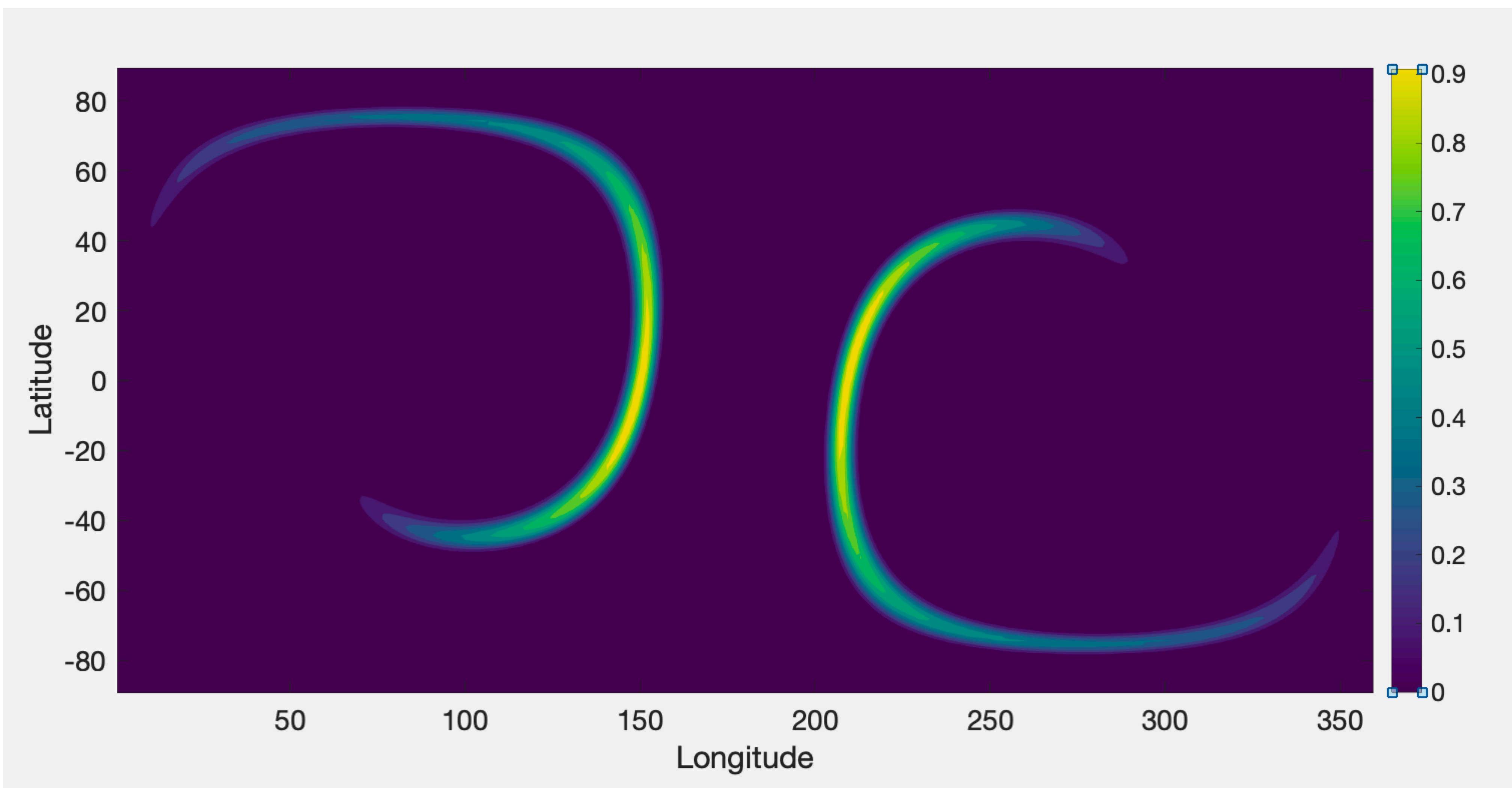
Topic 3

Numerical Solutions to the Advection-Diffusion Equations



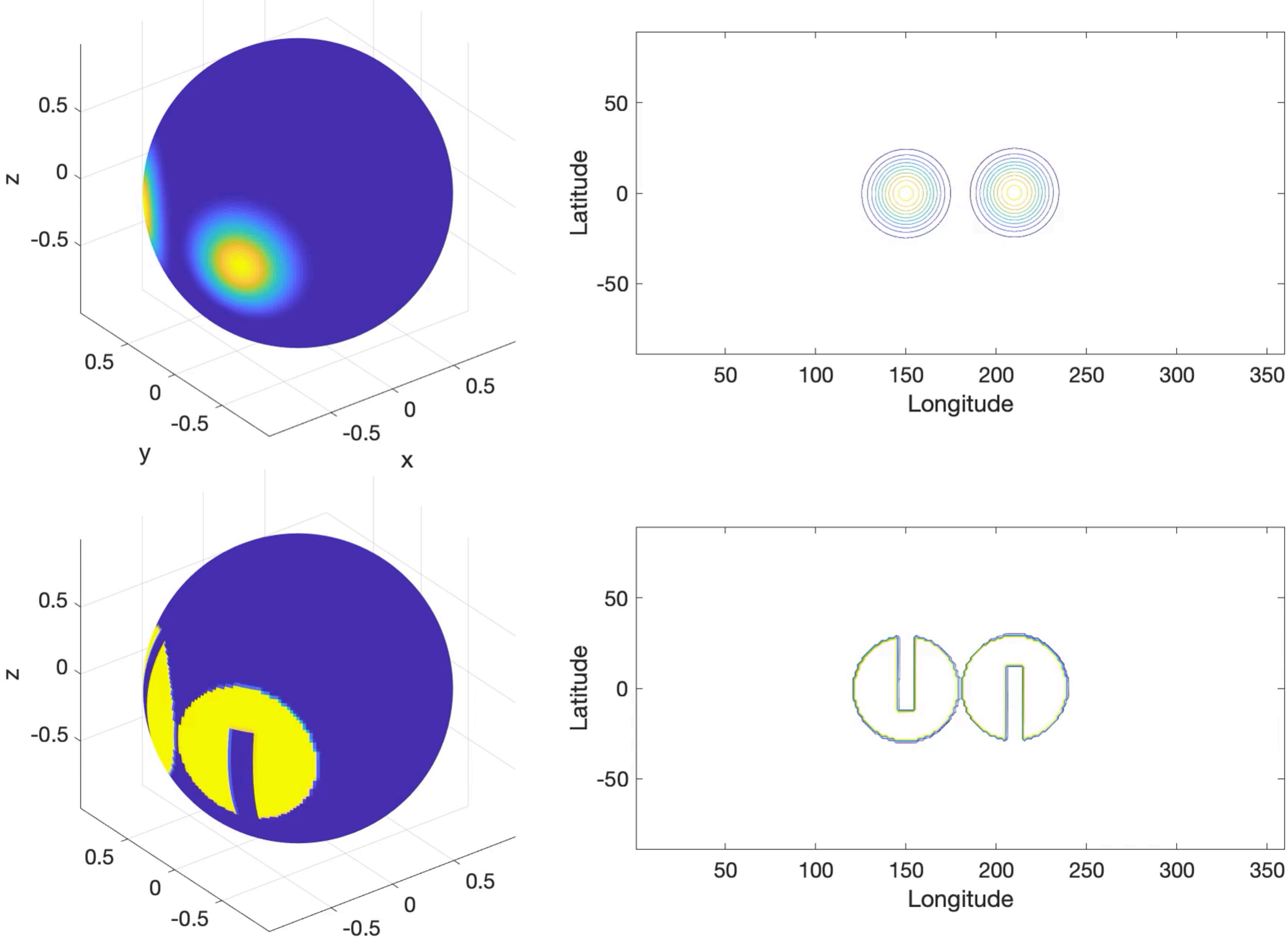
Outline

- Advection-Diffusion equations in plasma physics
- Why simple Finite difference methods do not work
- Introduction to Finite volume methods
- Reconstruction, slope limiting and flux limiting

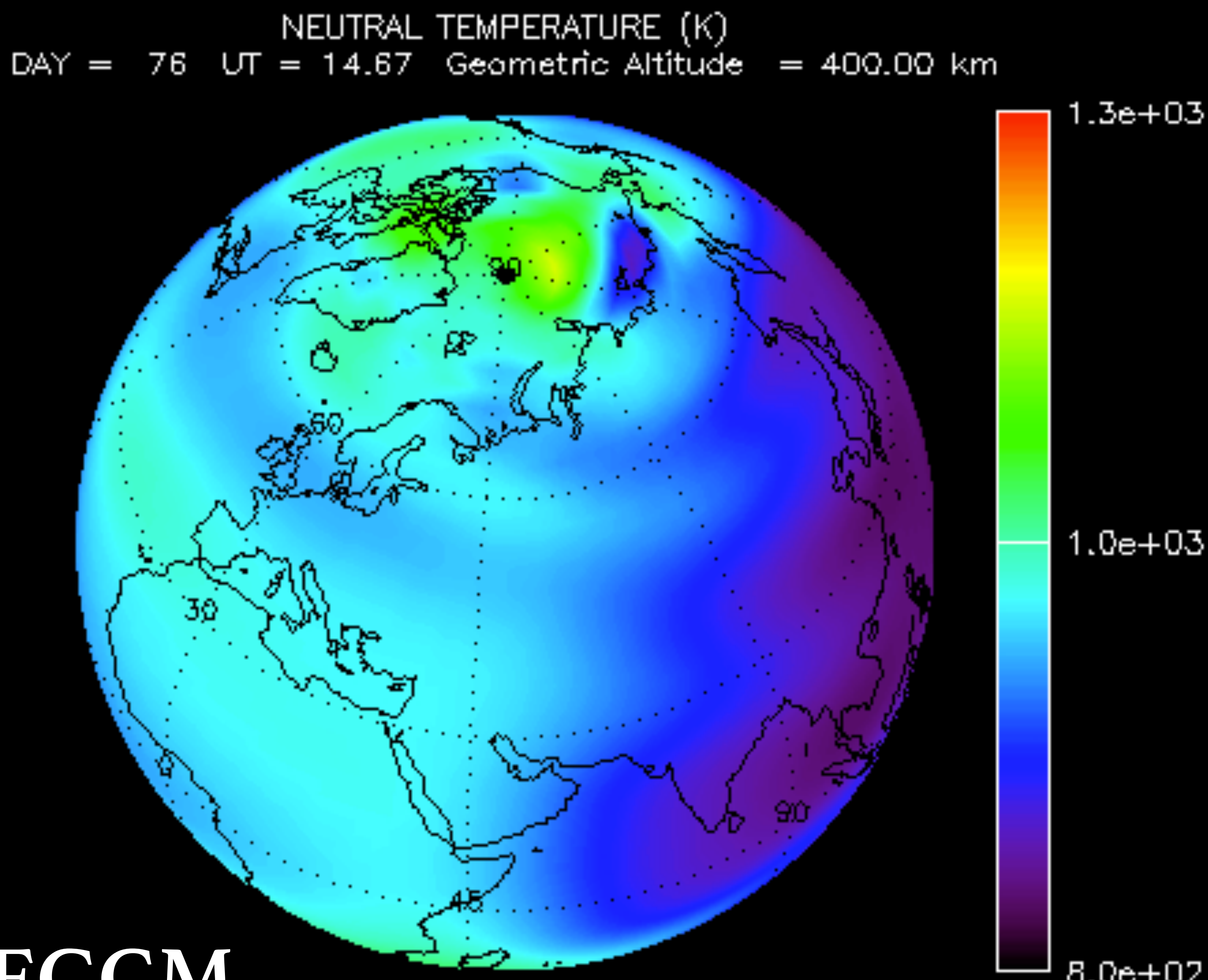
Course overview

- Introduction
- Finite difference schemes for 1-D MHD equations (3 Lectures)
- Finite volume methods for 1-D advection equations (2 Lectures)
- Vlasov simulations (Finite-volume based) (1 Lecture)
- Particle simulations (electrostatic PIC) (1 Lecture)
- Hybrid simulations (FD/FV electrons, PIC ions) (1 Lecture)

Advection of Trace Species on a Sphere



Thermosphere-Ionosphere Circulation



TIEGCM

Advection Diffusion Equations in TIEGCM

$$\frac{\partial Q}{\partial t} + \underbrace{u_0 \frac{\partial Q}{\partial x}}_{\text{Advection}} + \underbrace{D \frac{\partial^2 Q}{\partial x^2}}_{\text{Diffusion}} = 0$$

Mass Density

$$\frac{\partial \tilde{\Psi}}{\partial t} = -\mathbf{V} \cdot \nabla \tilde{\Psi} - \frac{e^Z}{\tau} \frac{\partial}{\partial Z} [\frac{\overline{m}}{m_{N_2}} (\frac{T_{00}}{T_n})^{0.25} \tilde{\alpha}^{-1} L \tilde{\Psi}] + e^Z \frac{\partial}{\partial Z} [K(z) e^{-Z} \frac{\partial}{\partial Z} (1 + \frac{1}{\overline{m}} \frac{\partial \overline{m}}{\partial Z}) \tilde{\Psi}] + \tilde{S} - \tilde{R} - w \frac{\partial \tilde{\Psi}}{\partial Z},$$

Zonal Velocity

$$\frac{\partial u_n}{\partial t} = -\mathbf{V} \cdot \nabla u_n + \frac{g e^Z}{p_0} \frac{\partial}{\partial Z} (\frac{\mu}{H} \frac{\partial u_n}{\partial Z}) + (f + \frac{u_n}{R_E} \tan \lambda) v_n + \lambda_{xx} (u_i - u_n) + \lambda_{xy} (v_i - v_n) - w \frac{\partial u_n}{\partial Z} - \frac{1}{R_E \cos \lambda} \frac{\partial \phi}{\partial \varphi},$$

Meridional Velocity

$$\frac{\partial v_n}{\partial t} = -\mathbf{V} \cdot \nabla v_n + \frac{g e^Z}{P_0} \frac{\partial}{\partial Z} (\frac{\mu}{H} \frac{\partial v_n}{\partial Z}) - (f + \frac{u_n}{R_E} \tan \lambda) u_n + \lambda_{yy} (v_i - v_n) + \lambda_{yx} (u_i - u_n) - w \frac{\partial v_n}{\partial Z} - \frac{1}{R_E} \frac{\partial \phi}{\partial \lambda},$$

Temperature

$$\frac{\partial T_n}{\partial t} = \underbrace{-\mathbf{V} \cdot \nabla T_n}_{\text{Advection}} + \underbrace{\frac{g e^Z}{p_0 C_p} \frac{\partial}{\partial Z} \left\{ \frac{K_T}{H} \frac{\partial T_n}{\partial Z}\right.}_{\text{Diffusion}} \left. + K_E H^2 C_P \rho \left[\frac{g}{C_P} + \frac{1}{H} \frac{\partial T_n}{\partial Z} \right] \right\} - w \left(\frac{\partial T_n}{\partial Z} + \frac{R^* T}{C_p \overline{m}} \right) + \frac{Q - L}{C_P},$$

Advection Equations in Space Plasmas

Fluid Description

$$\frac{\partial}{\partial t}(n_\alpha) + \nabla \cdot (n_\alpha \mathbf{u}_\alpha) = S_\alpha$$

Mass conservation

Momentum conservation

$$\frac{\partial}{\partial t}(n_\alpha \mathbf{u}_\alpha) + \nabla \cdot (n_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha + \mathbf{P}_\alpha) - \frac{n_\alpha q_\alpha}{m_\alpha}(\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B}) = \mathbf{R}_\alpha$$

Thermal Dynamics

$$\frac{\partial p_\alpha}{\partial t} + \mathbf{u}_\alpha \cdot \nabla p_\alpha + \gamma p_\alpha \nabla \cdot \mathbf{u}_\alpha = Q_\alpha$$

Maxwell's equation

$$\frac{\partial \mathbf{B}}{\partial \mathbf{t}} + \nabla \times \mathbf{E} = 0$$

$$\frac{\partial}{\partial t} : \text{ time derivative}$$

$$\nabla : \text{ spatial derivative}$$

$$= \frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial z}\hat{\mathbf{z}}$$

So the first key element of computation space plasma physics is to approximate these derivatives

Kinetic Description

Boltzmann equation

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = \left(\frac{\delta f_s}{\partial t}\right)_c$$

$$\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

Lorentz Force

$$\frac{\partial \mathbf{B}}{\partial \mathbf{t}} + \nabla \times \mathbf{E} = 0$$

Maxwell's equations

$$\mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \sum_s q_s \int_{-\infty}^{+\infty} v f_s d^3 v$$

Particle Description

$$m_s n_s \frac{d\mathbf{v}_s}{dt} = q n_s (\mathbf{E} + \mathbf{v}_\mathbf{s} \times \mathbf{B})$$

Equation of motion

$$\frac{\partial \mathbf{B}}{\partial \mathbf{t}} + \nabla \times \mathbf{E} = 0$$

Maxwell's equations

$$\mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \sum_s q_s n_s \mathbf{v}_s$$

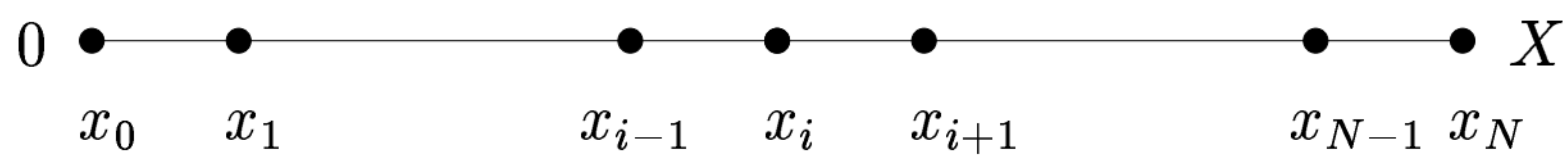
Recall: Numerical differentiation

Taylor's series expansion

Either the kinetic Vlasov equations of the fluid equations are solved numerically on a discrete set of spatial and temporal "grid points", this is called ***numerical discretization***:

$$\text{1D:} \qquad \Omega = (0, X), \qquad u_i \approx u(x_i), \qquad i = 0, 1, \ldots, N$$

$$\text{grid points} \quad x_i = i\Delta x \qquad \text{mesh size} \quad \Delta x = \tfrac{X}{N}$$



Recall the definition of derivatives:

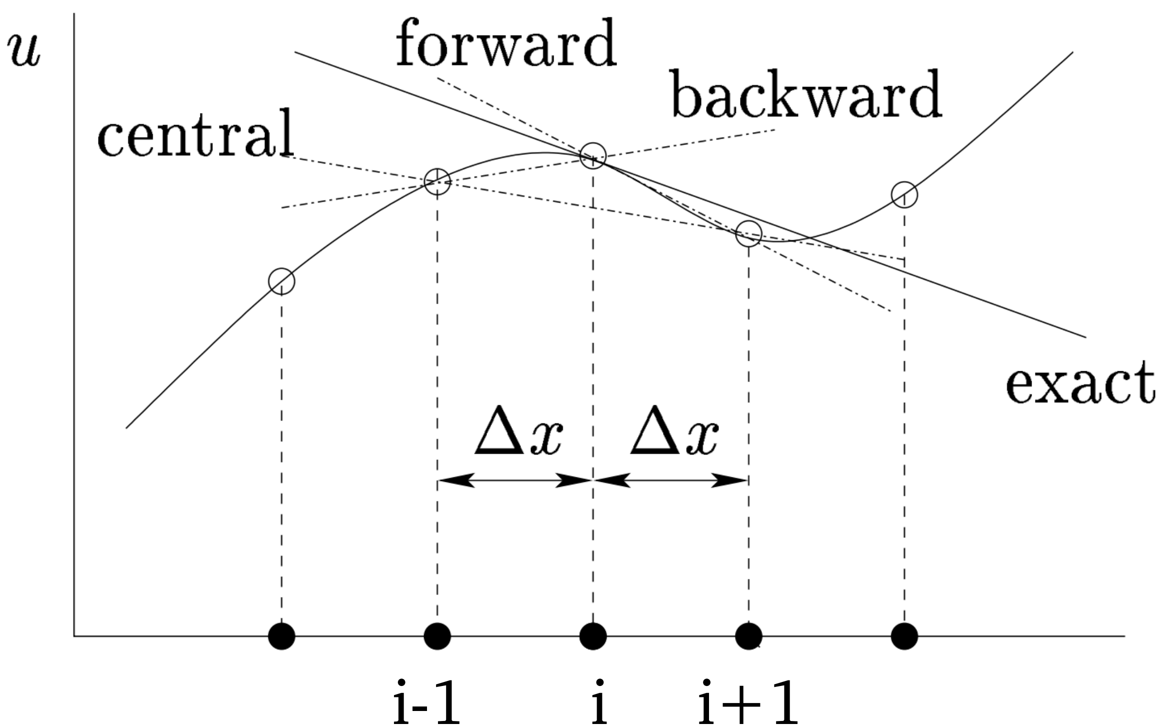
$$\left.\frac{dQ}{dx}\right|_{x=x_i} = \lim_{\Delta x \to 0} \frac{Q(x_i + \Delta x) - Q(x_i)}{\Delta x} = \lim_{\Delta x \to 0} \frac{Q(x_i) - Q(x_i - \Delta x)}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{Q(x_i + \Delta x) - Q(x_i - \Delta x)}{2\Delta x}$$

Finite Difference Approximation

Approximation of first-order derivatives

Geometric interpretation



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

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

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

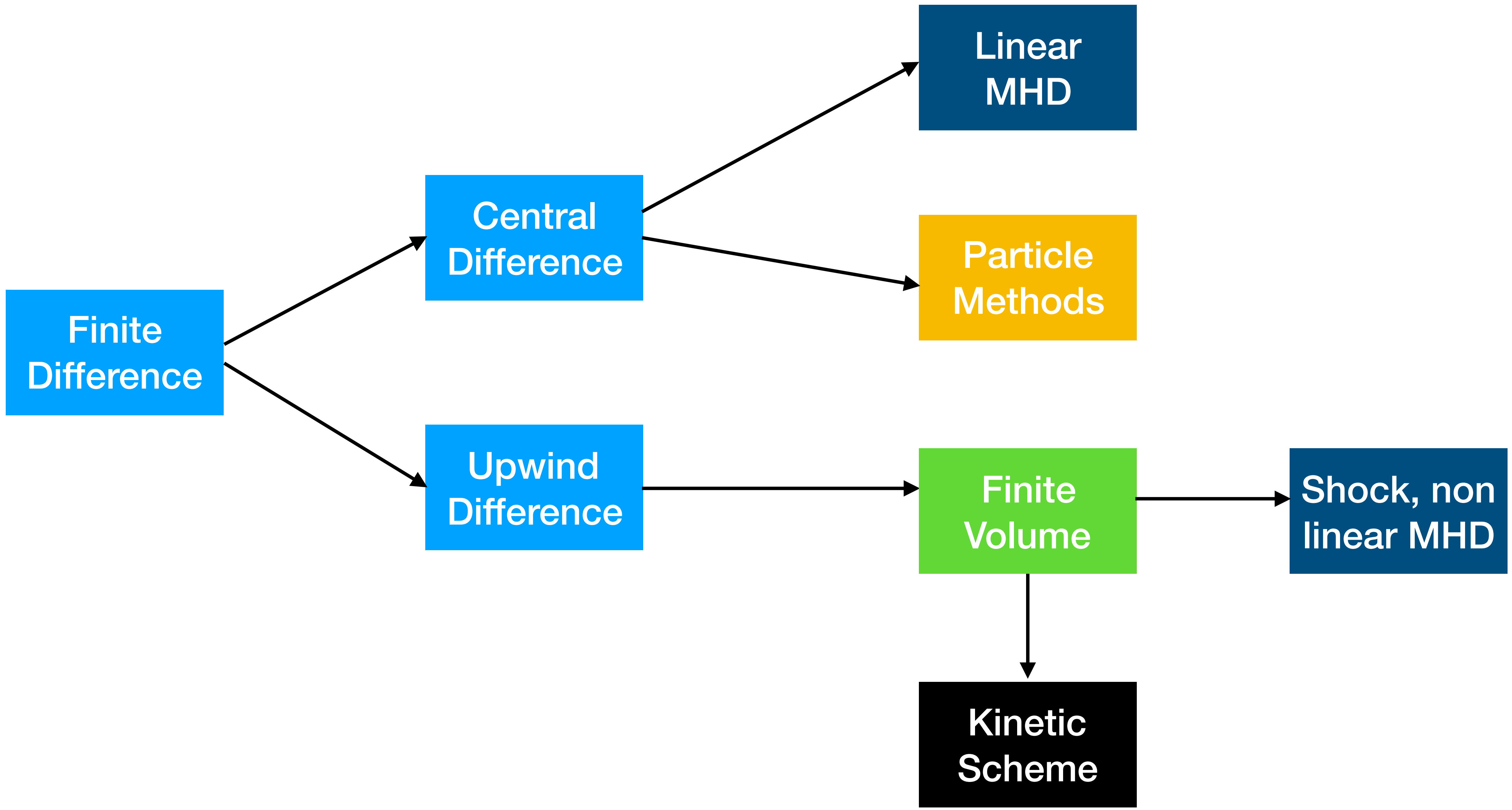
Recall Tayler series expansion: $u(x) = \sum_{n=0}^{\infty} \frac{(x - x_i)^n}{n!} \left(\frac{\partial^n u}{\partial x^n}\right)_i$

Let's try two expansions around x_i

T1: $$u_{i+1} = u_i + \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{1}{2}\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{1}{6}\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_i + \ldots$$

T2: $$u_{i-1} = u_i - \Delta x \left(\frac{\partial u}{\partial x}\right)_i + \frac{1}{2}\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{1}{6}\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_i + \ldots$$

Numerical Methods in Computation Space Plasma Physics



A simple example

Linear Advection Equation

Time derivative

$$\frac{\partial}{\partial t}(n_\alpha) + \nabla \cdot (n_\alpha \mathbf{u}_\alpha) = 0 \xrightarrow[\nabla = \frac{\partial}{\partial x}\hat{\mathbf{x}} \qquad \mathbf{u}_\alpha = u_0 \hat{\mathbf{x}}]{\textbf{1-D}} \frac{\partial n_\alpha}{\partial t} + u_0 \frac{\partial n_\alpha}{\partial x} = 0$$

u_0 is a constant, this equation is simply a linear PDE about n_\alpha

Spatial derivative

Now let's define a new notation for discretized n in both space and time

the n^{th} timestep

$$n_\alpha(t,x) \xrightarrow[\text{call it } Q]{\text{ignore } \alpha} Q(t,x) \xrightarrow{t = t_n \ x = x_i} Q(t = t_n, x = x_i) \xrightarrow{\text{define}} Q_i^n$$

the i^{th} grid point

Then let's take a look how to discretize the differential equation

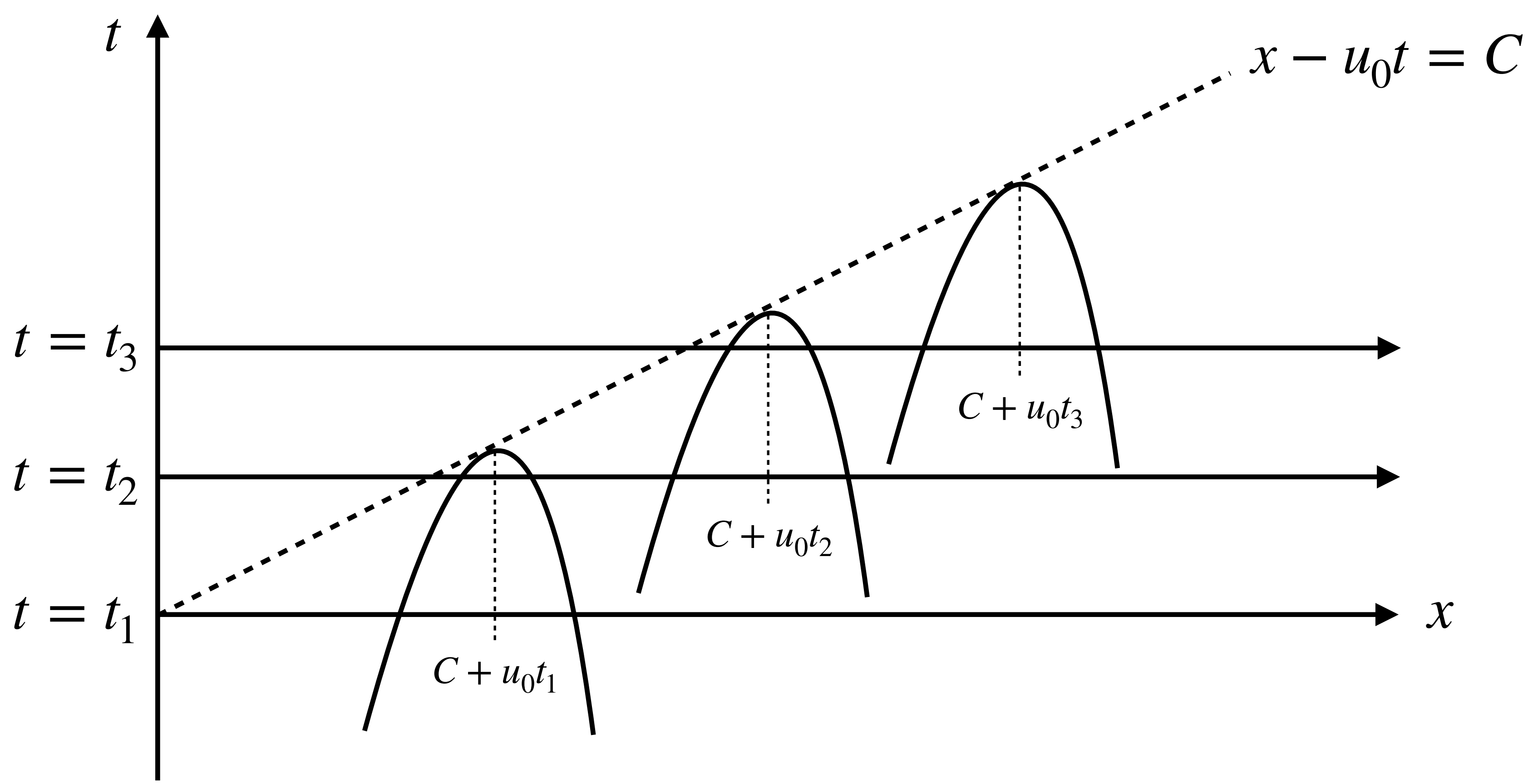
$$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0$$

first let's take a look at what the solution look like from the mathematical aspect

What does the linear advection equation do?

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

The solution goes like $Q(x,t) \sim f(x - u_0 t)$



A simple wave propagation towards +x direction:

- When $u_0 > 0$, to keep $(x-u_0t)$ constant, x ***increases*** with t -> wave propagates towards right
- When $u_0 < 0$, to keep $(x-u_0t)$ constant, x ***decreases*** with t -> wave propagates towards left

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

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

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

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

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

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

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

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

Finite-Difference Approximations

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

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

$$+\frac{1}{\rho^n_i}\left(\frac{p^n_{i+1} - p_{i-1}}{2\Delta x} - J^n_{z,i}B^n_{y,i}\right)$$

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

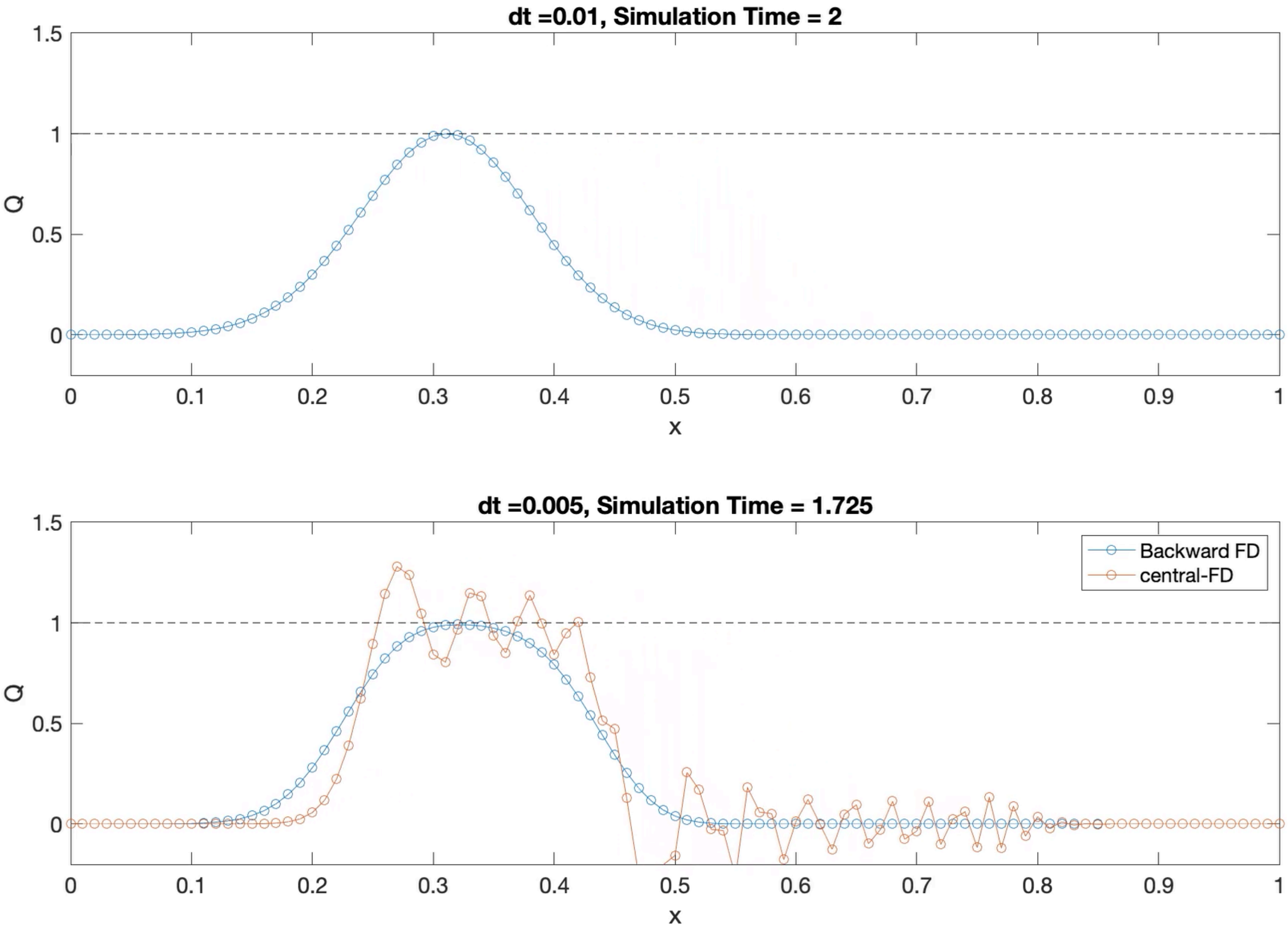
$$\frac{\partial B_y}{\partial t}\Big|_i = -\frac{E^n_{z,i+1} - E^n_{z,i-1}}{2\Delta x}$$

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

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

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

Results form Central-Difference Method



Why Central-Difference Method won't work

Von Neumann Analysis

Start with with the central difference scheme for the 1-D linear advection equation

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

Let's see the mathematical problem of this numerical update

Assume the solution goes like harmonic solutions with respect to space:

$$Q_i^n \sim e^{jkx_i} \longrightarrow Q_{i+1}^n \sim e^{jk(x_i+\Delta x)} = e^{jkx_i} \cdot e^{jk\Delta x}$$

$$= Q_i^n \cdot e^{jk\Delta x}$$

For the evolution, let's say $Q_i^{n+1} = g \cdot Q_i^n$ g: amplification factor

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

$$\longrightarrow g = 1 - \frac{u_0 \Delta t}{2\Delta x}(e^{jk\Delta x} - e^{-jk\Delta x})$$

Why Central-Difference Method won't work

Von Neumann Analysis

So the amplification factor g is calculated as

$$g = 1 - \frac{u_0 \Delta t}{2\Delta x}(e^{jk\Delta x} - e^{-jk\Delta x}) \quad = 1 - j\frac{u_0 \Delta t}{\Delta x}\sin k\Delta x$$

$$\longrightarrow \qquad |g|^2 = g \cdot g^* = 1 + \left(\frac{u_0 \Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x) \quad > 1 \text{ for all k} \neq 0$$

Which means that the solution of $Q_i^{n+1} = g \cdot Q_i^n$ grows exponentially. This is called

UNCONDITIONALLY UNSTABLE

Now think about this, in the above calculations of the amplification factor g; when k = 0, g=1 which means the solution is not going to be amplified exponentially. Does that mean the finite difference scheme is fine?

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

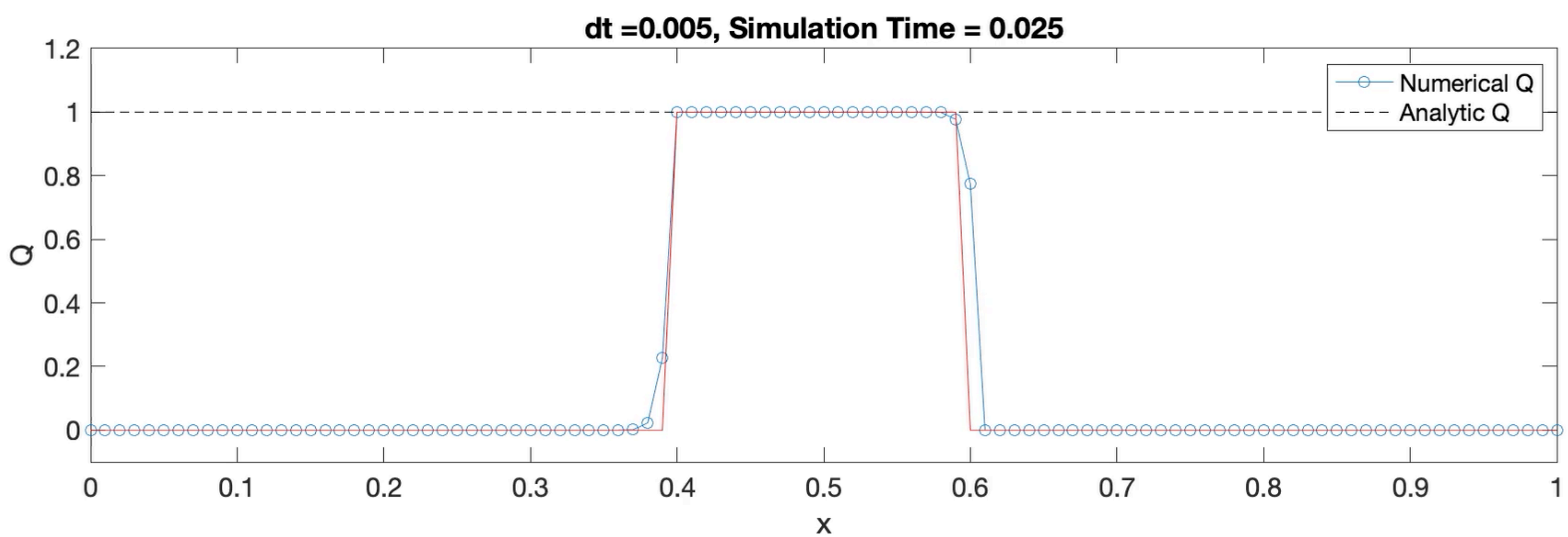
$$\left.\frac{\partial Q}{\partial t}\right|_{x=x_i} = \frac{Q_i^n - Q_{i-1}^n}{\Delta x} + \mathcal{O}(\Delta x)$$

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

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



What about Upwind-Difference Method?

Von Neumann Analysis

Start with with the upwind difference scheme for the 1-D linear advection equation

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

Let's do the same analysis

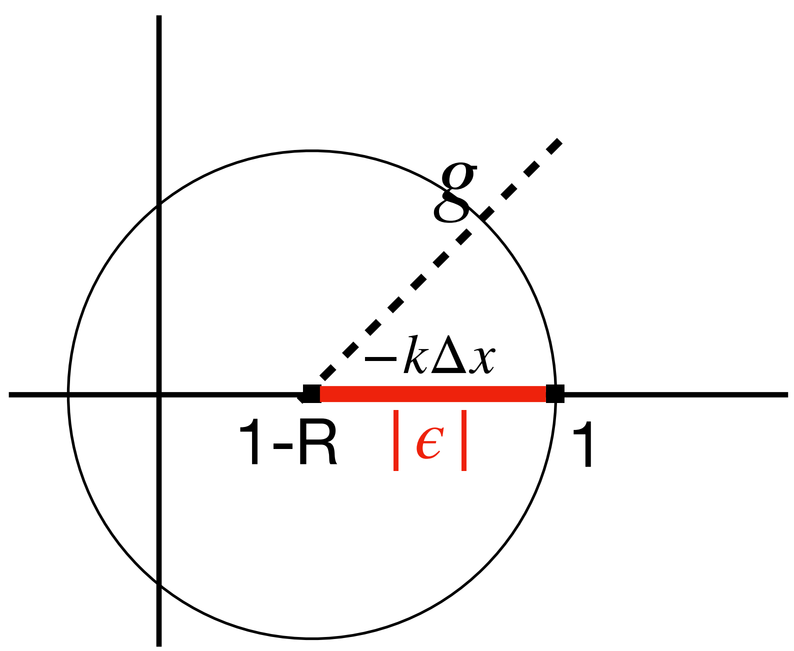
$$Q_i^n \sim e^{jkx_i} \qquad Q_{i-1}^n \sim Q_i^n \cdot e^{-jk\Delta x} \qquad Q_i^{n+1} = g \cdot Q_i^n$$

Substitute into the upwind scheme:

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

$$\longrightarrow g = 1 - \frac{u_0 \Delta t}{\Delta x}(1 - e^{-jk\Delta x})$$

$$= (1 - \epsilon) + \epsilon \cdot e^{-jk\Delta x}$$



It is straightforward to show that $|g| \leq 1$ with

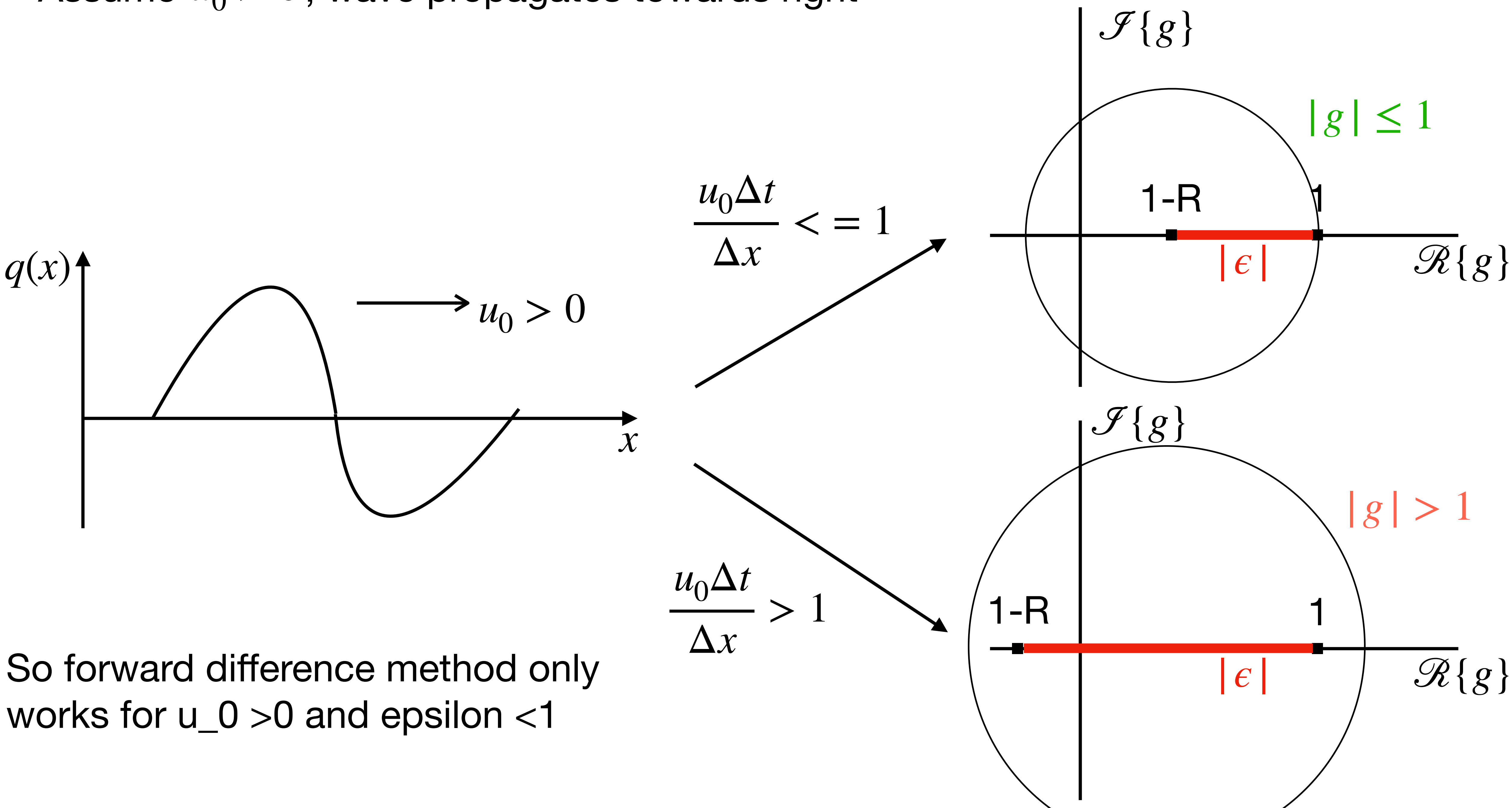
$$\epsilon \equiv \frac{u_0 \Delta t}{\Delta x} < 1$$

Stability Condition

The CFL condition

$$Q_i^{n+1} \approx Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) \longrightarrow g = (1-\epsilon) + \epsilon \cdot e^{-jk\Delta x} \qquad \epsilon \equiv \frac{u_0 \Delta t}{\Delta x}$$

Assume $u_0 > 0$, wave propagates towards right



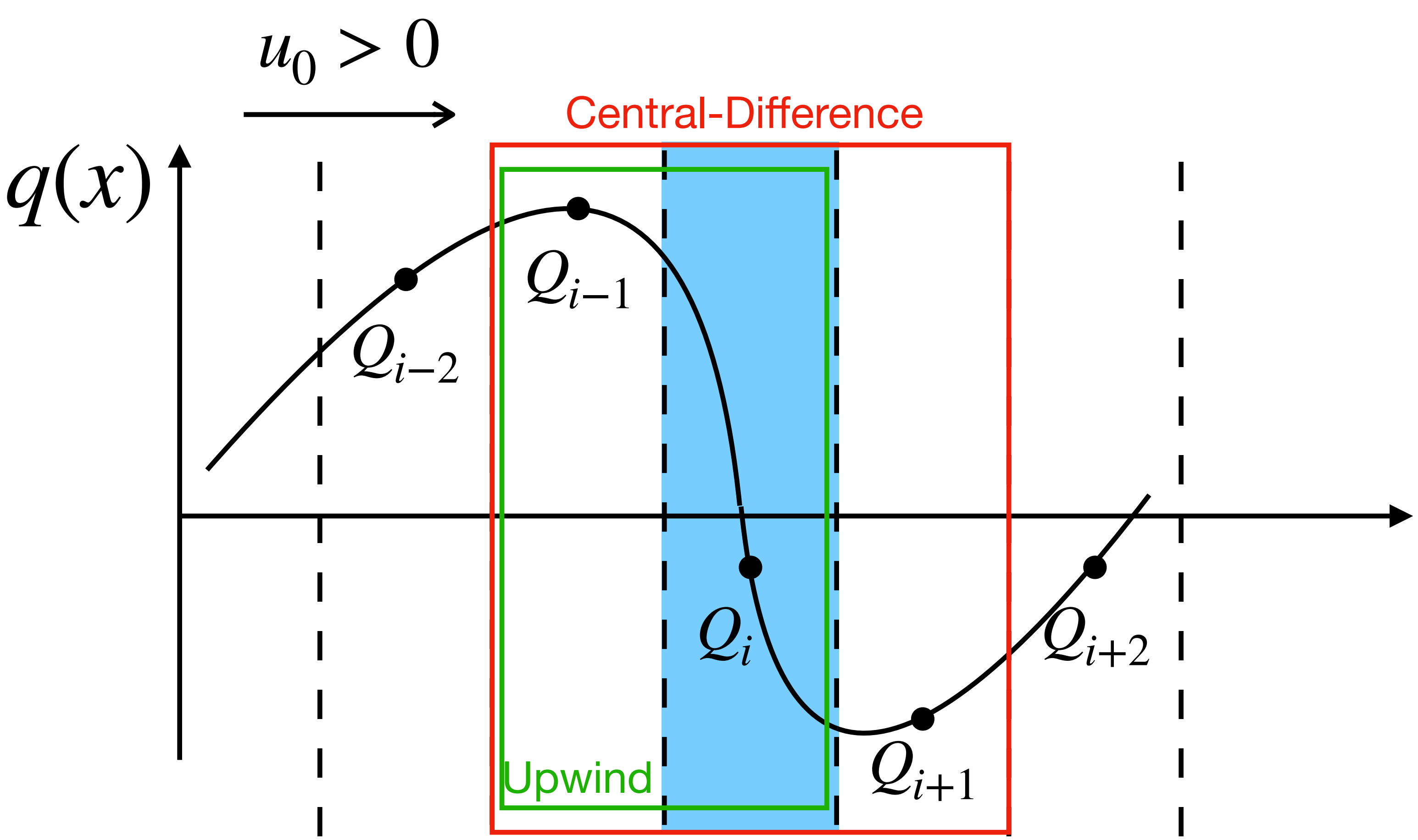
So forward difference method only works for u_0 >0 and epsilon <1

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:

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



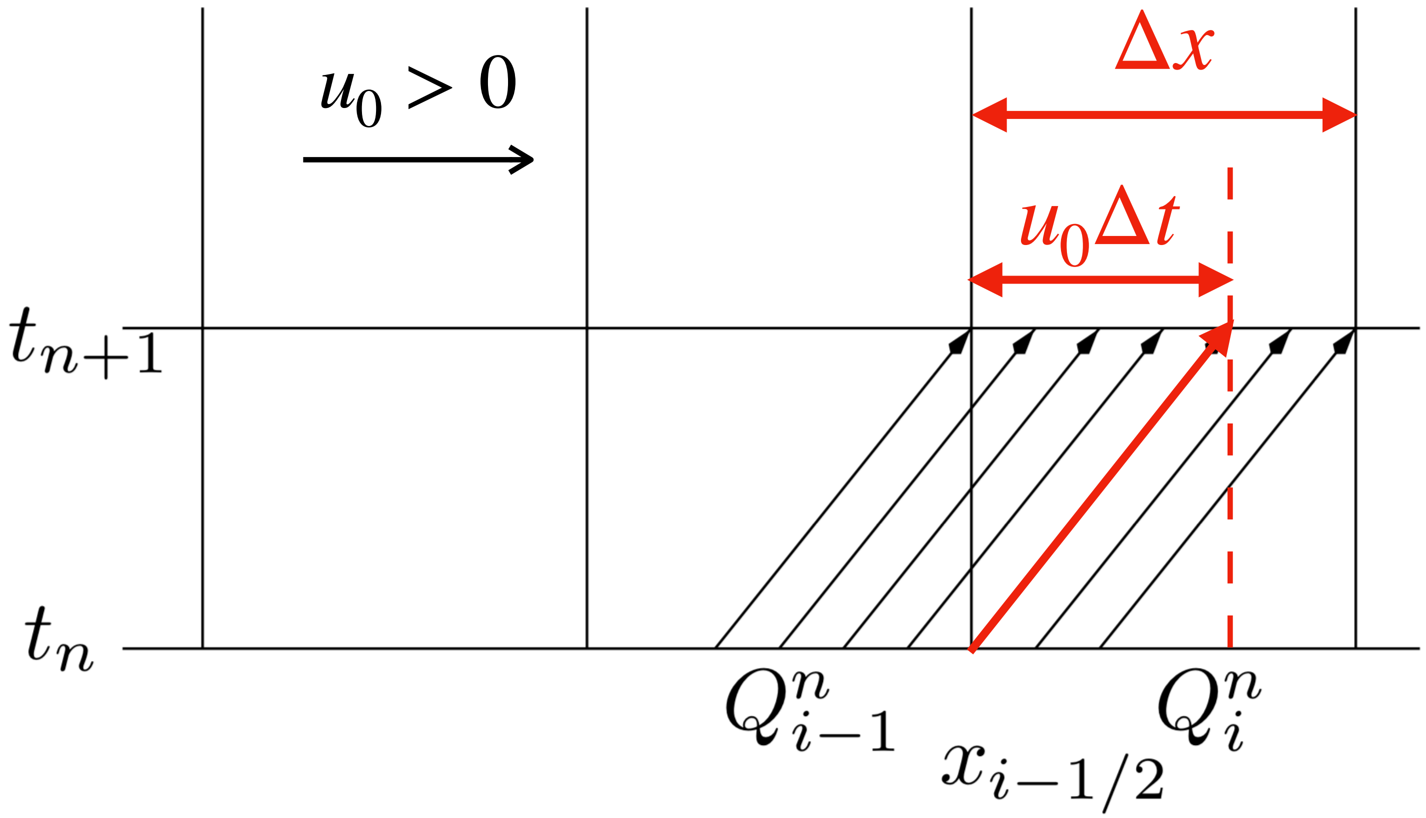
$$Q_i^{n+1} \approx Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n)$$

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

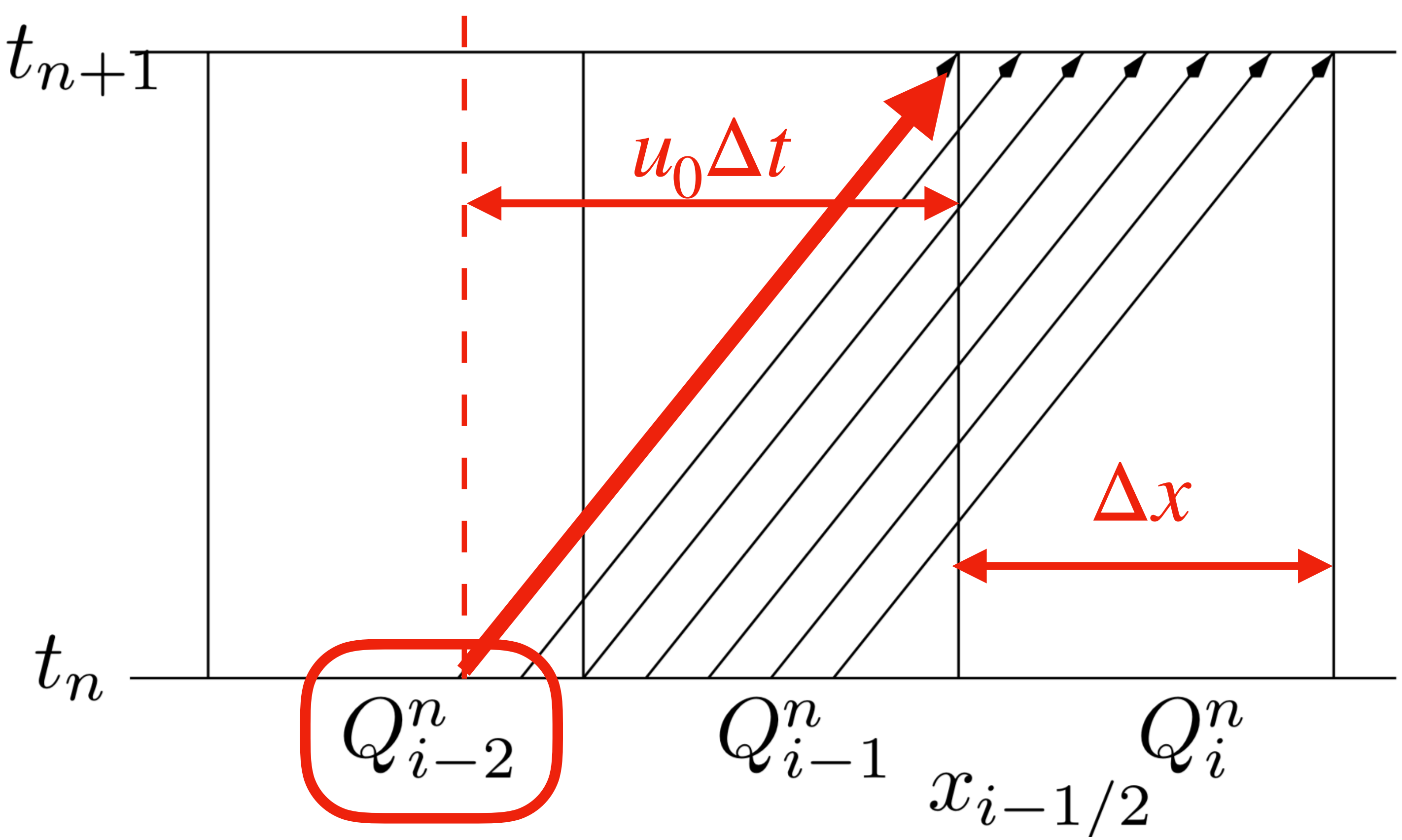


- Solution of Q_i is only affected by Q_{i-1} and Q_i

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

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

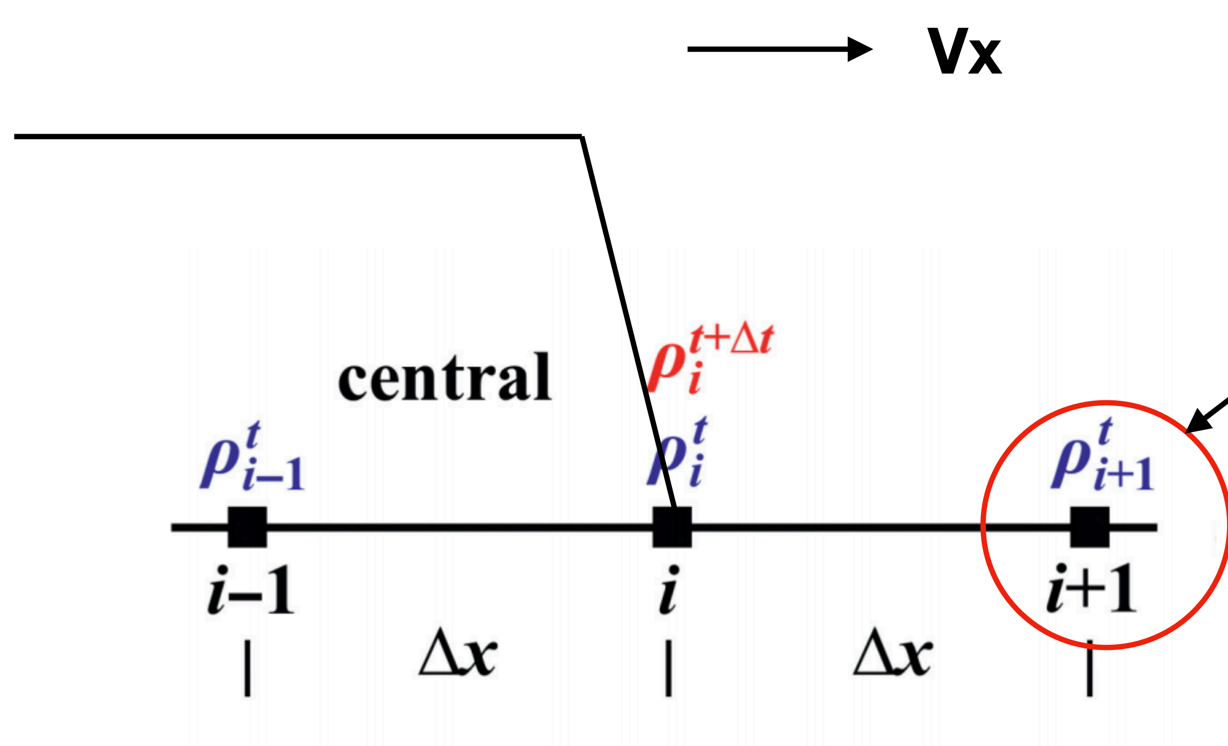
Mathematical reason:

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

The modified equation

Upwind method

The 1-D linear advection equation $$\frac{\partial Q}{\partial t} + u_0 \frac{\partial Q}{\partial x} = 0 \qquad (1)$$

is approximated by a numeric scheme: $$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) \qquad (2)$$

Now question is what is the level of accuracy when using (2) to approximate (1)

Let's say $Q_i^n = q(x,t)$ which satisfies the upwind scheme exactly:

$$q(x, t+\Delta t) = q(x,t) - \frac{u_0 \Delta t}{\Delta x}\left[q(x,t) - q(x-\Delta x, t)\right]$$

$\xrightarrow{\text{Re-form}}$

$$\frac{q(x,t+\Delta t) - q(x,t)}{\Delta t} + u_0 \frac{q(x,t) - q(x-\Delta x,t)}{\Delta x} = 0$$

Now consider the Taylor expansion in time:

$$q(x,t+\Delta t) = q(x,t) + \frac{\partial q}{\partial t}(\Delta t) + \frac{1}{2}\frac{\partial^2 q}{\partial t^2}(\Delta t)^2 + \ldots$$

The modified equation

Upwind method

The upwind equation $\dfrac{q(x,t+\Delta t)-q(x,t)}{\Delta t}+u_0\dfrac{q(x,t)-q(x-\Delta x,t)}{\Delta x}=0$ becomes

$$\left(\frac{\partial q}{\partial t}+\frac{1}{2}\frac{\partial^2 q}{\partial t^2}(\Delta t)+\frac{1}{6}\frac{\partial^3 q}{\partial t^3}(\Delta t)^2+\dots\right)+u_0\left(\frac{\partial q}{\partial x}-\frac{1}{2}\frac{\partial^2 q}{\partial x^2}(\Delta x)+\frac{1}{6}\frac{\partial^3 q}{\partial x^3}(\Delta x)^2+\dots\right)=0$$

Re-write the above equation:

$$\frac{\partial q}{\partial t}+u_0\frac{\partial q}{\partial x}=\underbrace{\frac{1}{2}\left(u_0\Delta x\frac{\partial^2 q}{\partial x^2}-\Delta t\frac{\partial^2 q}{\partial t^2}\right)-\frac{1}{6}\left[(u_0\Delta x)^2\frac{\partial^3 q}{\partial x^3}-(\Delta t)^2\frac{\partial^3 q}{\partial t^3}\right]+\dots}_{=R(q,q',q'',\dots)}$$

If $R(q,q',q'',\dots)\rightarrow 0$, the numerical solution q recovers the linear advection equation

Let's only keep the first order terms:

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

E

The modified equation

Upwind method

Let's only keep the first order terms:

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

$$\xrightarrow{\frac{\partial}{\partial t}} \quad \frac{\partial^2 q}{\partial t^2} + u_0\frac{\partial^2 q}{\partial t\partial x} = \frac{1}{2}\left(u_0\Delta x\frac{\partial^3 q}{\partial t\partial x^2} - \Delta t\frac{\partial^3 q}{\partial t^3}\right)$$

$$\xrightarrow{\frac{\partial}{\partial x}} \quad \frac{\partial^2 q}{\partial x\partial t} + u_0\frac{\partial^2 q}{\partial x^2} = \frac{1}{2}\left(u_0\Delta x\frac{\partial^3 q}{\partial x^3} - \Delta t\frac{\partial^3 q}{\partial x\partial t^2}\right)$$

$$\longrightarrow \quad \frac{\partial^2 q}{\partial t^2} = u_0^2\frac{\partial^2 q}{\partial x^2} + \mathcal{O}(\Delta t)$$

Substitute

Higher order error

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

$$\longrightarrow \quad \frac{\partial q}{\partial t} + u_0\frac{\partial q}{\partial x} \approx \underbrace{\frac{1}{2}u_0\Delta x\left(1 - \frac{u_0\Delta t}{\Delta x}\right)}_{\beta_{xx}}\frac{\partial^2 q}{\partial x^2} \quad \longrightarrow \quad \boxed{\frac{\partial q}{\partial t} + u_0\frac{\partial q}{\partial x} \approx \beta_{xx}\frac{\partial^2 q}{\partial x^2}}$$

Modified equation

A few things about the modified equation

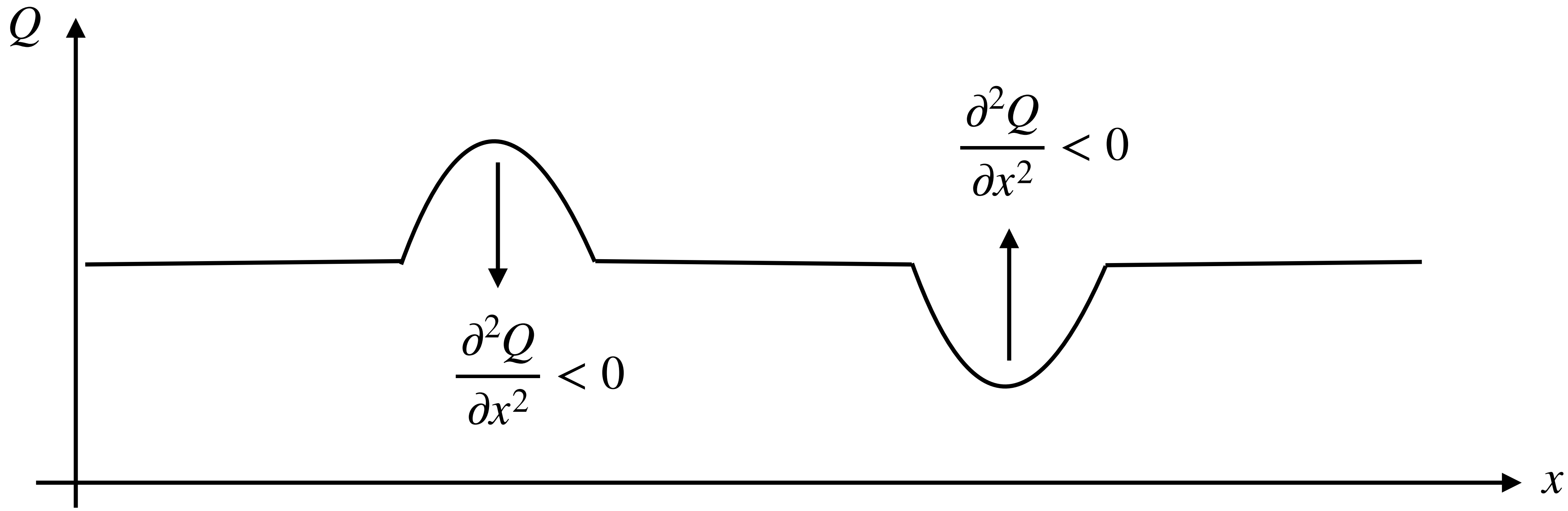
Upwind method

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

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 $\dfrac{u_0 \Delta t}{\Delta x} = 1 \longrightarrow \beta_{xx} = \dfrac{1}{2} u_0 \Delta x \left(1 - \dfrac{u_0 \Delta t}{\Delta x}\right) \equiv 0$ NO diffusion!
  - If $\Delta x \to 0 \longrightarrow \beta_{xx} \to 0$ Converged solution
  - If $0 < \dfrac{u_0 \Delta t}{\Delta x} < 1 \longrightarrow \beta_{xx} > 0$ 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

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

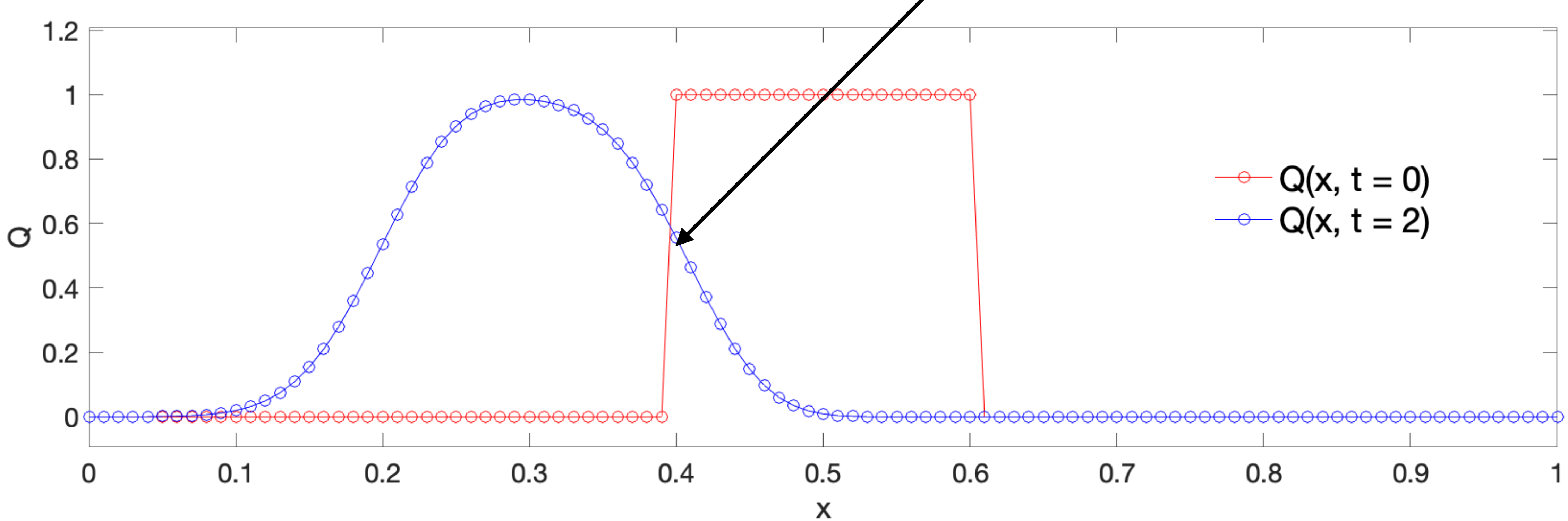
b) Run the linear_adv_lec_2.m code with a square wave as the initial profile: Q=1.0 for 0.4<x<0.6 and Q = 0.0 otherwise. Compare the final profile of Q with the initial condition and describe your result.

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)
```

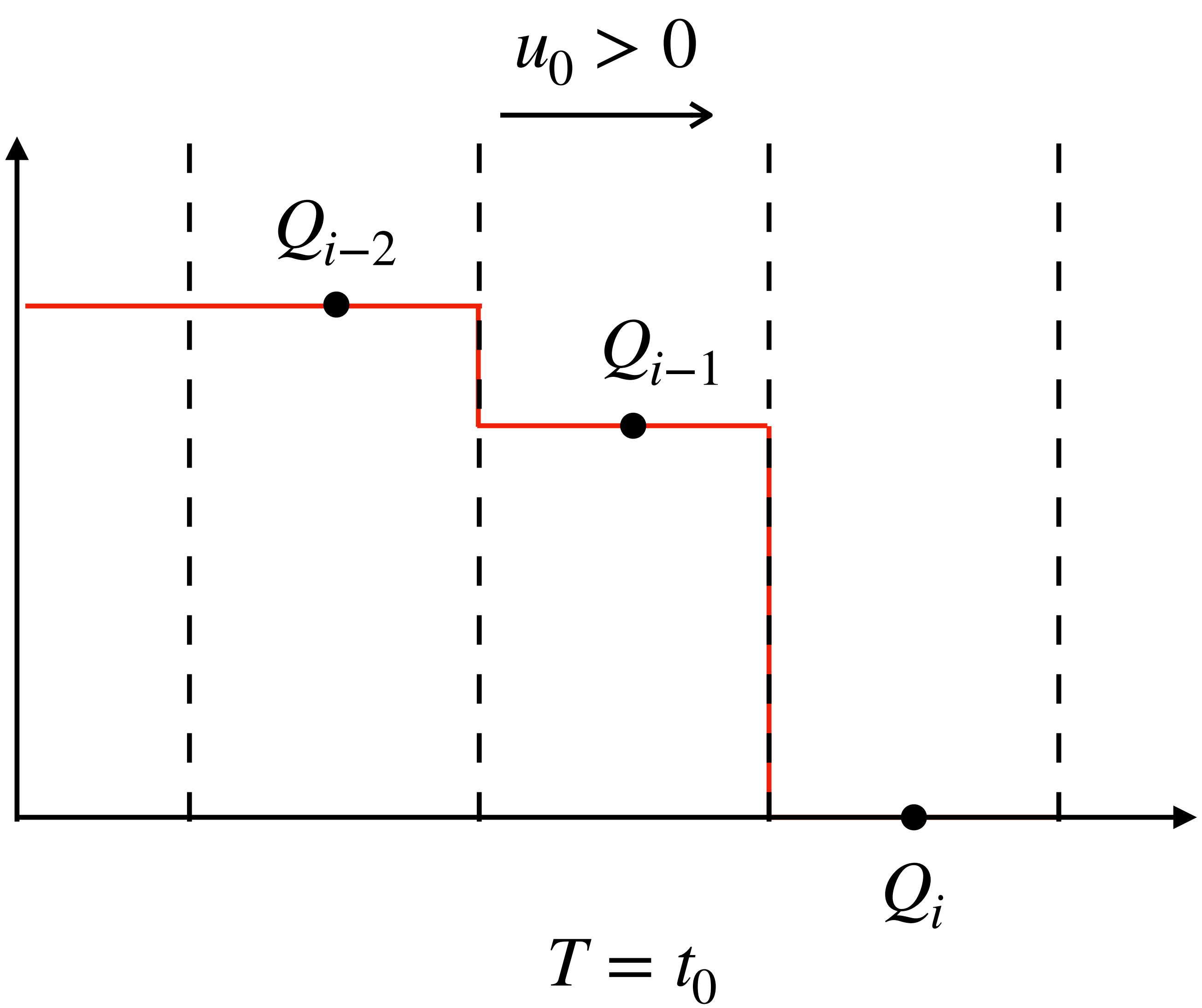
So the numerical solution of Q "spreads" in the x-direction - it deforms from a square function into something like a Gaussian function (mathematically it's the error function"

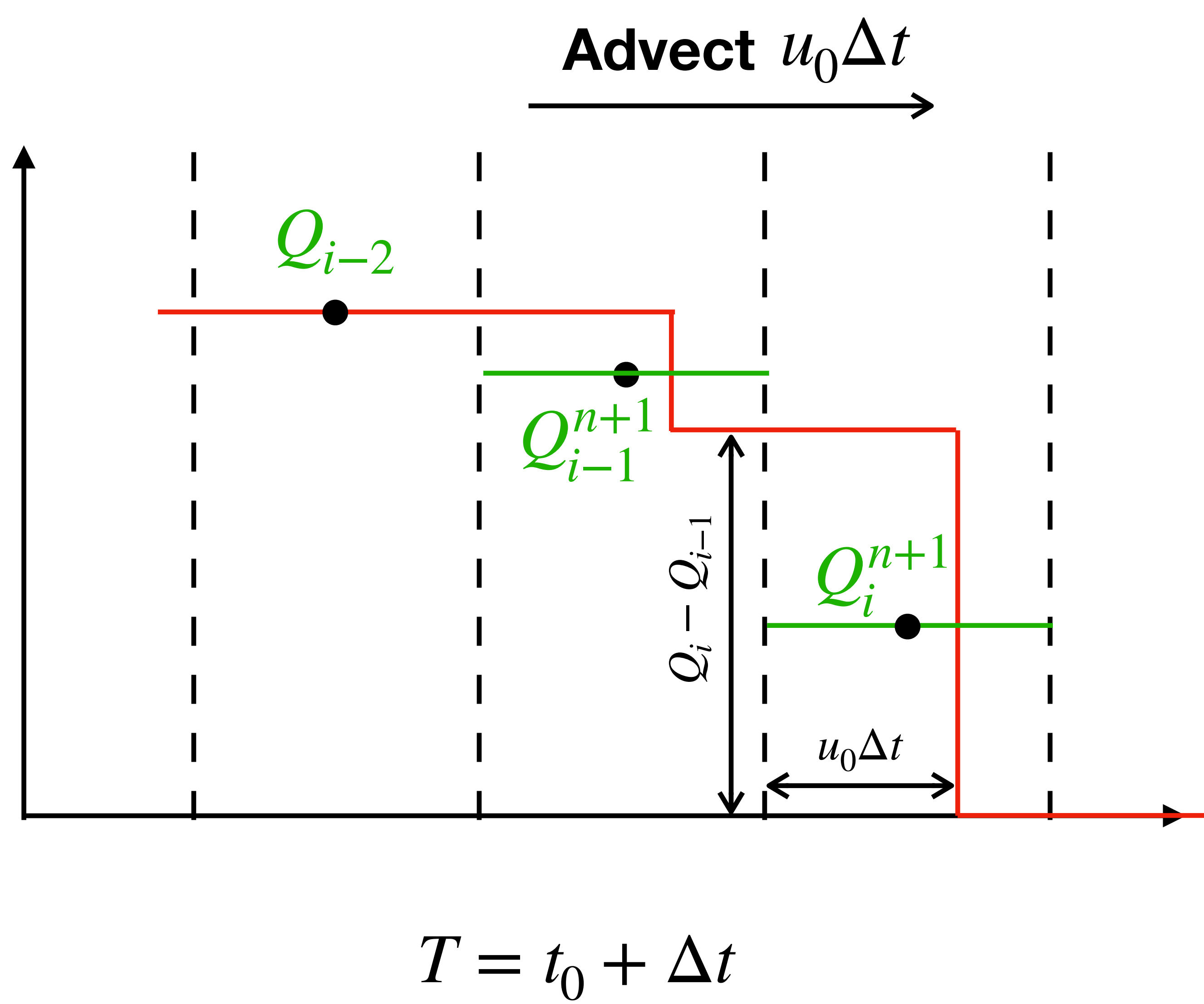
The Advection Nature of the equation

The REA framework

The upwind scheme can be written as $$Q_i^{n+1} = Q_i^n - \boxed{\frac{u_0 \Delta t (Q_i^n - Q_{i-1}^n)}{\Delta x}}$$ 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

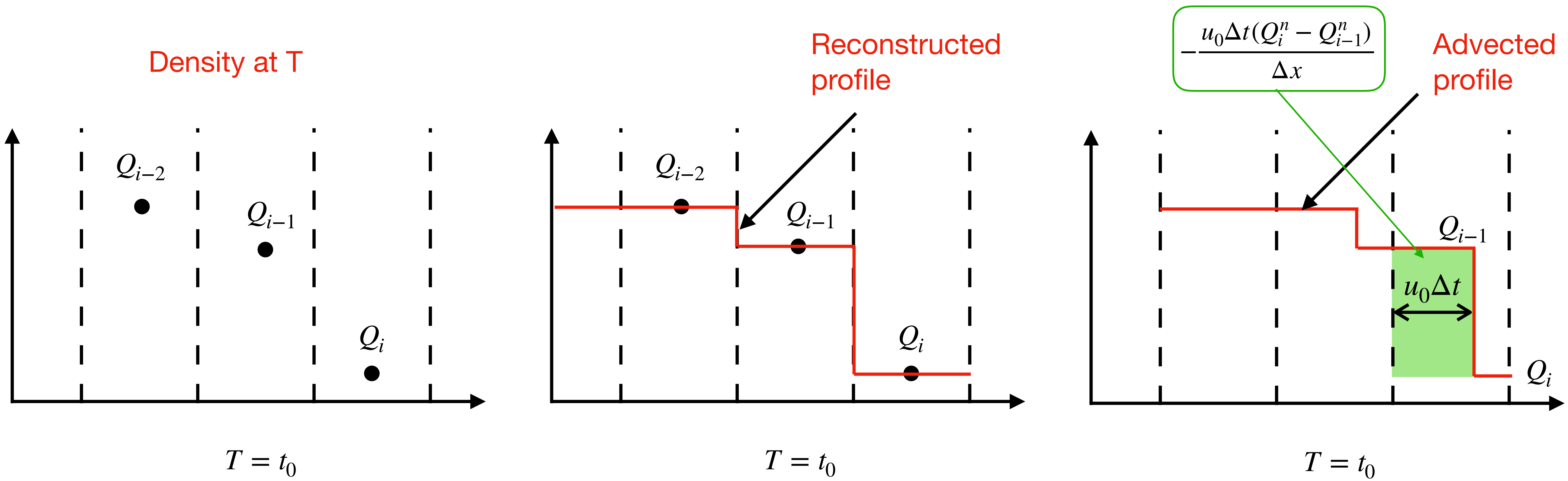




The Advection Nature of the equation

The REA framework

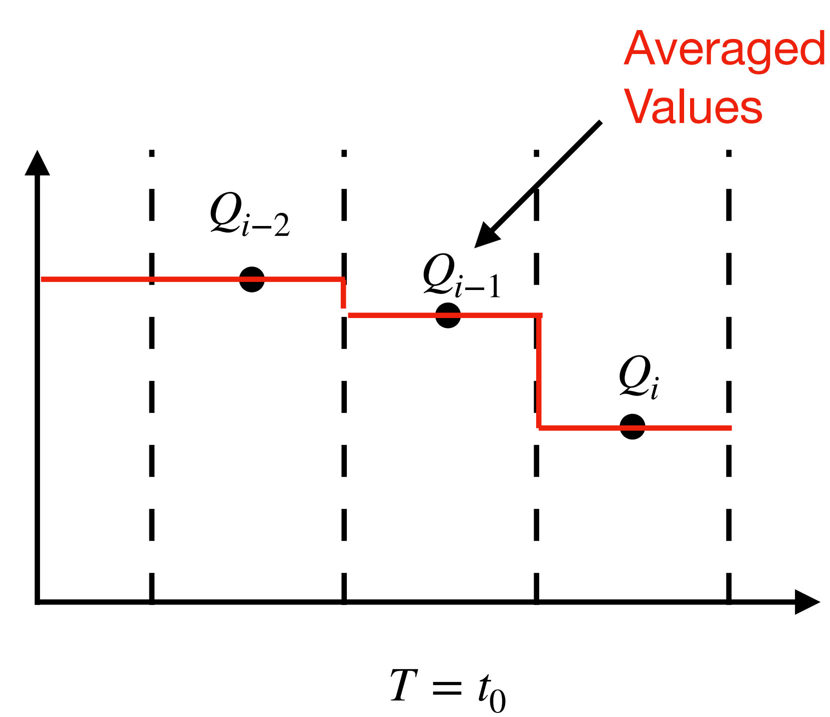
So the upwind scheme is basically an advection



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

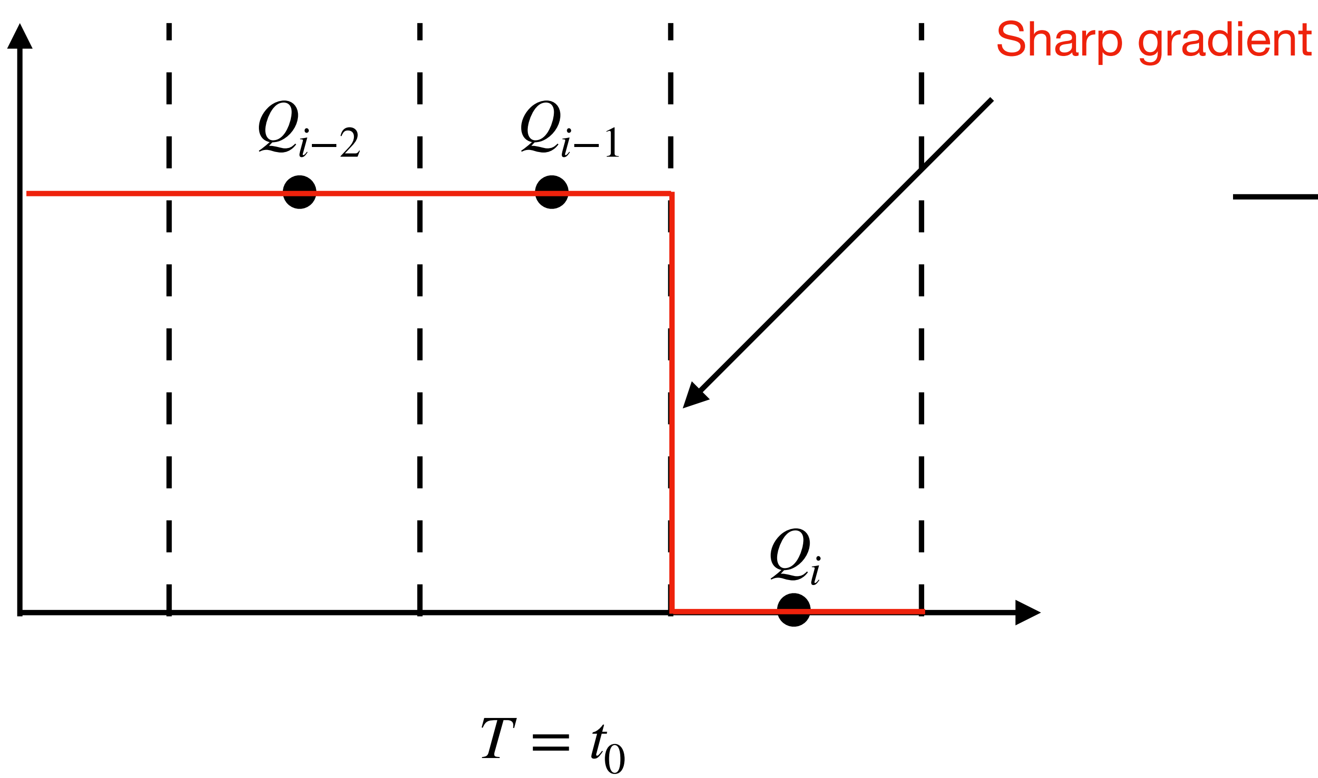
Reconstruct - ***Evolve*** - ***Average*** (REA framework)



The Advection Nature of the equation

Weak Solutions

From the REA framework, we know that the evolve-average step DOES NOT have requirement on the derivative of the profile:



$\longrightarrow$ Q(x) can even be a step function

How does this work with the PDE?

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

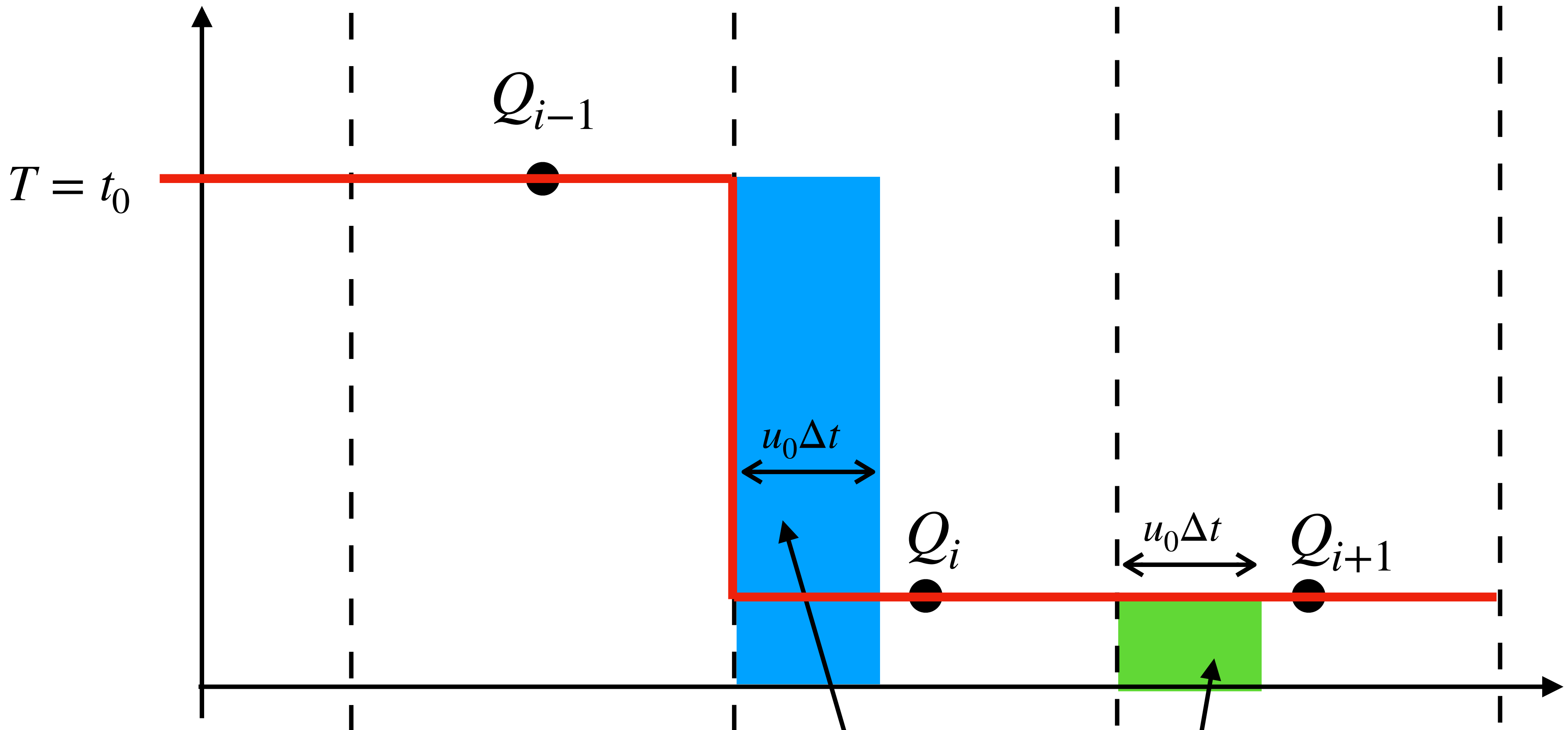
This is because the step-function profile satisfies the *integral form* of the advection equation

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

A solution Q that satisfies the integral form of the PDE is called a ***weak*** solution

The Transport Nature of the equation

The flux balance interpretation



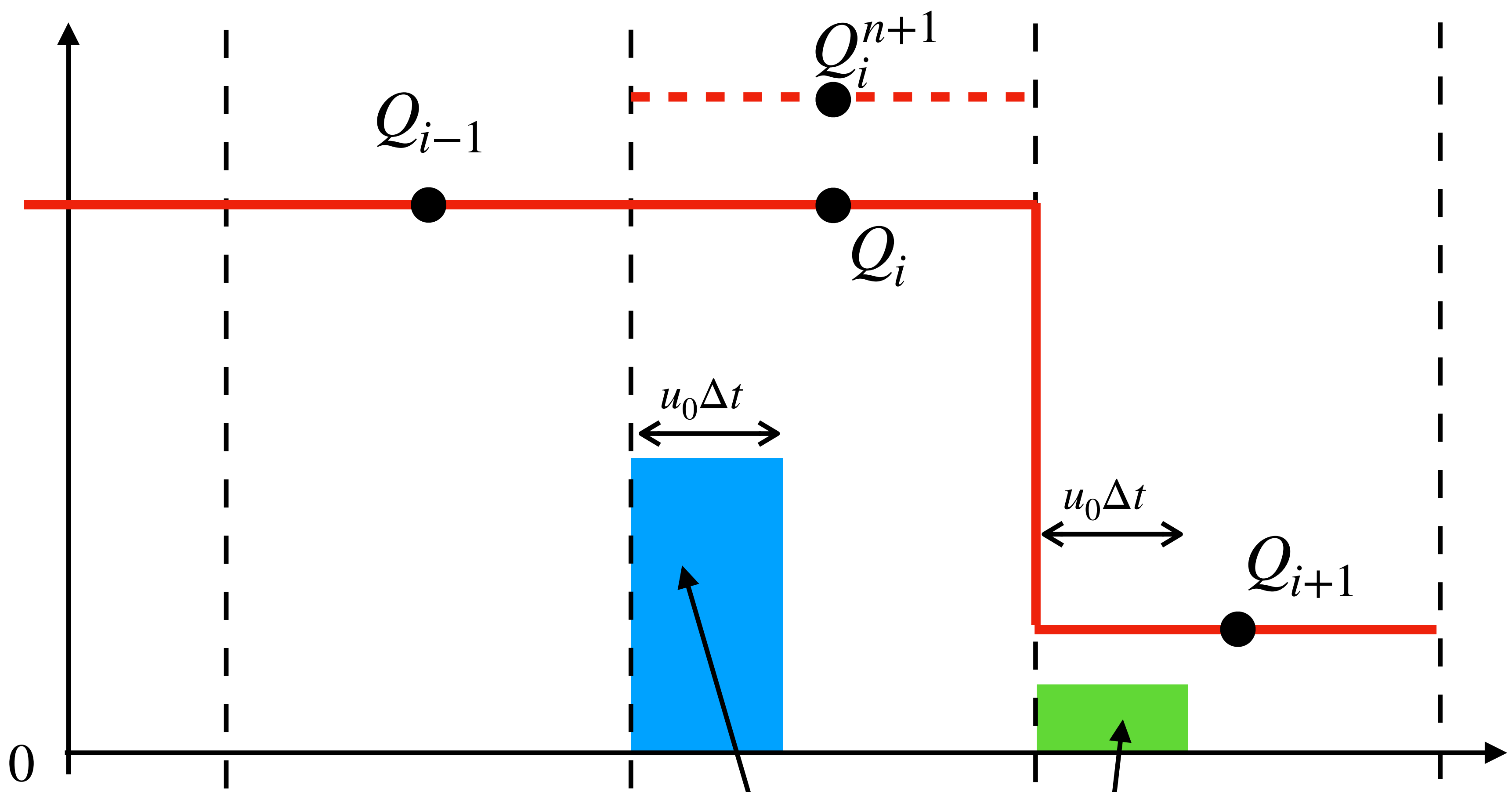
$$Q_i^{n+1} = Q_i^n - \frac{u_0 \Delta t (Q_i^n - Q_{i-1}^n)}{\Delta x} = Q_i^n + \left(\boxed{\frac{u_0 \Delta t}{\Delta x} Q_{i-1}^n} - \boxed{\frac{u_0 \Delta t}{\Delta x} Q_i^n} \right) \in (Q_{i-1}, Q_i)$$

Mass entering cell i

Mass leaving cell i

The Transport Nature of the equation

Why central scheme is unstable



$$Q_i^{n+1} = Q_i^n - \frac{u_0\Delta t(Q_{i+1}^n - Q_{i-1}^n)}{\Delta x} = Q_i^n + \left(\underbrace{\boxed{\frac{u_0\Delta t}{\Delta x}\frac{Q_{i-1}^n}{2}}}_{\text{Mass entering cell i}} - \underbrace{\boxed{\frac{u_0\Delta t}{\Delta x}\frac{Q_{i+1}^n}{2}}}_{\text{Mass leaving cell i}} \right) > Q_i^n$$

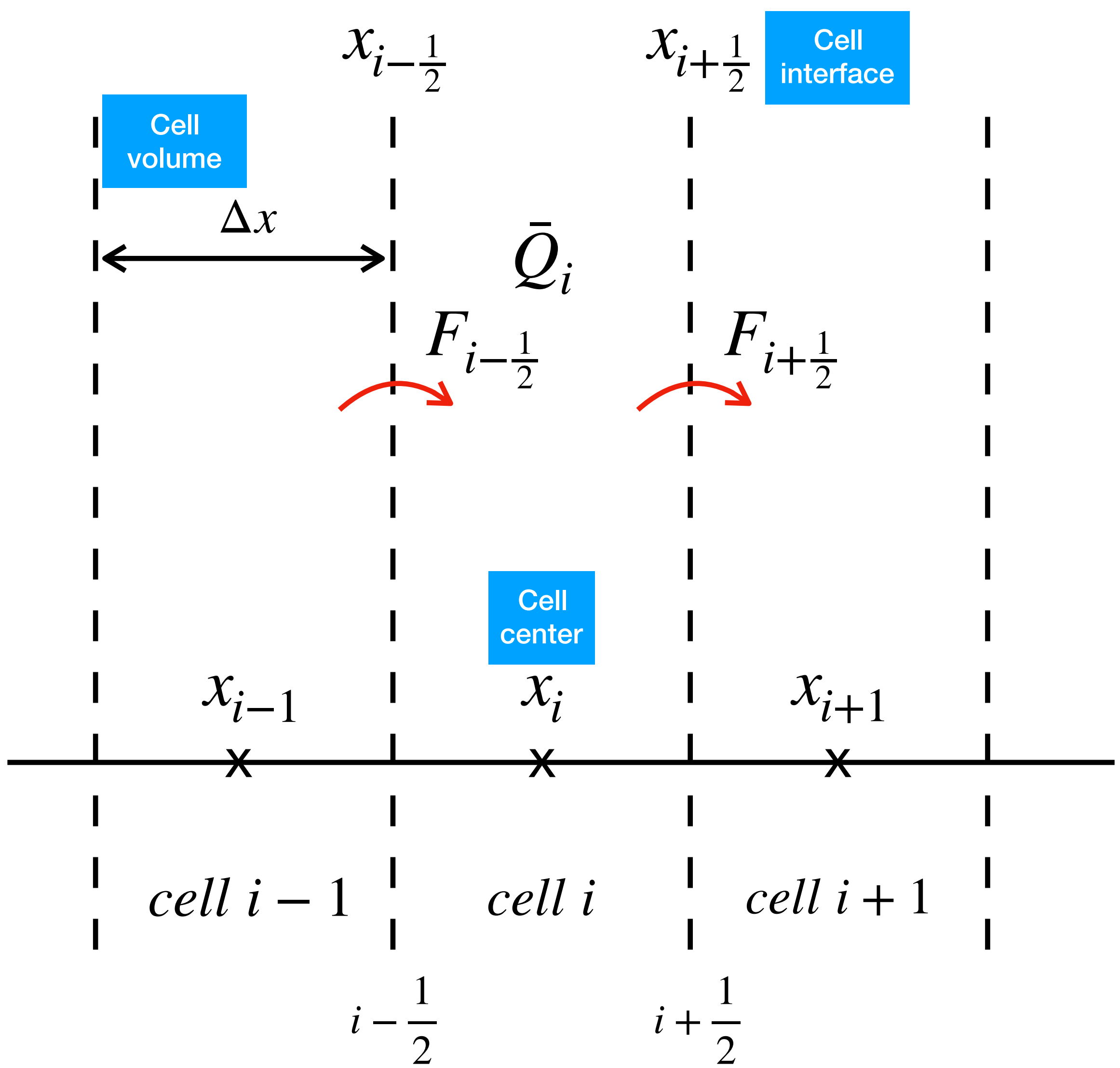
So in cell i, after one update, Q_i grows - oscillations which eventually leads to instability

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