0\Delta t)dx + \int_{x_{i-\frac{1}{2}}+u_0\Delta t}^{x_{i+\frac{1}{2}}} q_i(x - u_0\Delta t)dx\right)$$

Choice of Slope

A preview of limiting

The solution with the piecewise linear reconstruction method is

$$Q_i^{n+1} = -\frac{1}{\Delta x}\left(\int_{x_{i-\frac{1}{2}}}^{x_{i-\frac{1}{2}}+u_0\Delta t} q_{i-1}(x-u_0\Delta t)dx + \int_{x_{i-\frac{1}{2}}+u_0\Delta t}^{x_{i+\frac{1}{2}}} q_i(x-u_0\Delta t)dx\right)$$

$$= \frac{u_0\Delta t}{\Delta x}\left[Q_{i-1}^n + \frac{1}{2}(\Delta x - u_0\Delta t)\sigma_{i-1}^n\right] + \left(1-\frac{u_0\Delta t}{\Delta x}\right)(Q_i^n - \frac{1}{2}u_0\Delta t\sigma_i^n)$$

$$= \boxed{Q_i^n - \frac{u_0\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) - \frac{1}{2}\frac{u_0\Delta t}{\Delta x}(\Delta x - u_0\Delta t)(\sigma_i^n - \sigma_{i-1}^n) + \mathcal{O}(\Delta x^2)}$$

2nd-order
Piecewise Linear Method

Recall the modified equation for the upwind method (1st order)

$$\frac{\partial q}{\partial t} + u_0\frac{\partial q}{\partial x} \approx \frac{1}{2}u_0\Delta x\left(1-\frac{u_0\Delta t}{\Delta x}\right)\frac{\partial^2 q}{\partial x^2}$$

The term $-\frac{1}{2}\frac{u_0\Delta t}{\Delta x}(\sigma_i^n - \sigma_{i-1}^n)$ is anti-diffusion flux which reduces the diffusion in upwind

Choice of Slope

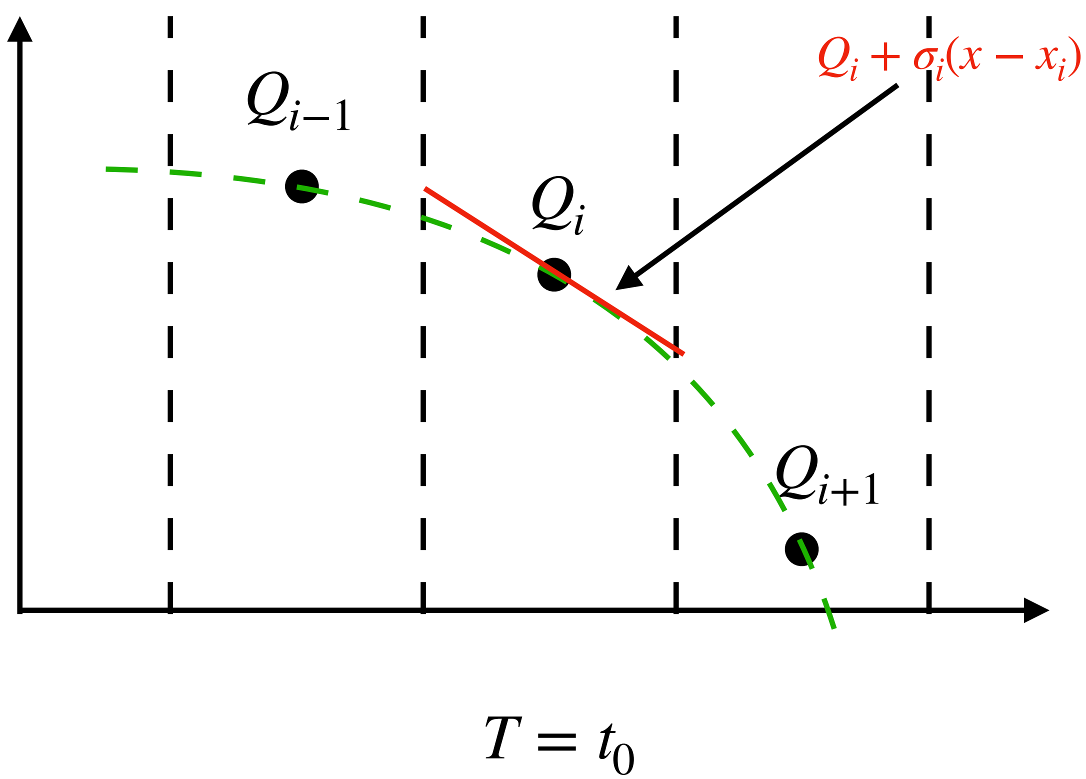
2nd-order methods:

$$\boxed{Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) - \frac{1}{2}\frac{u_0 \Delta t}{\Delta x}(\Delta x - u_0 \Delta t)(\sigma_i^n - \sigma_{i-1}^n) + \mathcal{O}(\Delta x^2)}$$

Our 1st order method

$$\sigma_i^n = 0$$ (Upwind method)

Some 2nd order methods



$$\sigma_i^n = \frac{Q_{i+1}^n - Q_{i-1}^n}{2\Delta x}$$ (Fromm's method)

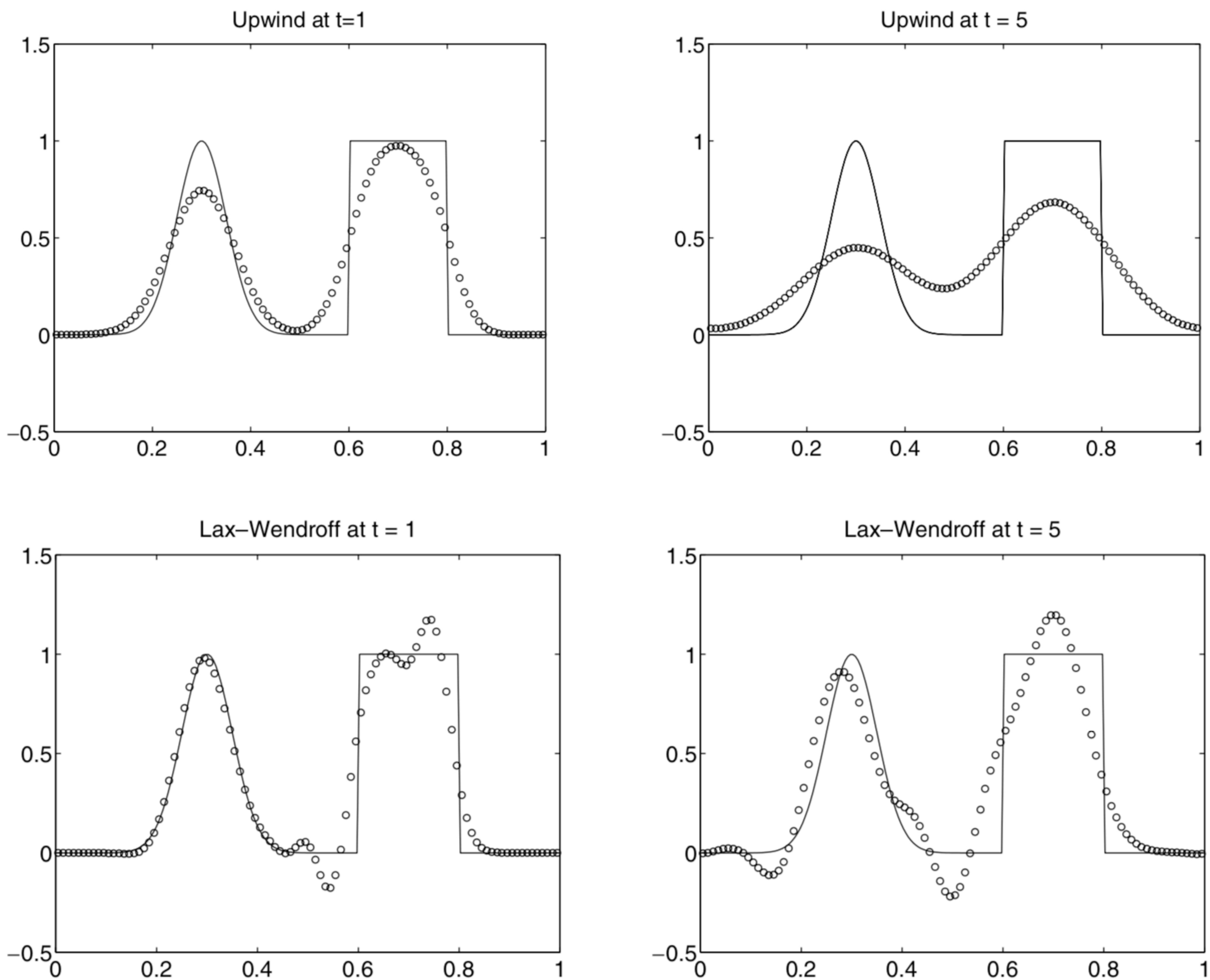
$$\sigma_i^n = \frac{Q_i^n - Q_{i-1}^n}{\Delta x}$$ (Beam-warming method)

$$\sigma_i^n = \frac{Q_{i+1}^n - Q_i^n}{\Delta x}$$ (Lax Wendroff method)

Results form Lax-Wendroff Method

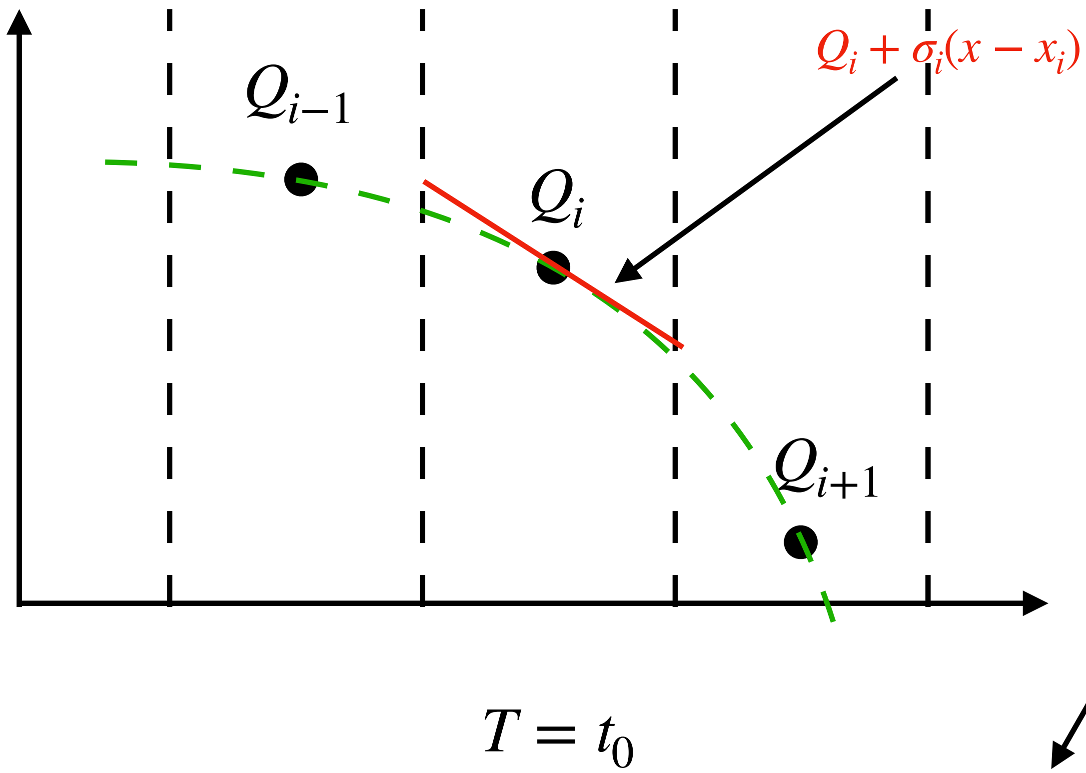
UPWIND

LAX-WENDROFF



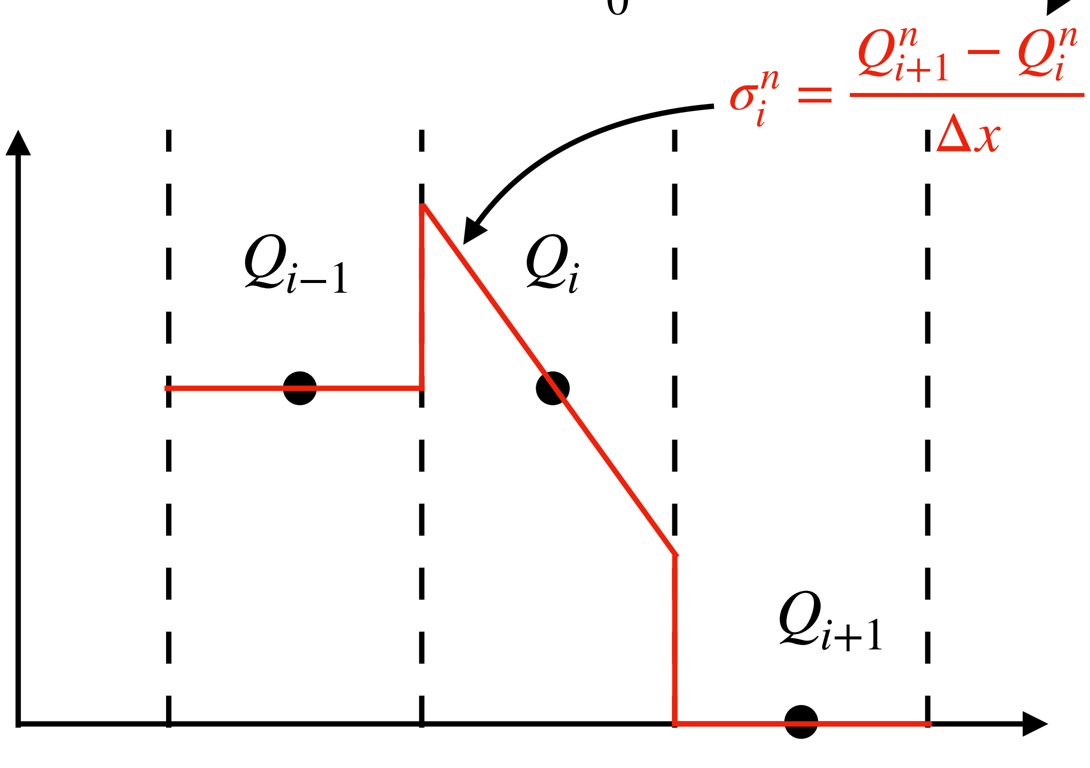
Why 2nd-order method oscillates?

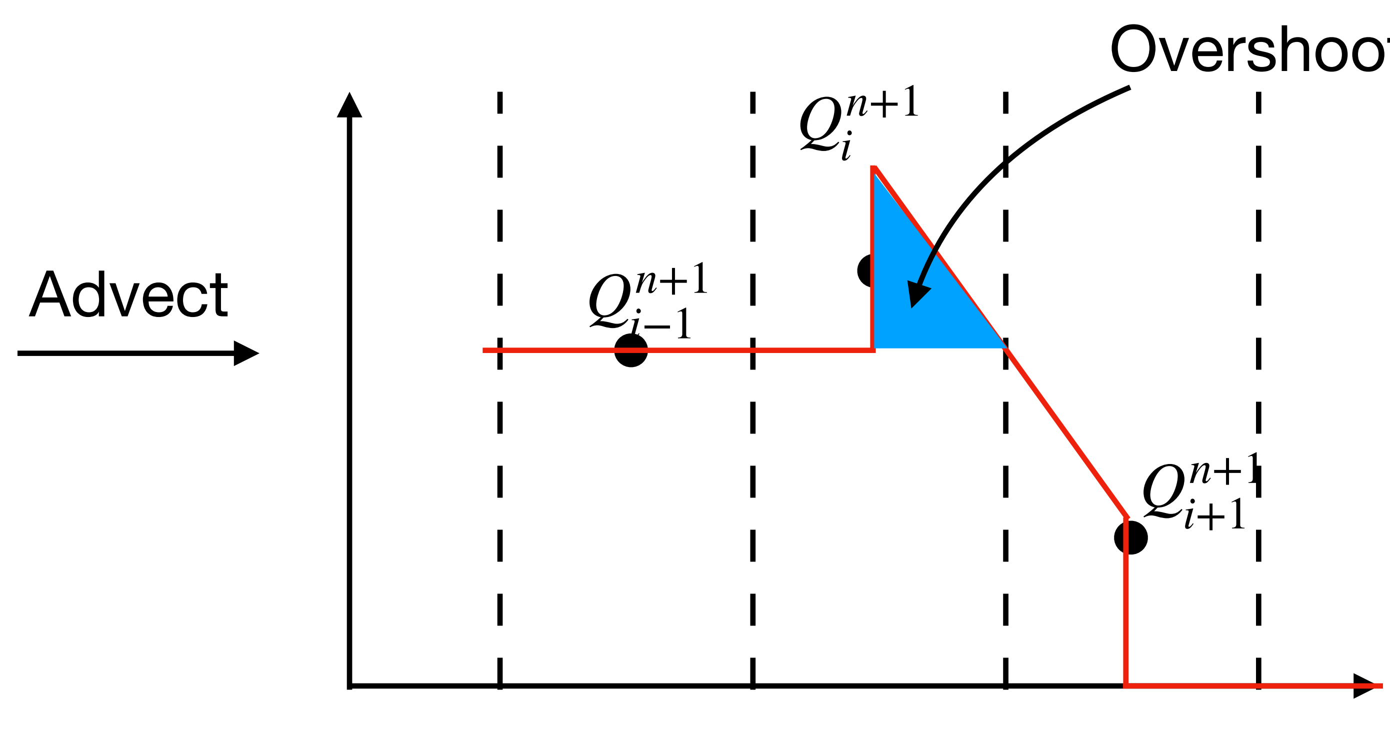
Lax-Wendroff



Use this slope in reconstruction

$$\sigma_i^n = \frac{Q_{i+1}^n - Q_i^n}{\Delta x} \quad \text{(Lax Wendroff method)}$$





What is Numerical Dispersion

Recall the modified equation for upwind method

Original Equation	Numerical Approximation	Modified Equation
$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$	$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$	$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \boxed{\beta_{xx} \frac{\partial^2 q}{\partial x^2}}$

Diffusion

For the 2nd-order Lax Wendroff method, we have

Original Equation	Numerical Approximation	Modified Equation
$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$	$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) + \frac{1}{2}\frac{u_0^2 \Delta t^2}{\Delta x^2}(Q_{i-1}^n - 2Q_i^n + Q_{i+1}^n)$	$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \boxed{\beta_{xxx} \frac{\partial^3 q}{\partial x^3}}$

Dispersion

What is Numerical Diffusion

Upwind method: $$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \boxed{\beta_{xx} \frac{\partial^2 q}{\partial x^2}}$$

Diffusion

Let's first take a look at the upwind method: $$\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \beta_{xx} \frac{\partial^2 q}{\partial x^2}$$

Only consider the numerical term: $$\frac{\partial q}{\partial t} \sim \beta_{xx} \frac{\partial^2 q}{\partial x^2}$$

Try harmonic analysis: $$q \sim e^{i(\omega t - kx)} \longrightarrow i\omega q \sim \beta_{xx}(-ik)^2 q \longrightarrow \omega = i\beta_{xx}k^2$$

This is a damping term: $$q \sim e^{i(\omega t - kx)} = e^{i(i\beta_{xx}k^2 t - kx)} = e^{-\beta_{xx}k^2 t} e^{-ikx}$$

Damping

This is why we say the leading error term in the upwind method is diffusion

What is Numerical Dispersion

Lax-Wendroff method: $\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \boxed{\beta_{xxx} \frac{\partial^3 q}{\partial x^3}}$

Dispersion

Let's first take a look at the upwind method: $\frac{\partial q}{\partial t} + u_0 \frac{\partial q}{\partial x} \approx \beta_{xxx} \frac{\partial^3 q}{\partial x^3}$

Only consider the numerical term: $\frac{\partial q}{\partial t} \sim \beta_{xxx} \frac{\partial^3 q}{\partial x^3}$

Try harmonic analysis:

$$q \sim e^{i(\omega t - kx)} \longrightarrow i\omega q \sim \beta_{xxx}(-ik)^3 q \longrightarrow \omega = \beta_{xxx} k^3 \longrightarrow \frac{\omega}{k} = \beta_{xxx} k^2$$

Phase speed

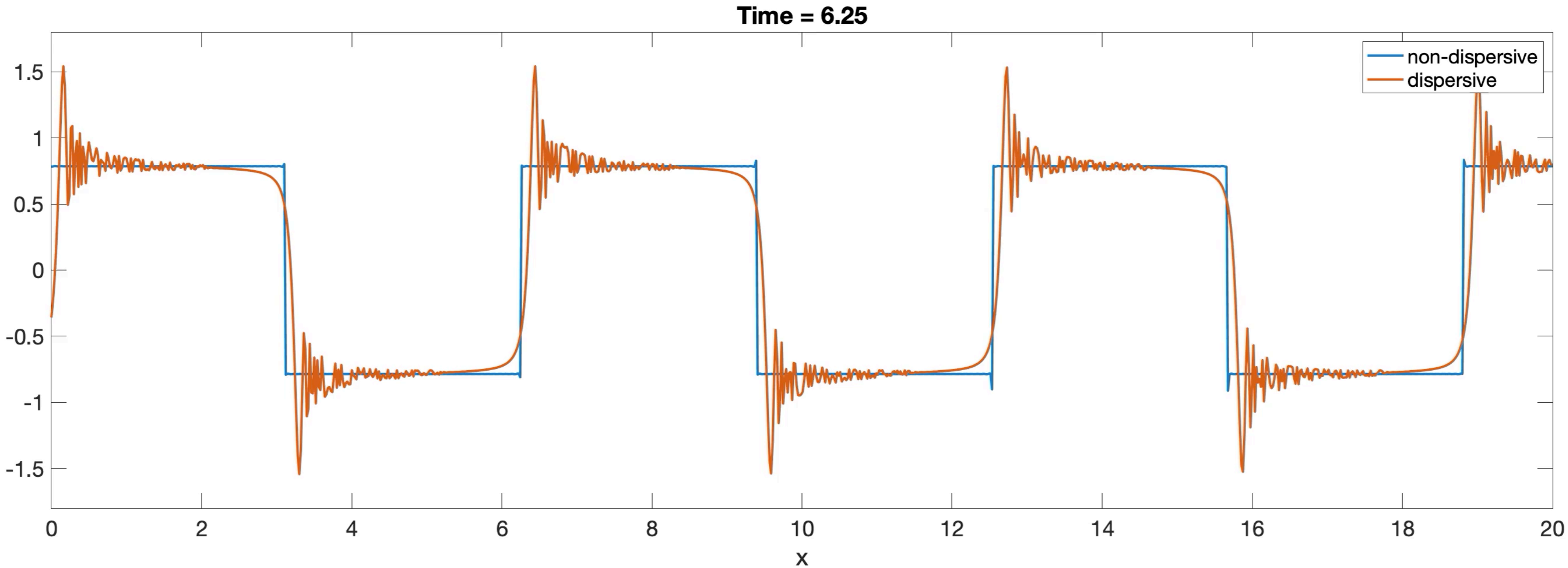
This is saying the phase speed of the wave is dependent on the wave number k - the shorter the wave length is, the faster the propagation speed is

This is why we say the leading error term in the upwind method is dispersion

Dispersion of waves

Non-dispersive : waves with different k travels at the same speed

dispersive : waves with different k travels at different speed



$$f(x-vt) = \sum_{n=0}^{\infty} \frac{1}{2n+1} \sin[(2n+1)(x-vt)]$$ Non-dispersive — "waveform" kept the same

$$= \sum_{n=0}^{\infty} \frac{1}{2n+1} \sin[(2n+1)(x-v(n)t)]$$ dispersive — "waveform" oscillatory

$$v(n) \sim \sqrt{2n+1}$$

Total Variation

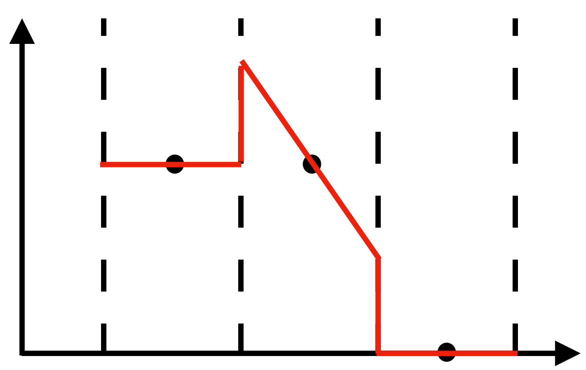
Definition: $TV \equiv \sum_{i=-\infty}^{+\infty} |Q_{i+1}^n - Q_i^n|$ For the linear advection equation, TV(Q) is a constant

Definition of TVD: a two-step method is TVD if $TV(Q^{n+1}) \leq TV(Q^n)$

So if a method is TVD, then if the initial profile is “monotonic”: $Q^{n+1} \geq Q^n$ for all i

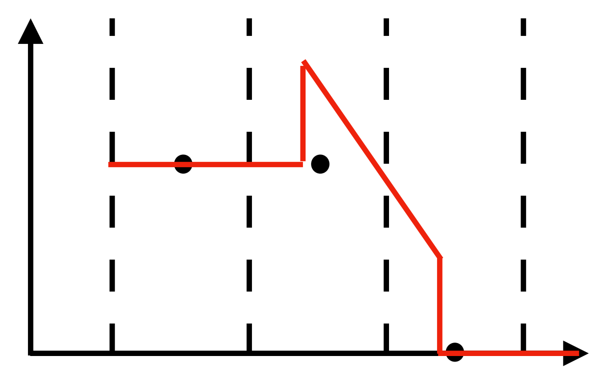
It will ***remain monotonic*** in all the future time steps (monotonicity preserving)

Reconstruct



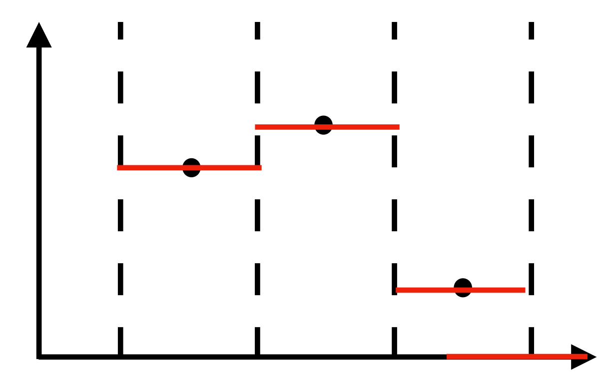
TV?

Evolve



$TV(q(x, t_{n+1}) = TV(q(x, t_n))$

Average

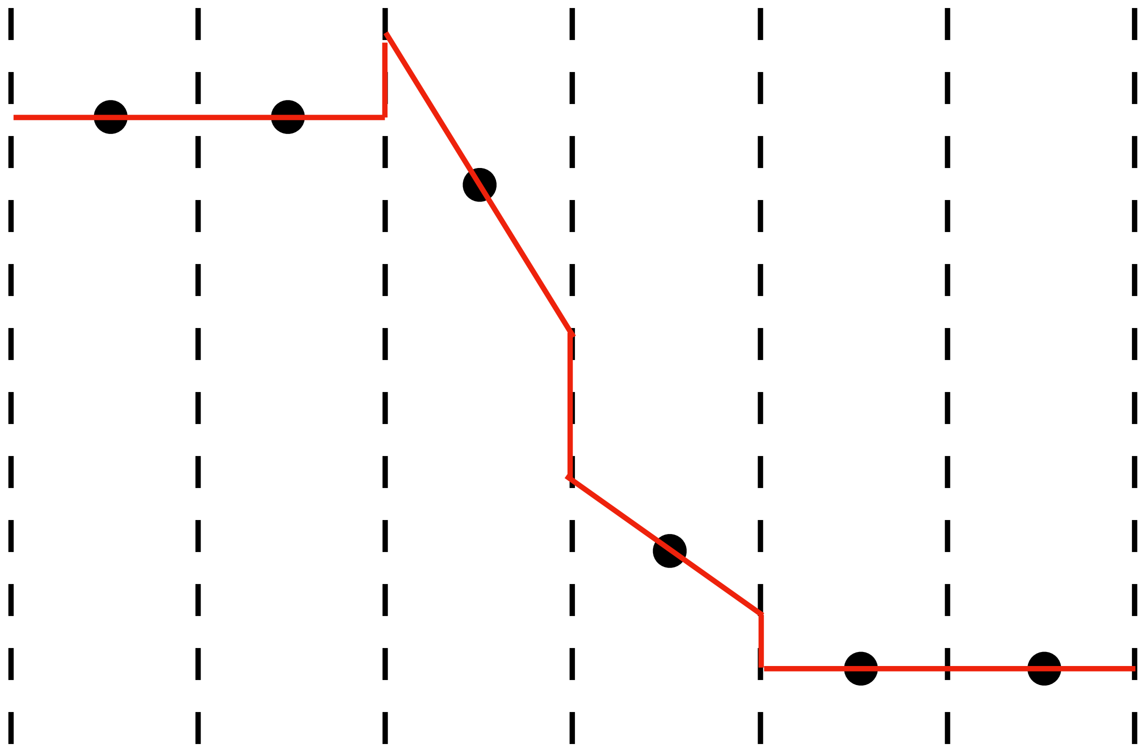


$TV(q(x, t_{n+1}) = TV(Q^{n+1})$

So it is the reconstruction step determines whether a scheme is TVD or not

Slope limiters for TVD solutions

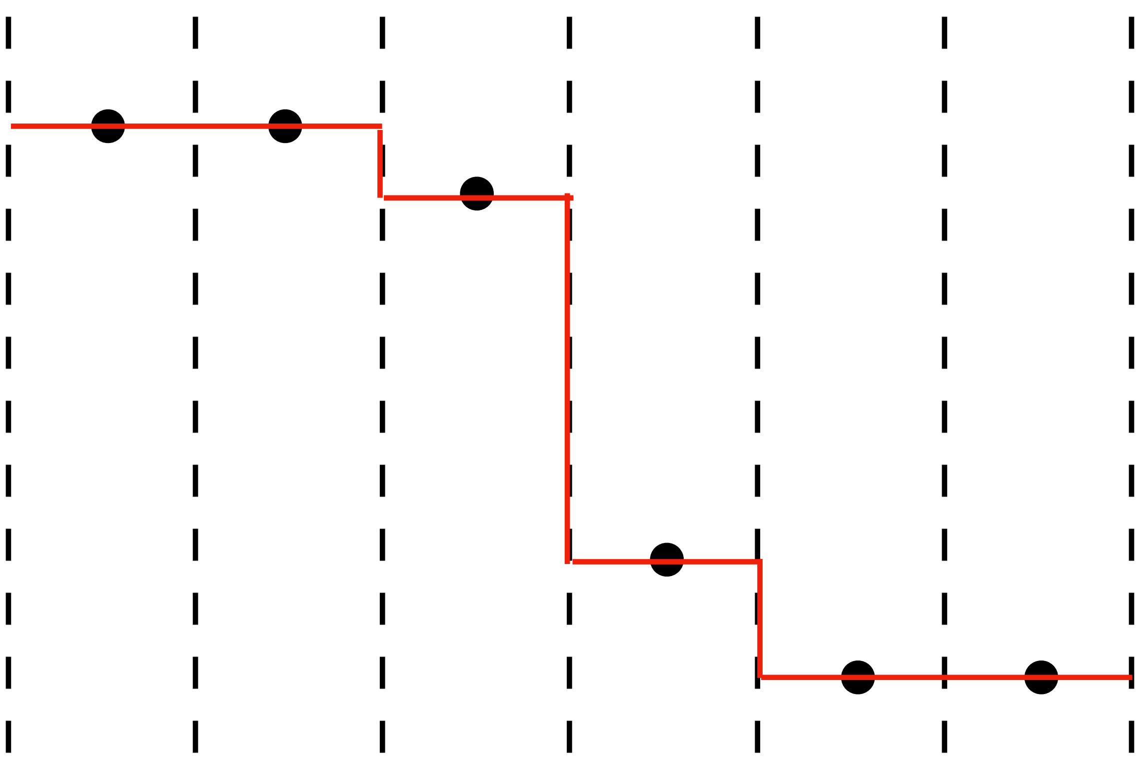
non-TVD reconstruction



$$\sigma_i^n = \frac{Q_{i+1}^n - Q_i^n}{\Delta x}$$ (Lax Wendroff method)

It's second-order but apparently non-TVD!

TVD reconstruction (PCM)



$$\sigma_i^n = 0$$ (first-order upwind)

It's TVD but apparently first-order

Slope Limiting for TVD solutions

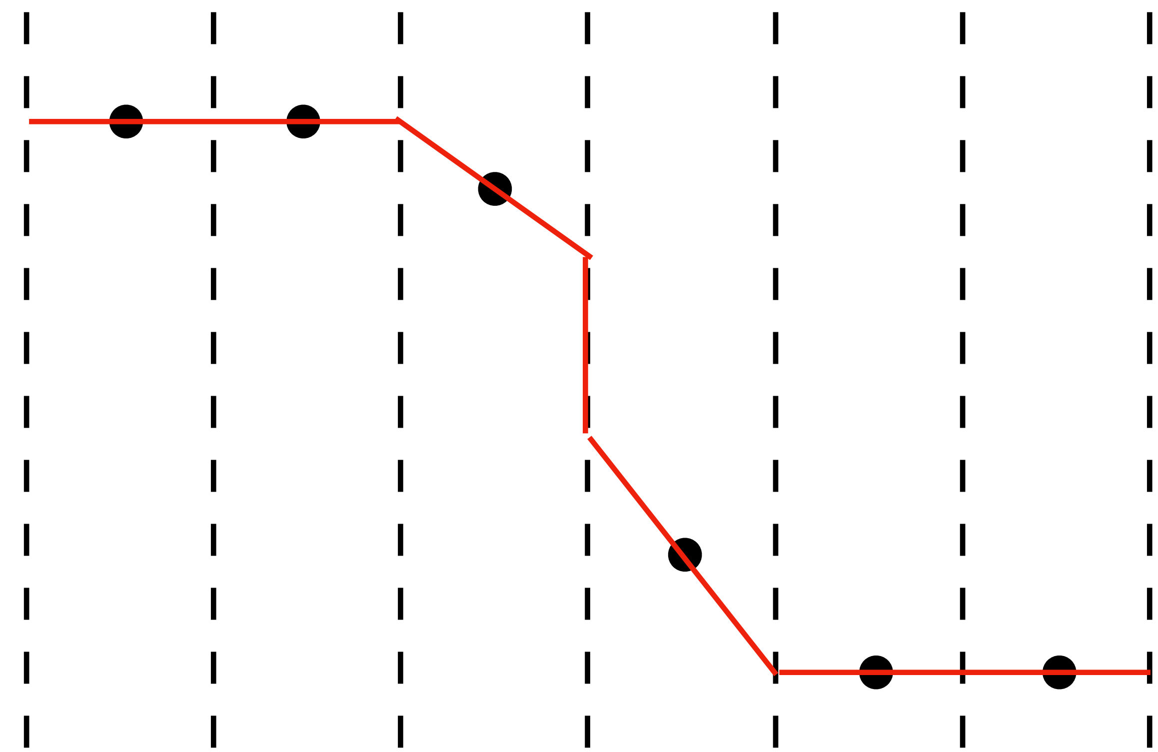
Super-bee Slope choice:

$$\sigma_i^n = \text{maxmod}(\sigma_i^{(1)}, \sigma_i^{(2)})$$

$$\sigma_i^{(1)} = \text{minmod}\left(\left(\frac{Q_{i+1}^n - Q_i^n}{\Delta x}\right),\ 2\left(\frac{Q_i^n - Q_{i-1}^n}{\Delta x}\right)\right),$$

$$\sigma_i^{(2)} = \text{minmod}\left(2\left(\frac{Q_{i+1}^n - Q_i^n}{\Delta x}\right),\ \left(\frac{Q_i^n - Q_{i-1}^n}{\Delta x}\right)\right).$$

TVD reconstruction (super-B)

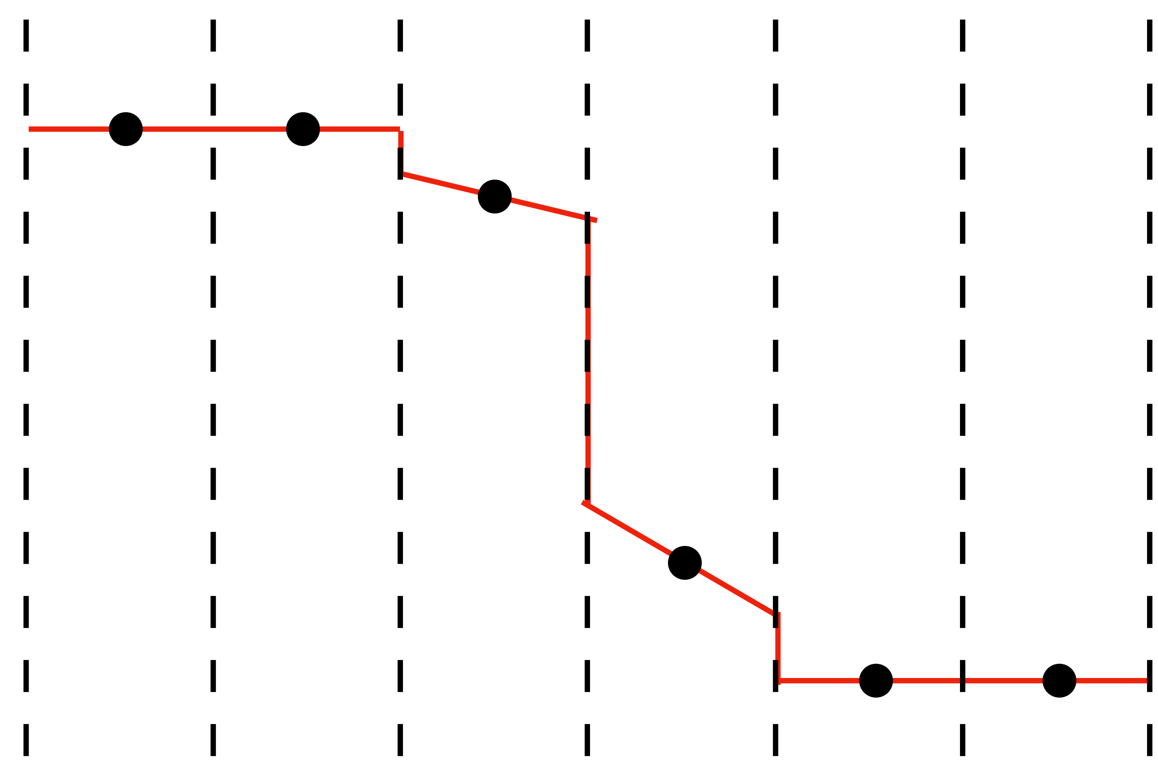


Minmod Slope choice:

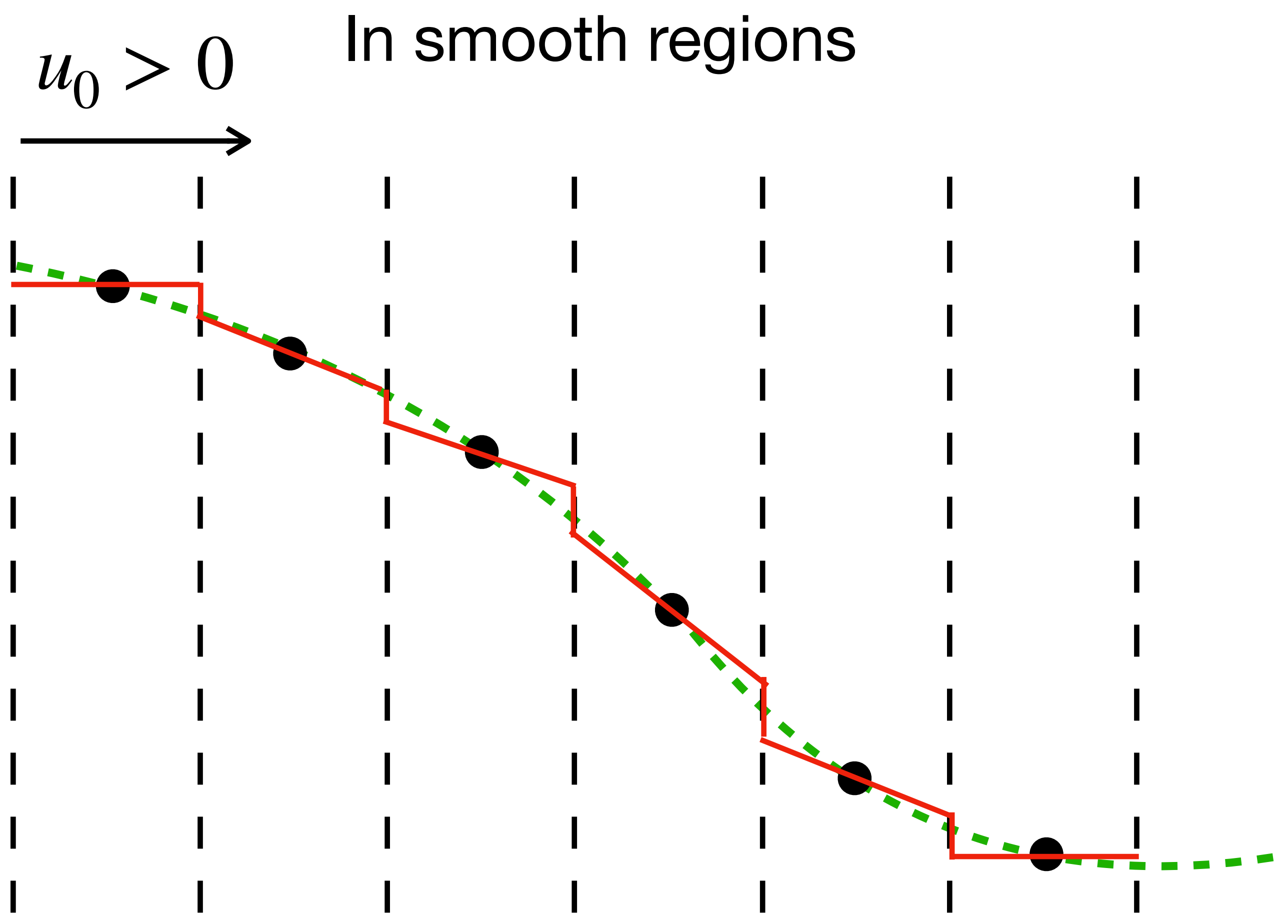
$$\sigma_i^n = \text{minmod}\left(\frac{Q_{i+1}^n - Q_i^n}{\Delta x}, \frac{Q_i^n - Q_{i-1}^n}{\Delta x}\right)$$

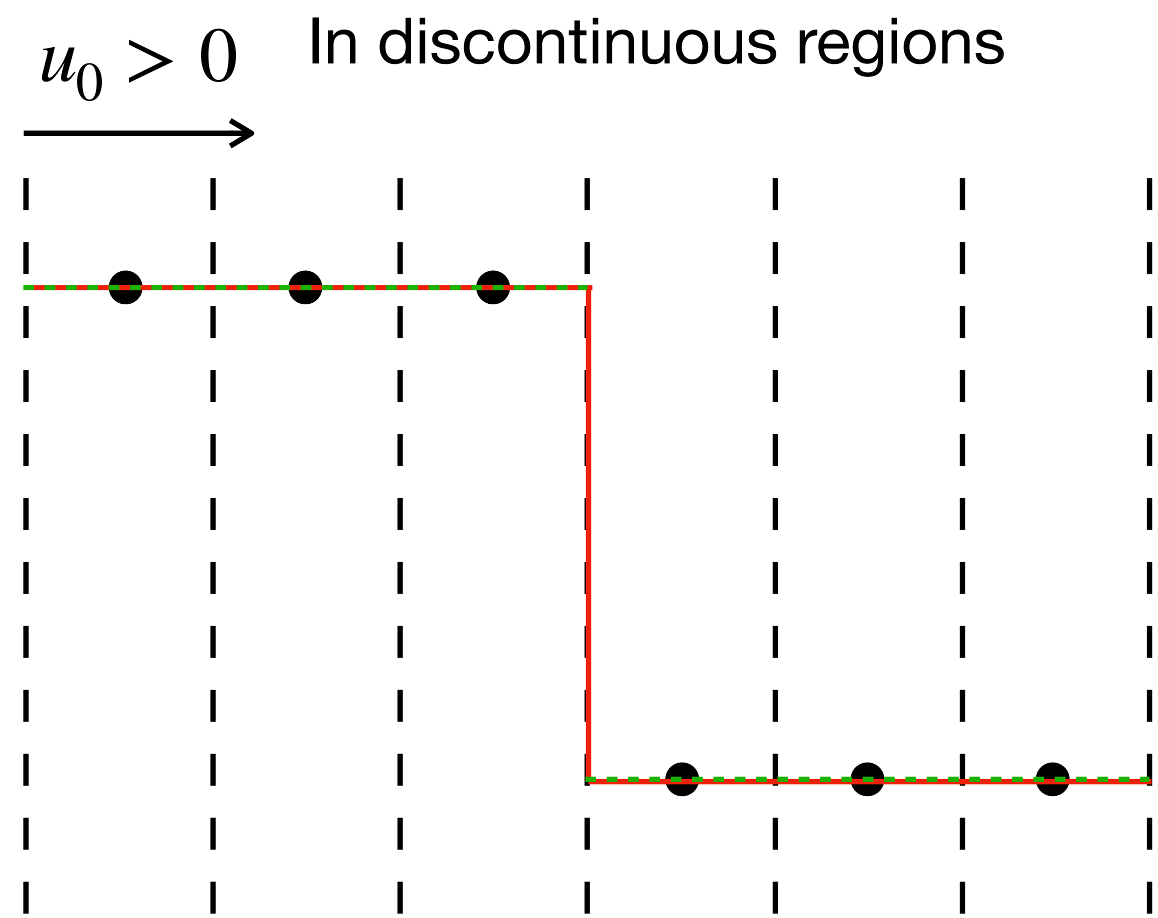
$$\text{minmod}(a,b) = \begin{cases} a & \text{if } |a| < |b| \text{ and } ab > 0, \\ b & \text{if } |b| < |a| \text{ and } ab > 0, \\ 0 & \text{if } ab \le 0. \end{cases}$$

TVD reconstruction (minmod)



What does slope limiters do?



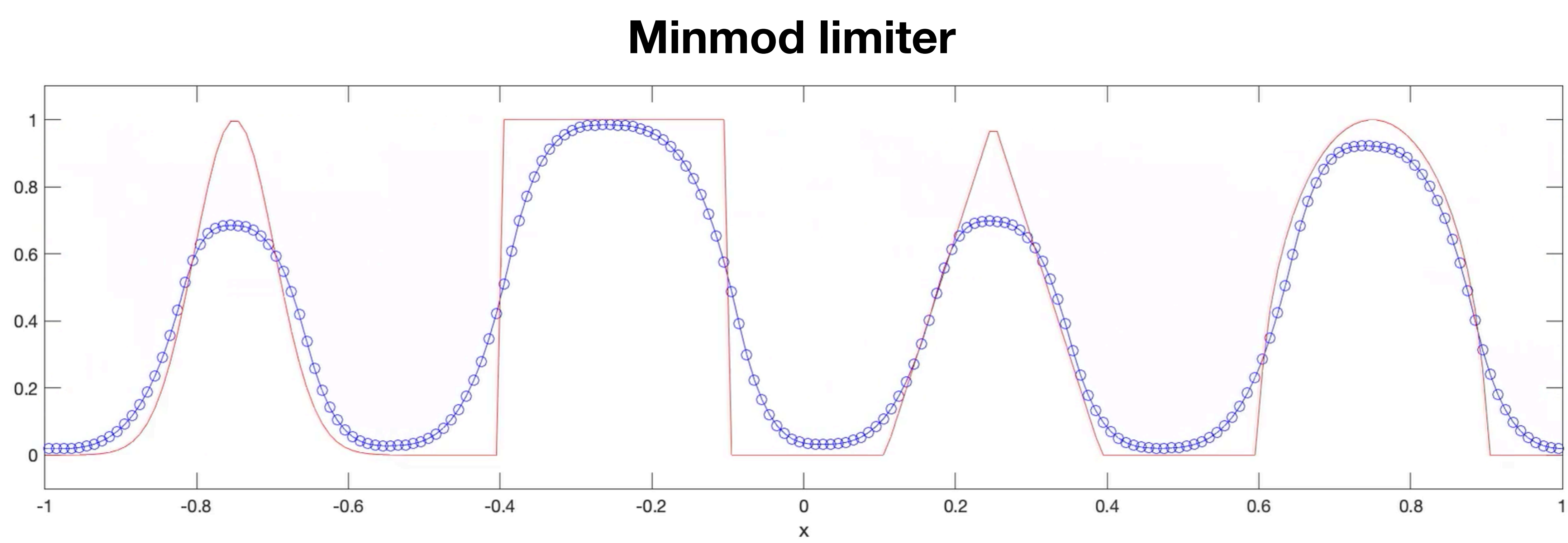


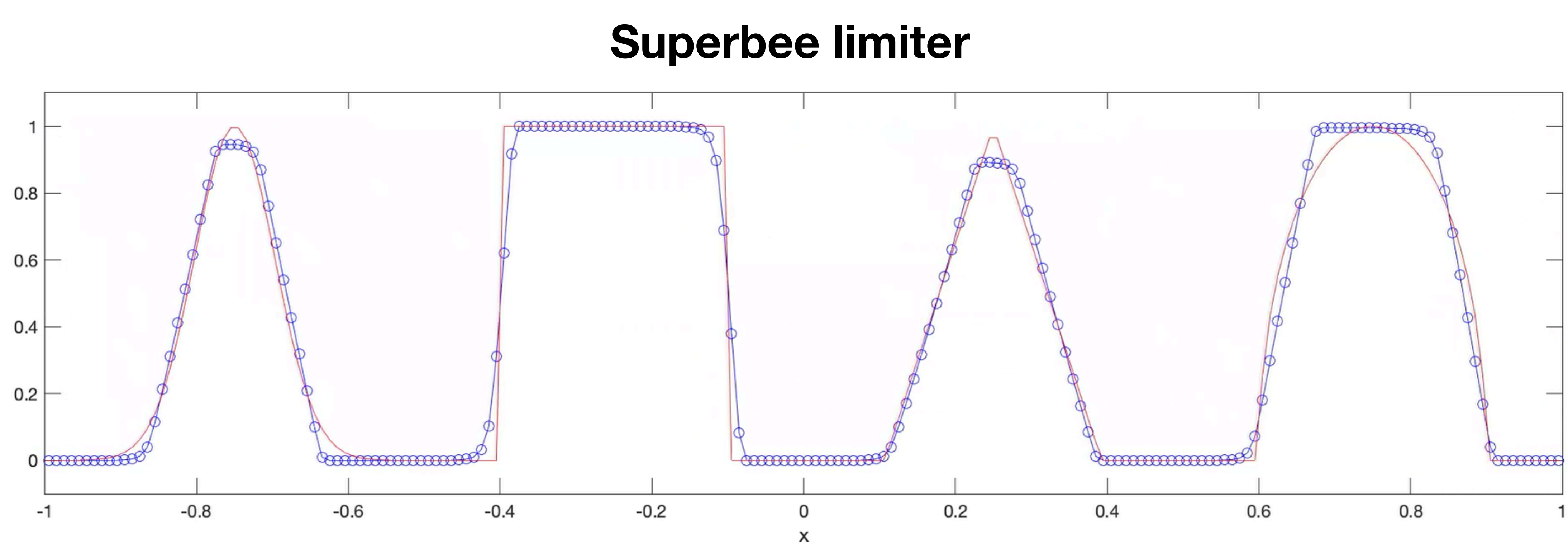
$$\sigma_i^n = \text{minmod}\left(\frac{Q_{i+1}^n - Q_i^n}{\Delta x}, \frac{Q_i^n - Q_{i-1}^n}{\Delta x}\right)$$

$$\text{minmod}(a, b) = \begin{cases} a & \text{if } |a| < |b| \text{ and } ab > 0, \\ b & \text{if } |b| < |a| \text{ and } ab > 0, \\ 0 & \text{if } ab \le 0. \end{cases}$$

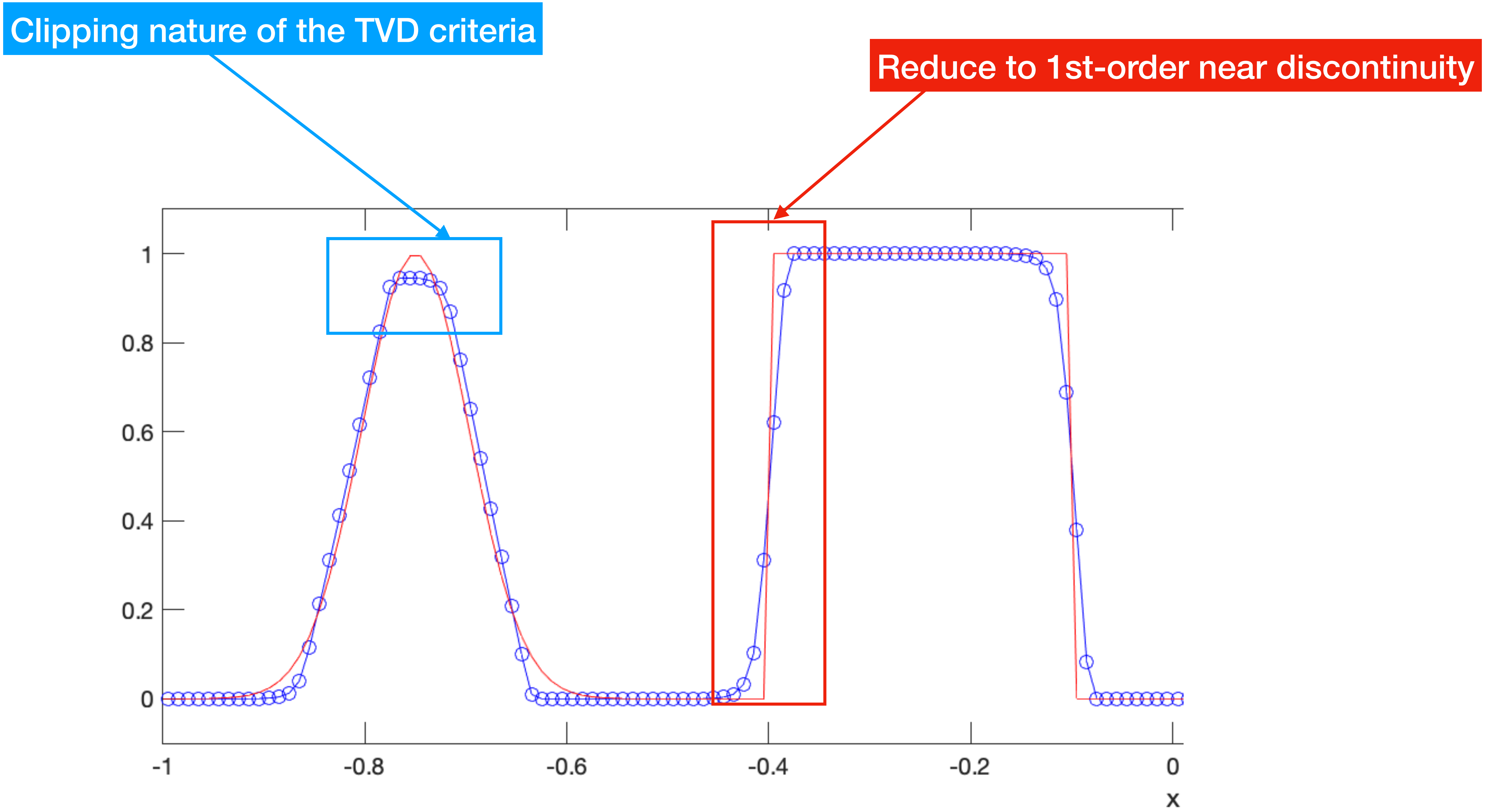
- In smooth regions, the minmod slope limiter gives a profile that approximates the true profile with piecewise linear functions (2nd-order accuracy)
- In discontinuous regions, the minmod slop limiter chooses the smaller slope which is degenerated to the 1st-order upwind method (guaranteed TVD)

Results form minmod/super-B Methods



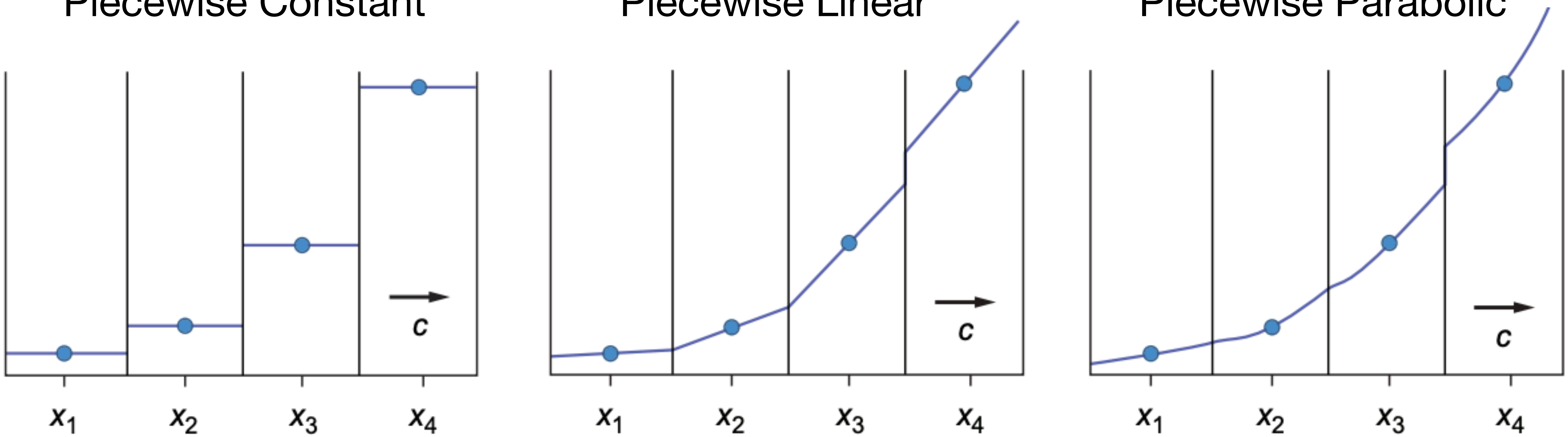


The Issue of typical TVD methods



Other Methods of Reconstruction (PPM)

Piecewise Constant | Piecewise Linear | Piecewise Parabolic

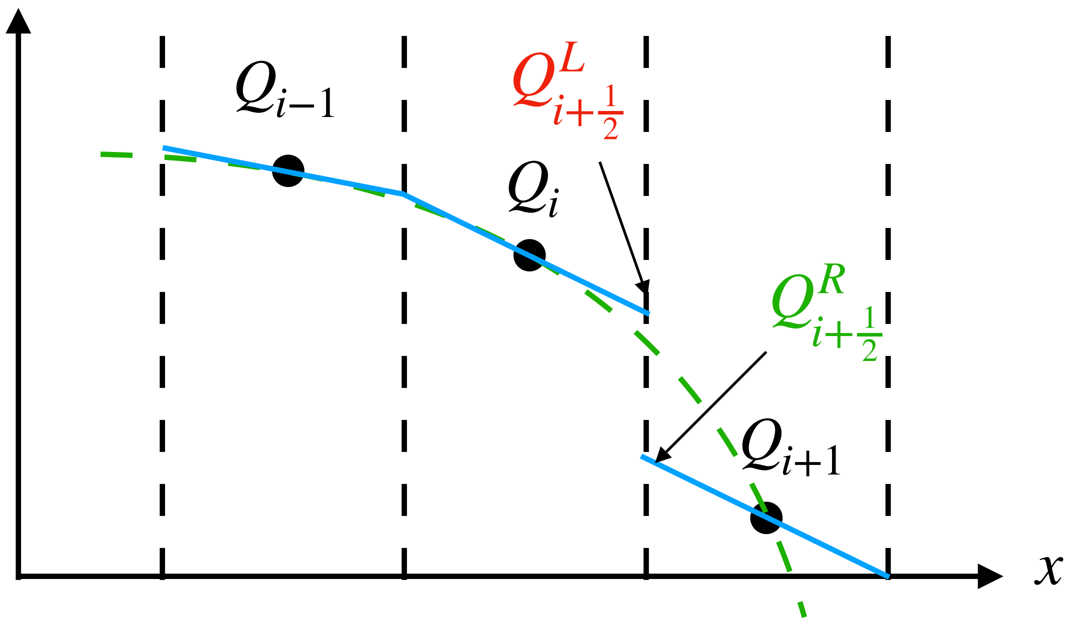


Upwind Scheme | MUSCL Schemes | PPM Schemes

Summary of the Finite Volume framework

Step 1: Interface Reconstruction

purpose: get interface values



INPUT:	Q_i	
OUTPUT:	$Q^L_{i+\frac{1}{2}}$	$Q^R_{i+\frac{1}{2}}$

Step 2: Flux calculation

$$F_{i+\frac{1}{2}}(Q^L_{i+\frac{1}{2}}, Q^R_{i+\frac{1}{2}}) = \frac{1}{2}(F(Q^L_{i+\frac{1}{2}}) + F(Q^R_{i+\frac{1}{2}})) - \frac{1}{2}|u_{max}|(Q^R_{i+\frac{1}{2}} - Q^L_{i+\frac{1}{2}})$$

INPUT:	$Q^L_{i+\frac{1}{2}}$	$Q^R_{i+\frac{1}{2}}$
OUTPUT:	$F_{i+\frac{1}{2}}$	

Step 3: Finite Volume Update

$$\frac{\partial}{\partial t}\bar{Q}_i = -\frac{1}{\Delta x}(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})$$

INPUT:	Q_i^n	$F_{i+\frac{1}{2}}$
OUTPUT:	Q_i^{n+1}	

$$Q_i^n \xrightarrow{\text{Reconstruct}} Q^L_{i+\frac{1}{2}},\ Q^R_{i+\frac{1}{2}} \xrightarrow{\text{Flux calculation}} F_{i+\frac{1}{2}} \xrightarrow{\text{F-V update}} Q_i^{n+1}$$