Computational Astrophysics

1b. Numerical Solutions of PDEs

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Topics today [Ch. 2.1-2.7, 6.3.1-6.3.2]

- Numerical solutions: finite difference / finite volume
- The integral equations for finite volume
- The simple advection problem
- Courant-Friedrich-Lewy condition
- Upwind method
- higher order space and time updates
- van Leer method
- **Assignment 1d:**
  - Implement a slope limiter for the van Leer method
- **Assignment 1e:**
  - Stability analysis of schemes for solving the advection equation

Numerical Solutions to Differential Equations

- Partial differential equations come in three different types:
  - Hyperbolic: Solution depends on the ***initial value***

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

  - Elliptic: Solution depends on the ***boundary values***

$$\nabla^2\phi = 4\pi G\rho$$

  - Parabolic equations: Solution depends on the initial value, but it is irreversible (e.g. heat equation), and needs boundary values

- Today we will be concerned with the first type; elliptic equations are the topic of week 4, and radiative transfer can be formulated as a parabolic equation (week 6) In a general physics problem, the system of equations will contain all types

Numerical Solutions to Differential Equations

- To solve differential equations; for example the advection equation

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

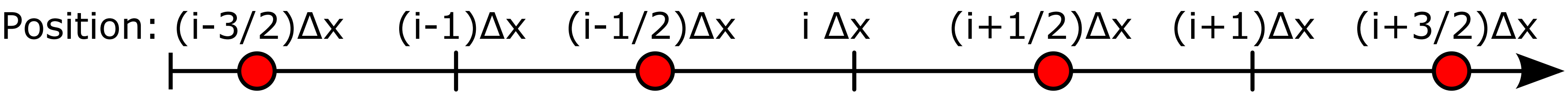
on a mesh there are two popular approaches:

Finite Difference and ***Finite Volume*** methods

- You play with both in this week's exercises
- In the course we will spend some time on the Finite Volume method
- While related, the mathematical theories behind the two techniques are very different

Finite Difference Method

- Assume the solution is known ("sampled") at a distinct set of points:



- ***$q(x_i,t)$*** is the value at each point ***$x_i = (i+1/2)\Delta x$*** at time ***t***

- Derivatives in time and space are approximated by differences, f.x.:

$$\frac{\partial q(x,t)}{\partial x}\bigg|_{x=x_i} \rightarrow \frac{q(x_i+\Delta x,t)-q(x_i-\Delta x,t)}{2\Delta x}$$

- This is essentially what you do in ***exercise 1c*** using a *second order in time, second order in space* approximation:

$$dqdt(x_i,t) = -A\frac{q(x_i+\Delta x,t)-q(x_i-\Delta x,t)}{2\Delta x}$$

$$q(x_i,t+\Delta t) = q(x_i,t)+\Delta t\left(\frac{3}{2}dqdt(x_i,t)-\frac{1}{2}dqdt(x_i,t-\Delta t)\right)$$

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Why do we call it 2nd order (?)

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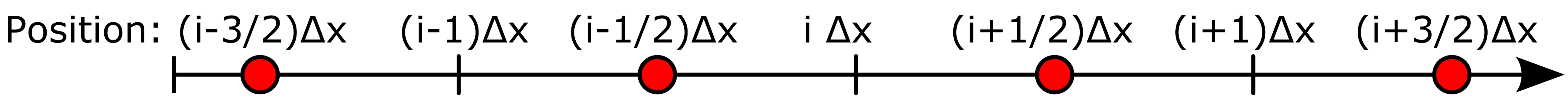

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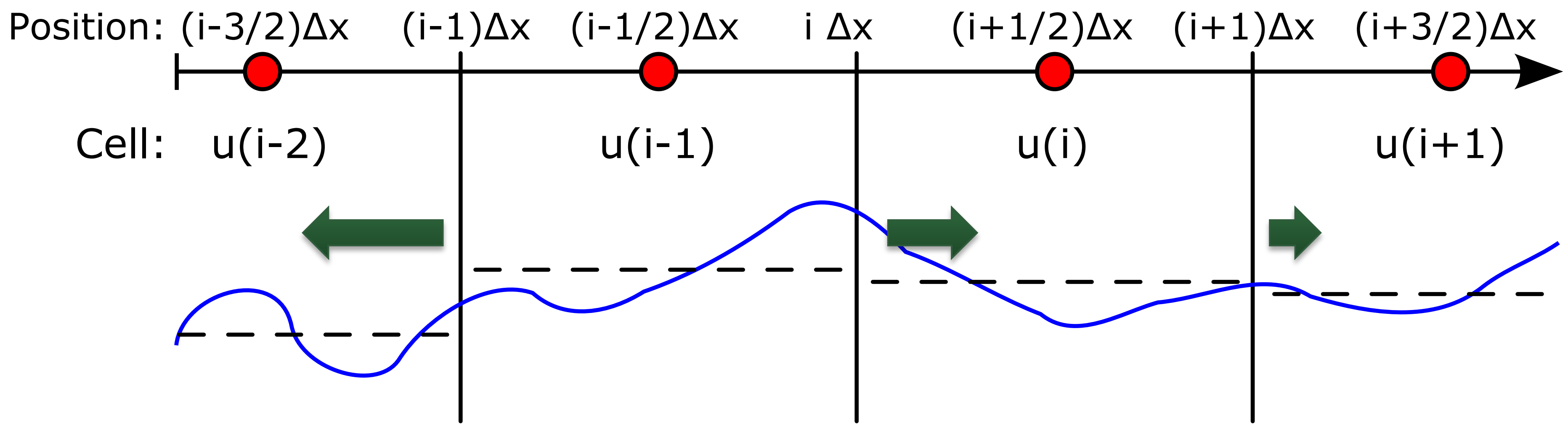
- The advantage of finite difference methods is that they are conceptually simple, and very fast. For smooth flows, high order methods can be extremely precise. For non-smooth flows, viscosity must be added by hand.

- The disadvantage is that they do not always respect the properties of the equations, because they consider point values.

Finite Volume Method

- In the finite volume method the **fundamental variable is the *volume average*** of the function inside a cell:



- ***u(x$_i$,t)*** is the average value in the interval [$\boldsymbol{x_{i-1/2}}$, $\boldsymbol{x_{i+1/2}}$] at time ***t***

$$u(x_i,t) = \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2} q(x,t)\mathrm{d}x$$

- To find the solution to the volume average we have to consider the ***flux through the surface*** of each cell.

Finite Volume Method – Evolution on Integral Form

- To find the evolution of the *volume average* we integrate the differential equation:

$$\int_t^{t+\Delta t} dt \int_{x_i-\Delta x/2}^{x_i+\Delta x/2} dx \frac{\partial q}{\partial t} + \frac{\partial F}{\partial x} = 0, \qquad F(x,t) = A\, q(x,t)$$

- We can do the spatial integral to find

$$\int_t^{t+\Delta t} dt\, \Delta x \frac{\partial u_i}{\partial t} + (F_{i+1/2} - F_{i-1/2}) = 0$$

where $F_{i+1/2} = F\big(x_{i+1/2}, q\big(x_{i+1/2}, t\big), t\big)$ is called the flux

- Finally doing the time-integral we find

$$u(t+\Delta t) - u(t) = -\frac{\Delta t}{\Delta x}\big(\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}\big)$$

where $\tilde{F}_{i+1/2} = \frac{1}{\Delta t}\int_t^{t+\Delta t} dt\, F_{i+1/2}(x_{i+1/2}, t)$ is the time-averaged flux.

General Finite Volume Method – an excursion

- In general, we can imagine a problem that is written as:

$$\frac{\partial q(x,t)}{\partial t} + \frac{\partial F(q,t)}{\partial x} = S(q,x,t)$$

- The solution to the evolution will be the result of **fluxes *F*** moving things around, while **sources *S*** are changing the values inside the cells:

$$u(x_i, t+\Delta t) - u(x_i, t) = \frac{\Delta t}{\Delta x}\left[\Delta x\, \tilde{S}_i - \left(\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}\right)\right]$$

where the ***time averaged flux*** and **time and space averaged source** are:

$$\tilde{F}_{i+1/2} = \frac{1}{\Delta t}\int_t^{t+\Delta t} dt\, F_{i+1/2}(x_{i+1/2}, t)\,,$$

$$\tilde{S}_i = \frac{1}{\Delta t\, \Delta x}\int_t^{t+\Delta t}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2} dt\, dx\, S(x,t)$$

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- **Fluxes *F*** are related to conserved quantities, while **sources *S*** corresponds to the creation, destruction or transfer of a quantity. Examples are
  - Mass, momentum and total energy of a system (fluxes)
  - Energy cooling and heating (sources); Gravitation (source or flux!)
  - Geometric source terms (e.g. in a spherical coordinate system, or non-inertial forces in an accelerated system)

Finite Volume Method – Evolution equation

- The integral evolution equation of the *volume average*

$$u(t+\Delta t) - u(t) = -\frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}\right)$$

is exact.

- ***Derivatives*** are converted into ***differences***
  - This is ***in principle*** well suited for numerical evaluation
  - The absence of partial derivatives means the equations are well defined even for discontinuous functions

Finite Volume Method

- The problem is to find an expression for the time averaged fluxes

$$\tilde{F}_{i+1/2} = \frac{1}{\Delta t}\int_t^{t+\Delta t} dt\, F\left[x_{i+1/2}, t, q\left(x_{i+1/2}, t\right)\right]$$

- Problems:
    - The flux is calculated from the actual point values ***q*** at the interface, not the cell-averaged values ***u***.
    - We need to approximate the time integral.

- Solutions:
    - We need to reconstruct the value at the interface based on the cell average. This is called ***slope reconstruction***.
    - For the time evolution we can use f.x. Adams Bashforth, but a better estimate would be through ***implicit methods*** (difficult) or some kind of ***predictor-corrector*** scheme to get a ***time-centered*** approximation.

time-stepping and flow of information

The Advection Problem

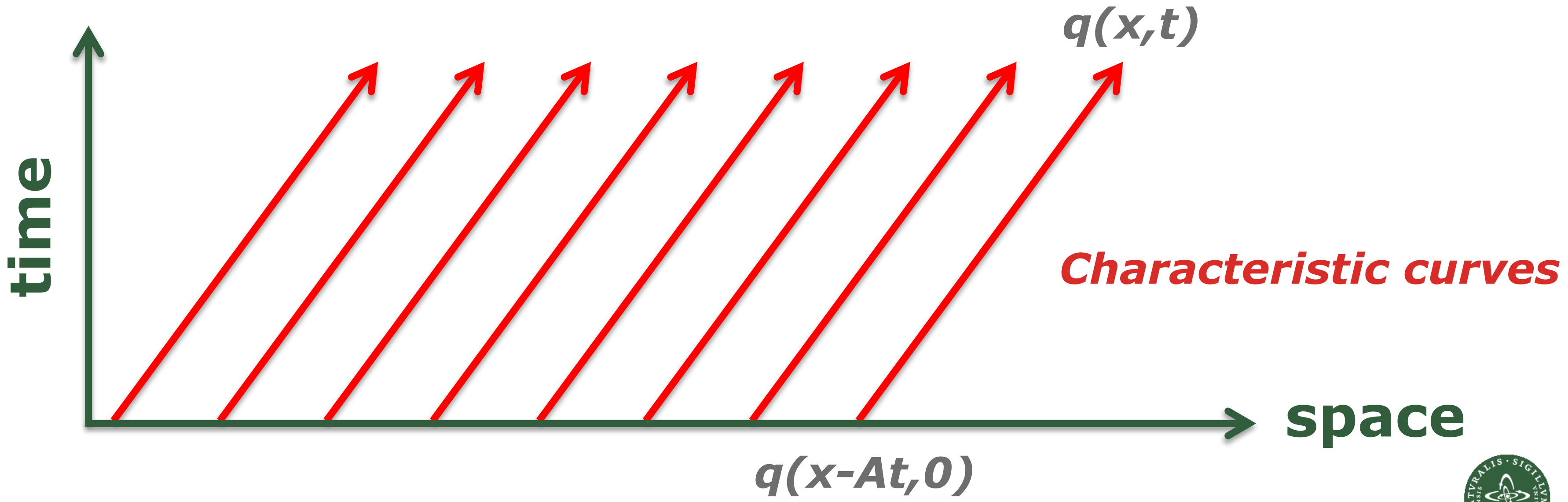
- The evolution is given by

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

- With the basic solution

$$q(x,t) = q(x - At, 0)$$

- This can also be sketched in a space-time diagram



Solving the Advection Problem

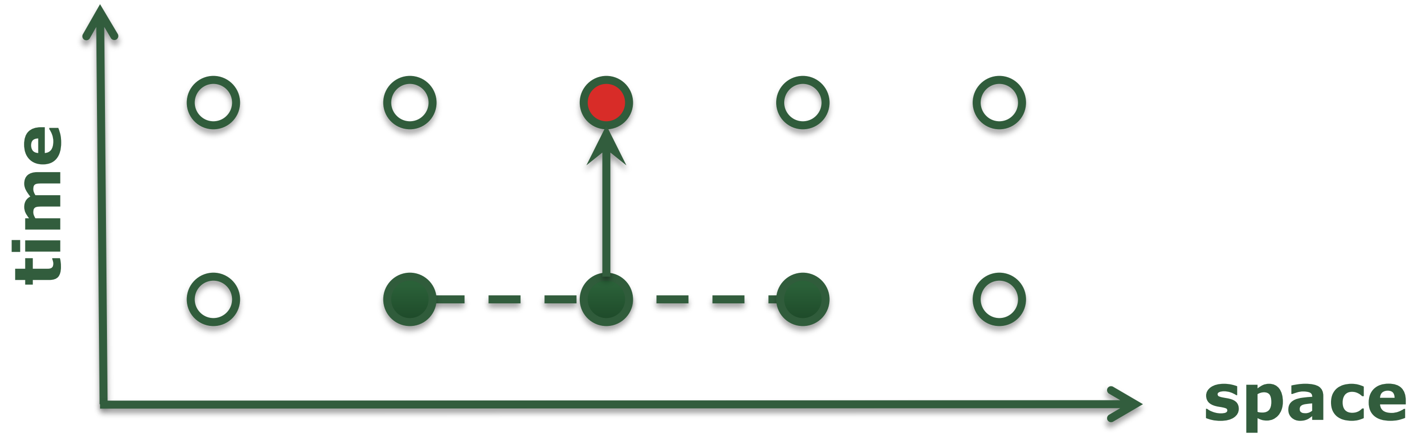
- Let us try with a simple numerical solution (exercise 1c)

$$dqdt(x_i,t) = -A\frac{q(x_i+\Delta\mathrm{x},t)-q(x_i-\Delta x,t)}{2\Delta x}$$

- This gives the prescription

$$q(x_i,t+\Delta t) = q(x_i,t)+\Delta t\left(\frac{3}{2}dqdt(x_i,t)-\frac{1}{2}dqdt(x_i,t-\Delta t)\right)$$

- We can sketch the method in a discrete space-time diagram (ignoring points at t-Δt for simplicity; they just extend the triangle)



The Courant-Friedrich-Lewy condition

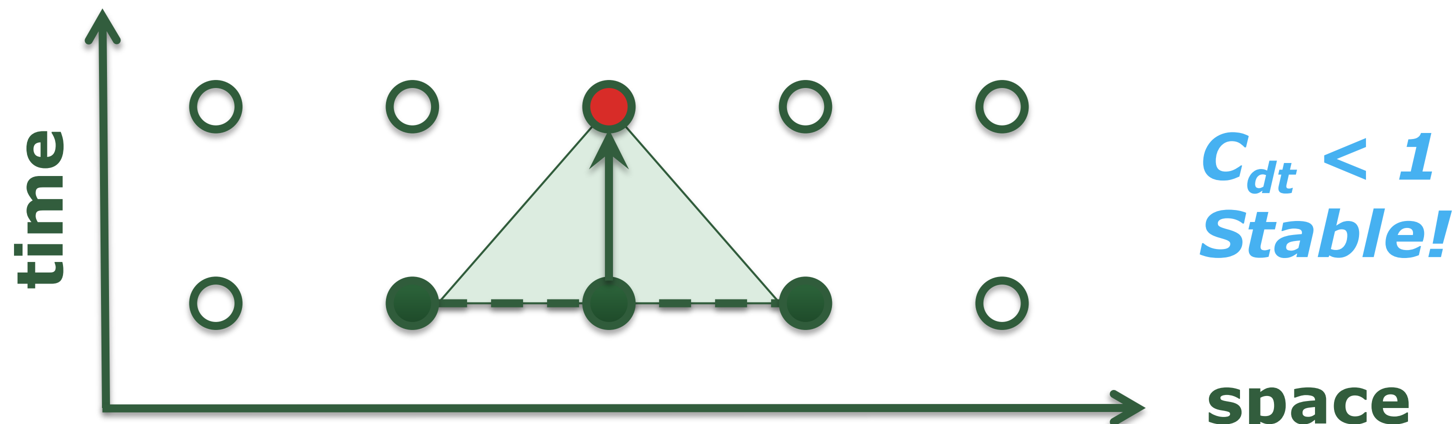
- The characteristics tell us the domain of dependence, or how fast information travel. In this case the travel speed is simply ***A***

- This can be compared with the "numerical domain of dependence", and the corresponding "numerical velocity" $\Delta x/\Delta t$.

- The ratio between the two is called the Courant number

$$C_{dt} = \frac{A}{\Delta x/\Delta t}$$

- If $C_{dt} < 1$ we are including the full physical domain of dependence in the numerical domain



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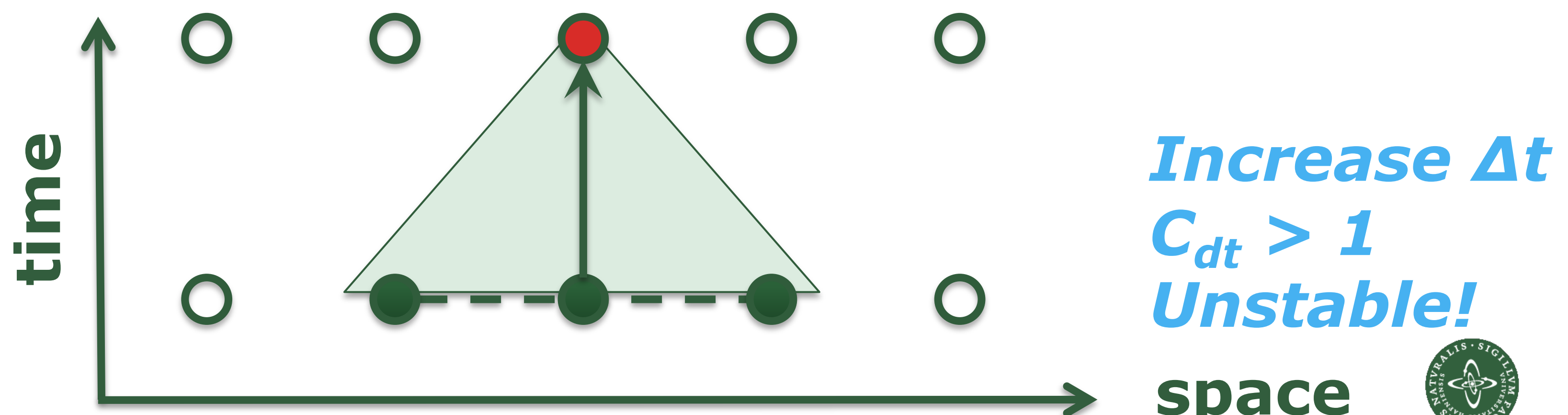
$$C_{dt} = \frac{A}{\Delta x/\Delta t}$$

- If $C_{dt} > 1$ we are *not* covering the full physical domain of dependence in the numerical domain. It is unstable



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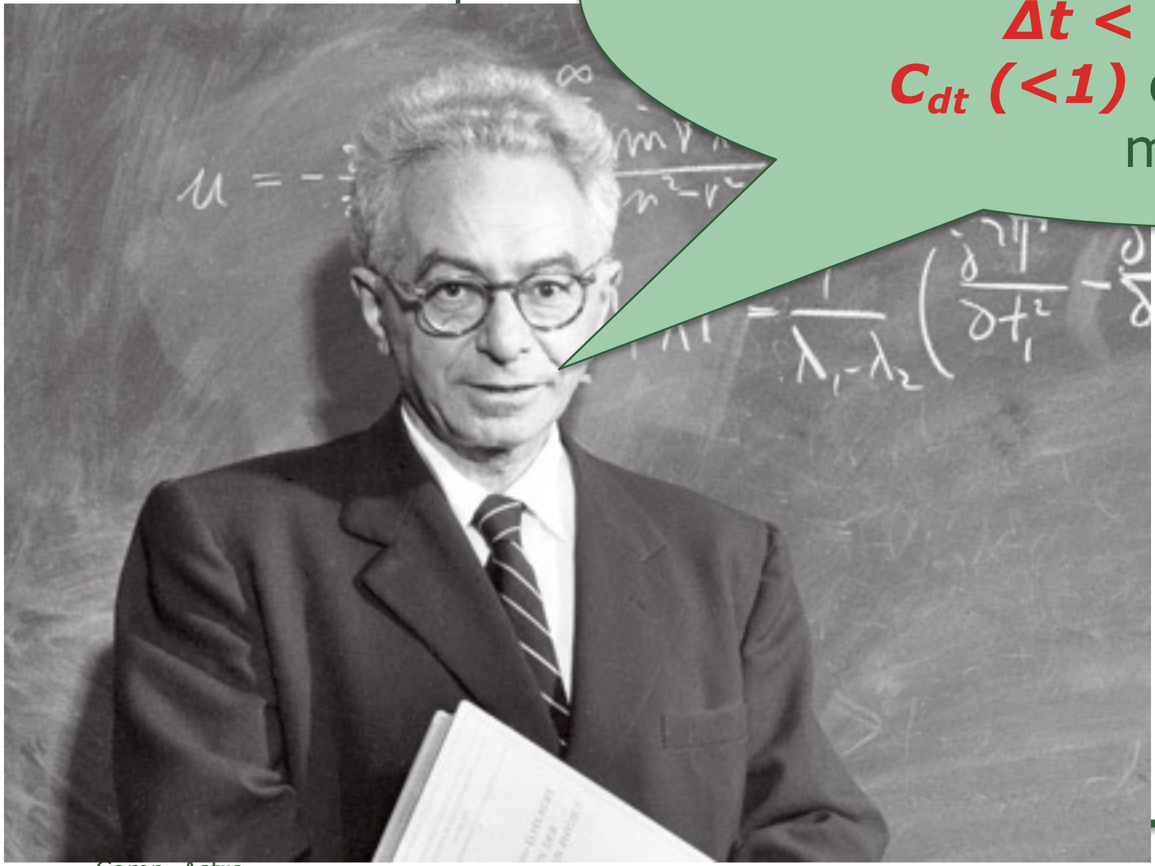


You can easily test this in your notebook: If ***A*** is the fastest speed of propagation, you need

$$\Delta t < C_{dt}\, \Delta x / A$$

C_{dt} **(<1)** depends on the method

cal domain of dependence

Increase Δt

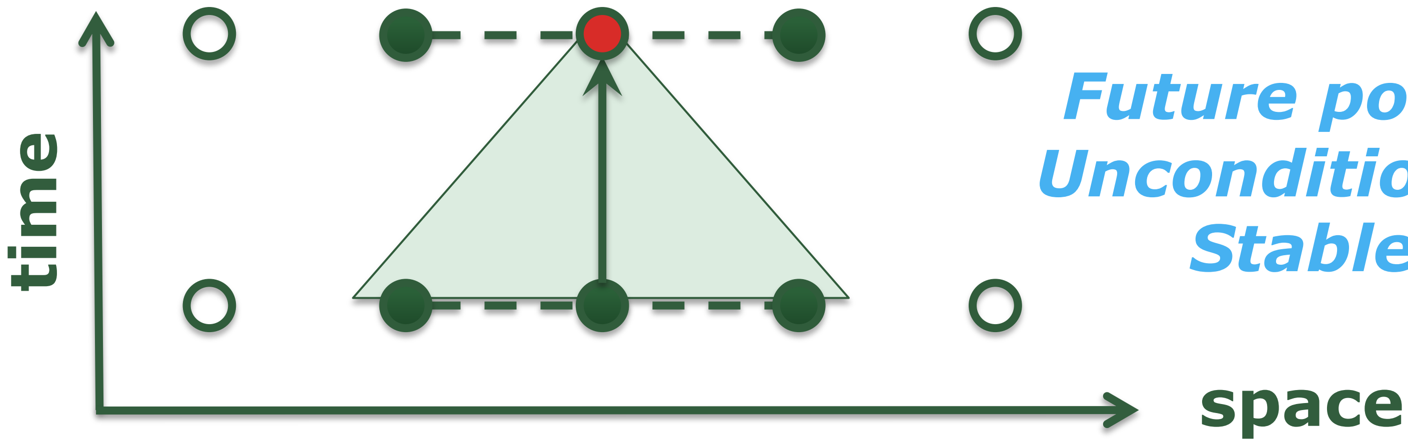
$C_{dt} > 1$

Unstable!

space

The Courant-Friedrich-Lewy condition

- Notice that if we use information from a future time level the method is called **implicit** and can often be unconditionally stable



Future points: Unconditionally Stable!

- Formal stability analysis is more complicated and require considering how perturbations with different wavelengths behave. This is called a Von Neumann analysis and is discussed in chap. 2.4 – 2.6.

- Von Neumann analysis is useful for understanding how/why a scheme is unstable, but difficult for large systems (e.g. MHD)

- Rule of thumb: signals should not propagate more than one cell.

Overview of CFL conditions from chap 2.6

$$\boxed{\frac{\partial q}{\partial t} + \nabla \cdot F = 0}$$

- In the solution of the one-dimensional hydrodynamic equations by explicit techniques, the continuity equation leads to a time step limit of

$$\Delta t < \min \frac{\Delta x}{|v|}, \tag{2.89}$$

where v is the (in general, variable) velocity. The minimum is taken across the entire grid. Furthermore, the linearized stability analysis of a simple explicit hydrodynamic system gives the time step limit

$$\Delta t < \min \frac{\Delta x}{c_s}, \tag{2.90}$$

where c_s is the sound speed and the minimum is taken across the entire grid.

- In a general Eulerian hydrodynamic system, where the velocity is not necessarily small compared with the sound speed, the two criteria are usually combined according to the equation

$$\Delta t < \min \frac{\Delta x}{\left(c_s^2 + v^2\right)^{1/2}} \tag{2.91}$$

or

$$\Delta t < \min \frac{\Delta x}{(c_s + |v|)}. \tag{2.92}$$

Overview of CFL conditions from chap 2.6

$$\boxed{\frac{\partial q}{\partial t} + \nu_d \nabla^2 q = 0}$$

- In the solution of a one-dimensional diffusion equation by an explicit technique, the time step is limited, by considerations of stability, to

$$\Delta t < 0.5 \frac{(\Delta x)^2}{\nu_d} \tag{2.87}$$

where Δx is the smallest space interval on the grid and ν_d is the diffusion coefficient.

- If the diffusion equation is to be solved in N-space dimensions, the time step limit becomes

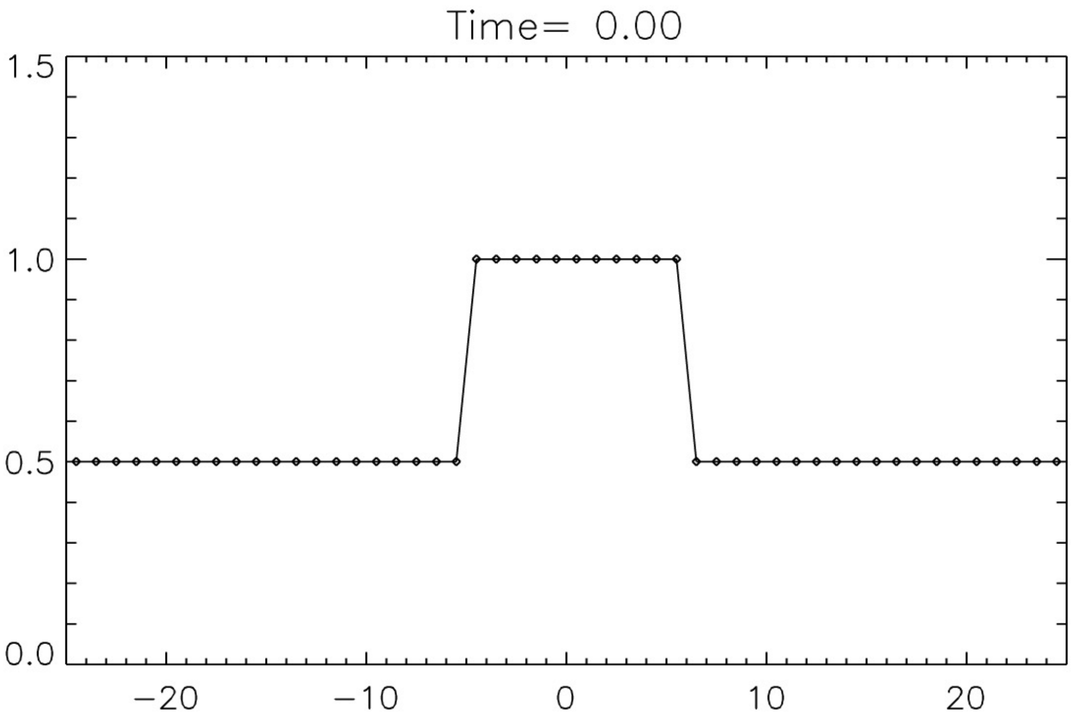
$$\Delta t < \frac{0.5}{N} \frac{(\Delta x)^2}{\nu_d}. \tag{2.88}$$

This restriction may make the explicit technique inappropriate for many problems. In contrast, the implicit Crank–Nicolson scheme and other implicit schemes are numerically stable for all Δt, and the time step is limited only by the physical time scale of the problem.

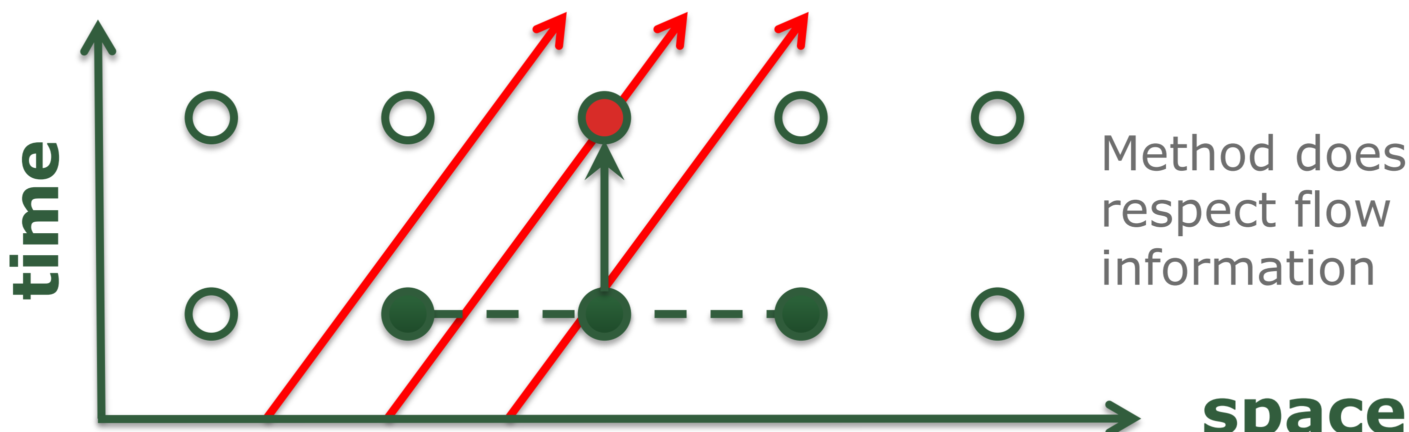
- Danger! Diffusion limits timestep at high resolution: $\Delta t \propto \Delta x^2$
  - Implicit methods or sub-cycling in time may be needed

Upwind / Donor Cell Method

Forward-in-Time-Centered-in-Space Advection

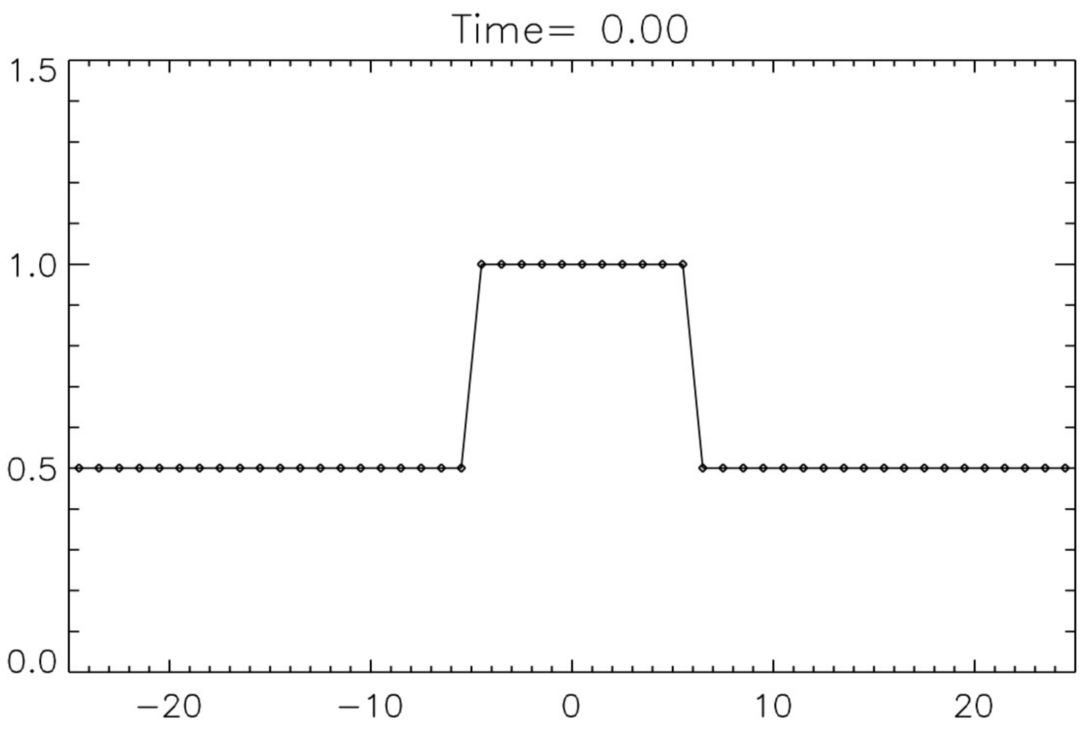


$$\frac{\partial q(x,t)}{\partial x} \rightarrow \frac{q(x+\Delta x)-q(x-\Delta x)}{2\Delta x}$$

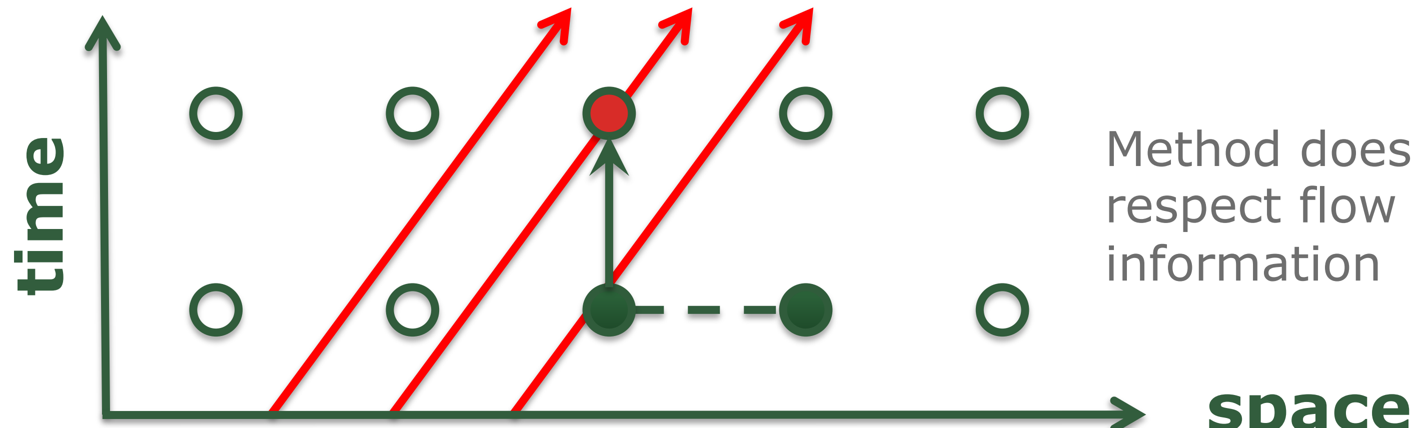


Method does not respect flow of information

Try 2: Forward-in-Time-Forward-in-Space

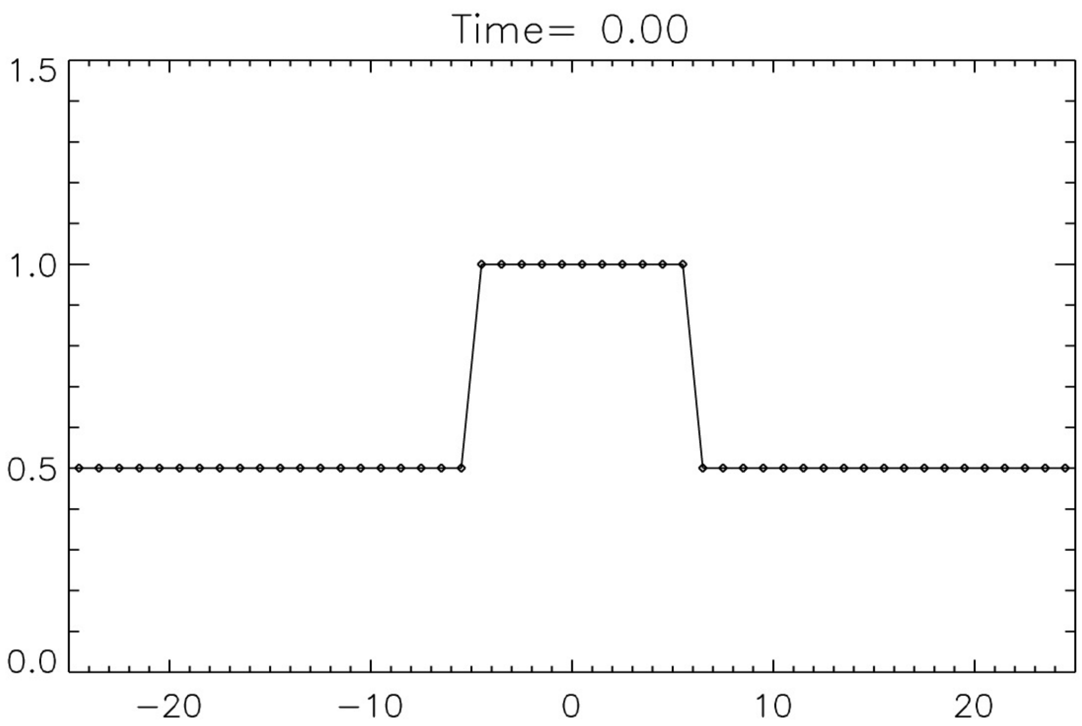


$$\frac{\partial q(x,t)}{\partial x} \rightarrow \frac{q(x+\Delta x)-q(x)}{\Delta x}$$

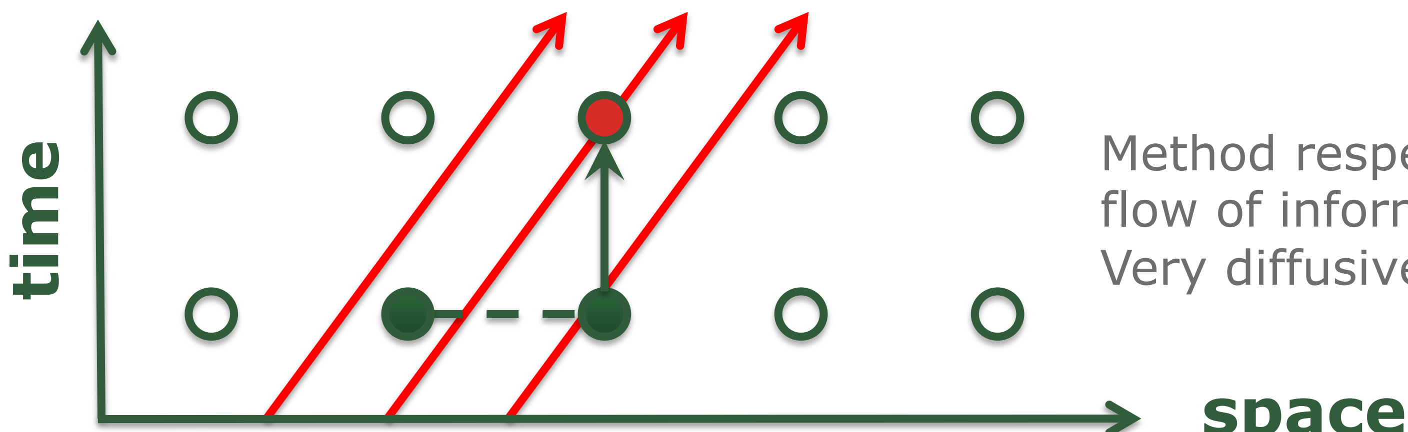


Method does not respect flow of information

Try 3: Forward-in-Time-Backward-in-Space



$$\frac{\partial q(x,t)}{\partial x} \rightarrow \frac{q(x)-q(x-\Delta x)}{\Delta x}$$



Method respects flow of information.
Very diffusive!

The Upwind / Donor Cell Method

- This observation can be generalized into the so-called Upwind or Donor cell method.

- Use a difference operator that respects the flow of information

$$\frac{\partial q(x,t)}{\partial x} \rightarrow \begin{cases} \dfrac{q(x)-q(x-\Delta x)}{\Delta x}, A>0 \\ \dfrac{q(x+\Delta x)-q(x)}{\Delta x}, A<0 \end{cases}$$

Ex: von Neumann analysis of the FinT-FinS scheme

- Space-time diagrams give us an intuitive understanding of what goes on, but a formal stability analysis can be done relatively easy

- Advection equation is linear: $q_j^{n+1} - q_j^n = \alpha\left(q_{j+1}^n - q_j^n\right), \alpha = -A\,\Delta t/\Delta x$
- Consider a small perturbation with a wavenumber k: $\mathrm{q}_j^n = \epsilon^n e^{-ikj}$
- Advection equation becomes:
$$\epsilon^{n+1}e^{-ikj} = \epsilon^n e^{-ikj} + \alpha\left(\epsilon^n e^{-ik(j+1)} - \epsilon^n e^{-ikj}\right) = \epsilon^n e^{-ikj}\left[1 + \alpha\left(e^{-ik} - 1\right)\right]$$
- The amplification function (matrix in chap 2.4) is then:
$$g(k) = 1 + \alpha\left(e^{-ik} - 1\right) = 1 + \alpha(\cos(k) - 1) - i\,\alpha\sin(k)$$
- Every time a timestep is taken the mode is amplified by this factor. If α can be chosen such that $|\mathrm{g(k)}| < 1$ then the amplitude will be bounded. Otherwise, the solution is unstable. Condition is:

$$|g(k)|^2 = (1 + \alpha(\cos(k) - 1))^2 + \alpha^2\sin^2(k) < 1$$

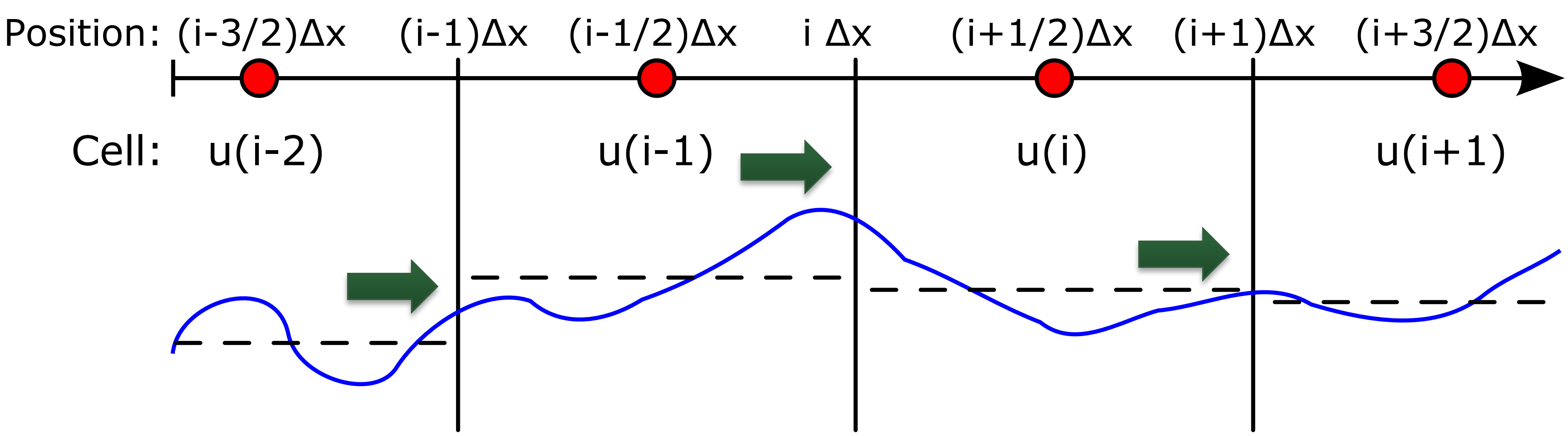
if A>0 is it possible to choose α such that $\forall k$: $|\mathrm{g(k)}| < 1$?

Recap: Finite Volume Method

- The problem was to find an expression for the time averaged fluxes

$$\tilde{F}_{i+1/2} = \frac{1}{\Delta t}\int_t^{t+\Delta t} dt\, F\left[x_{i+1/2}, t, q\left(x_{i+1/2}, t\right)\right]$$

- In the case of the advection problem, we just found a lowest order solution: ***Use the upwind method to approximate the flux.***



$$\tilde{F}_{i+1/2} = F\left[x_i, t, u(x_i, t)\right]$$

Higher Order Methods

Higher Order Finite Volume Solvers:

- Make a better prediction for the flux integral by for example

$$\tilde{F}_i(t+\Delta t/2) = \frac{1}{2}\left[F_i(x_{i-1/2},t) + F_i(x_{i-1/2},t+\Delta t)\right]$$

- The problem is that we do not know the value of ***u(x,t+Δt)***

- Use a ***predictor scheme:***

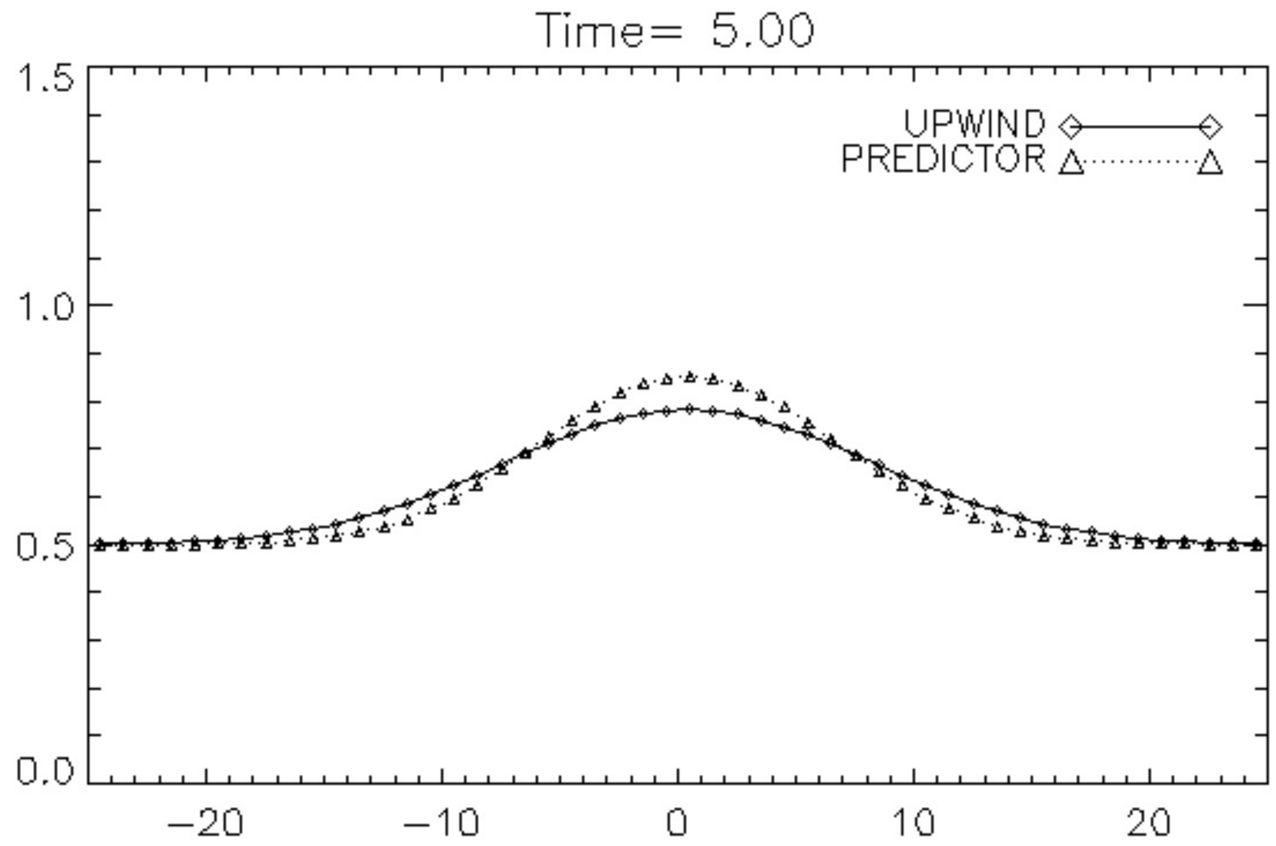
u* = u(x,t)+Δt/2 Centered Difference

Calculate F from u*

Higher Order Finite Volume Solvers:

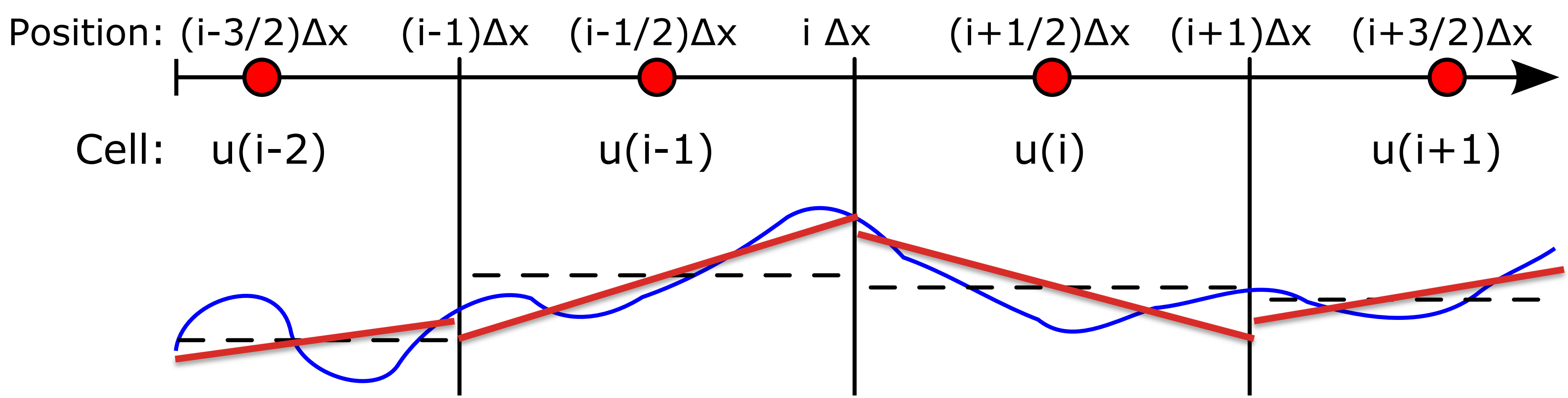
- Make a better prediction for the flux integral by for example

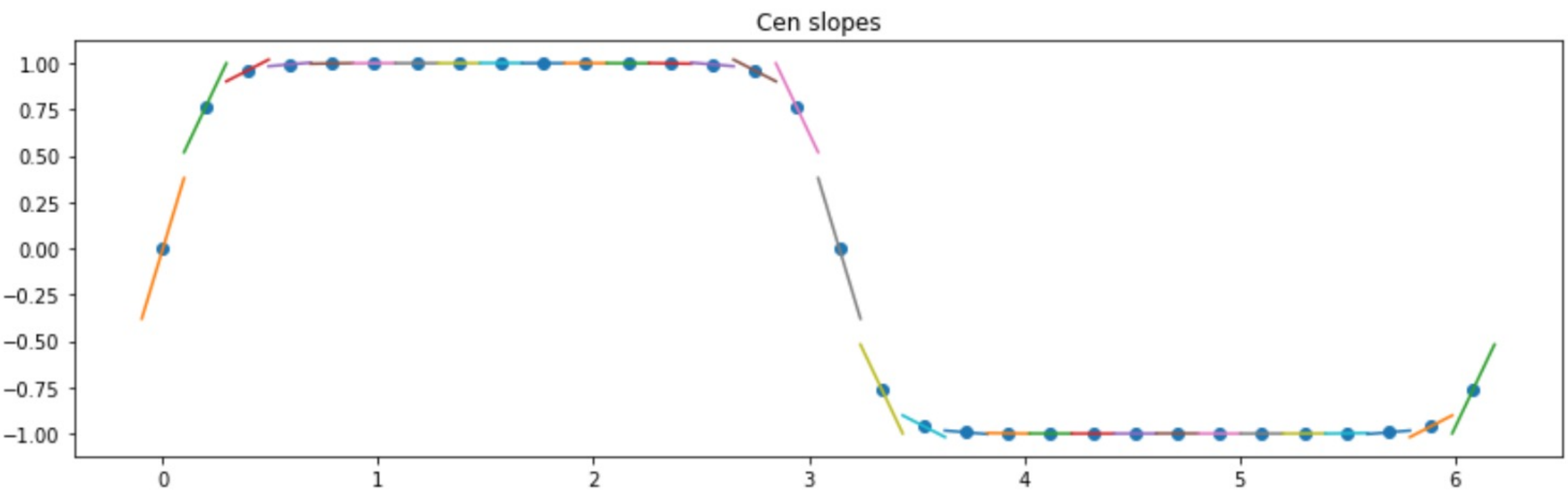
$$\tilde{F}_{i+1/2} = F\left[x_{i+1/2}, u^*\left(x_{i+1/2}\right)\right]$$



Higher Order in Space – Slope reconstruction

- As we have seen the Upwind method is very diffusive. Van Leer got the idea (1979) to also use spatial reconstruction for the Flux





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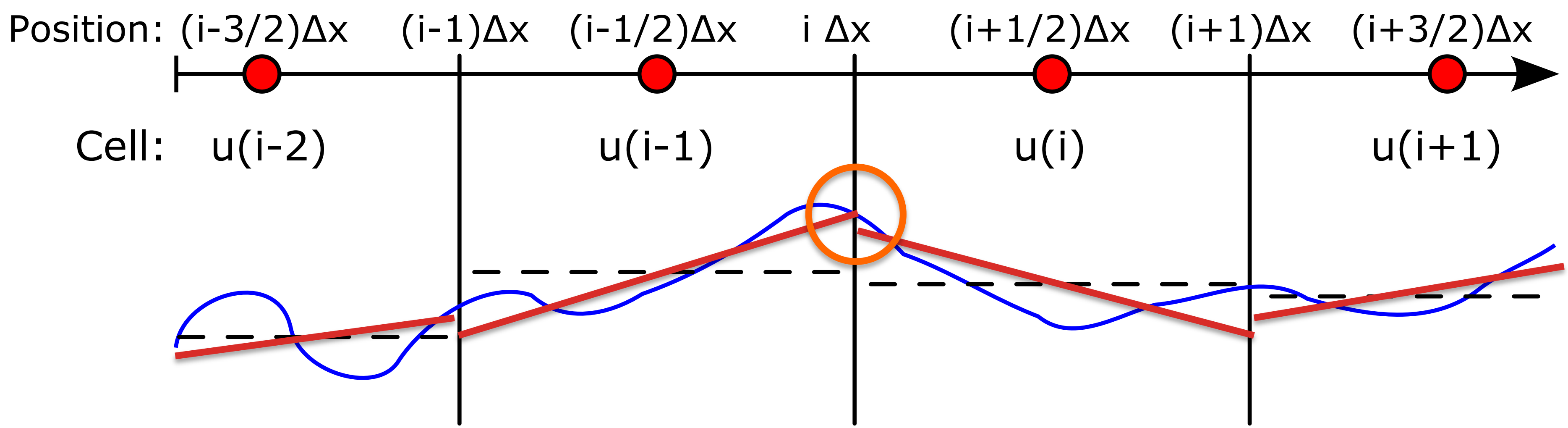

- A slope reconstruction has to be ***Total-Variation-Diminishing (TVD) [Harten 1983]***. It cannot introduce new maxima, at the interface. This would lead to oscillations in the solution.

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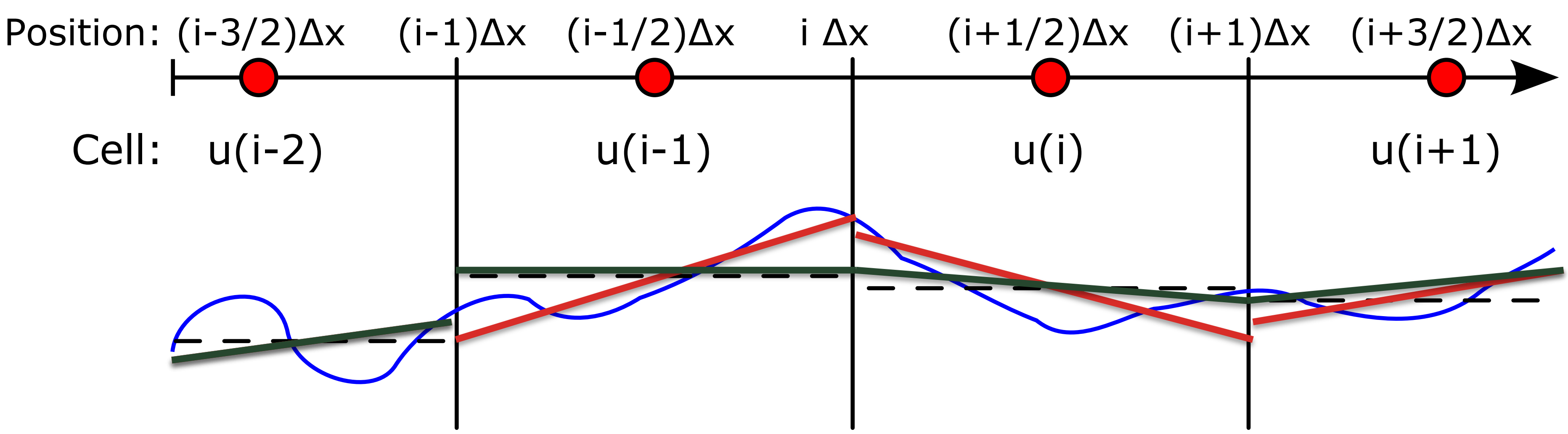

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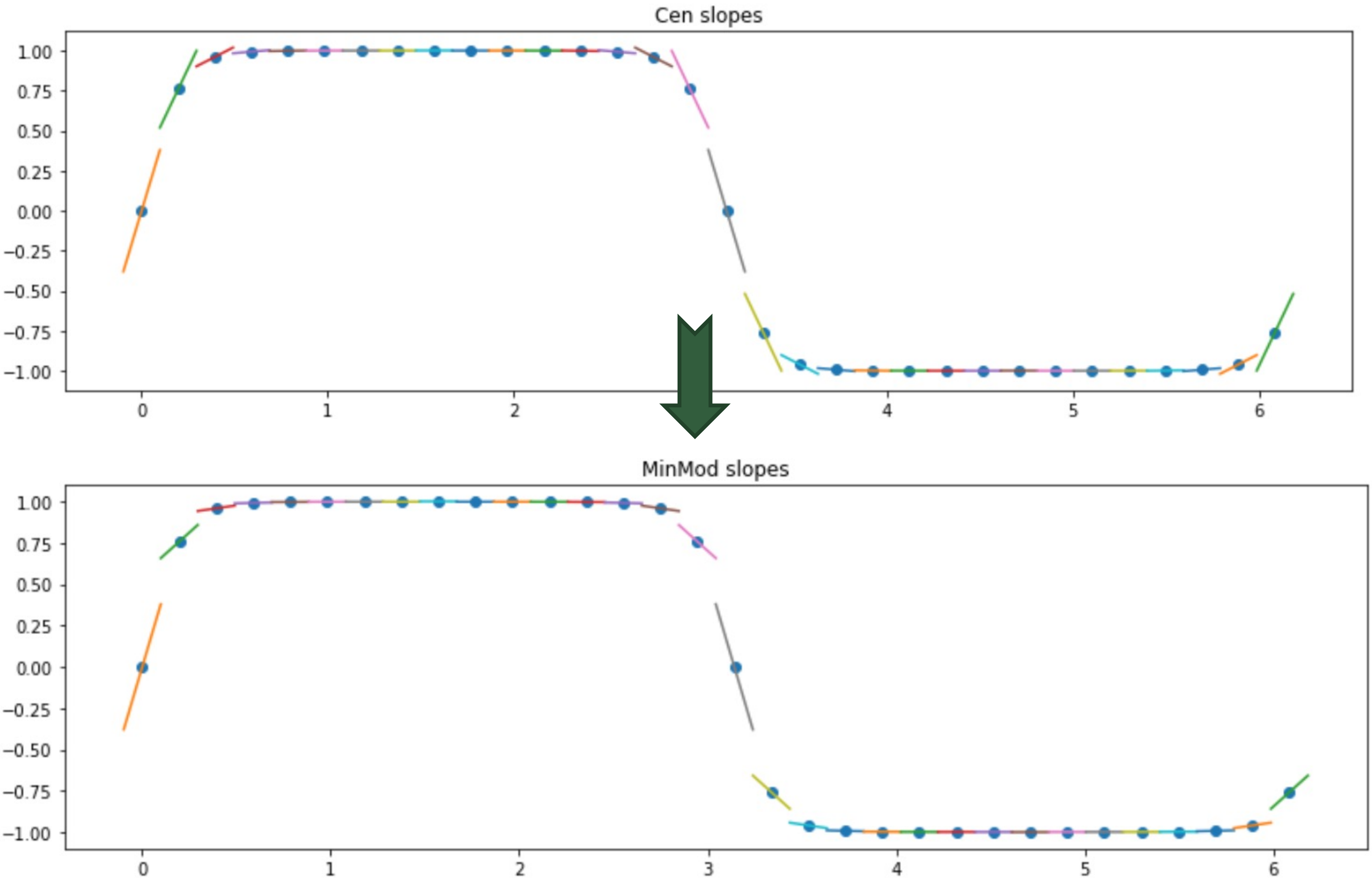
- Different slope limiters are more or less aggressive in limiting the state at the interface.

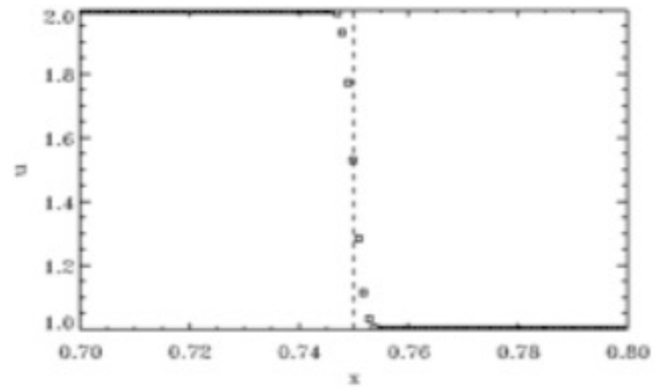
Higher Order in Space – Slope reconstruction



Higher Order in Space – Slope reconstruction

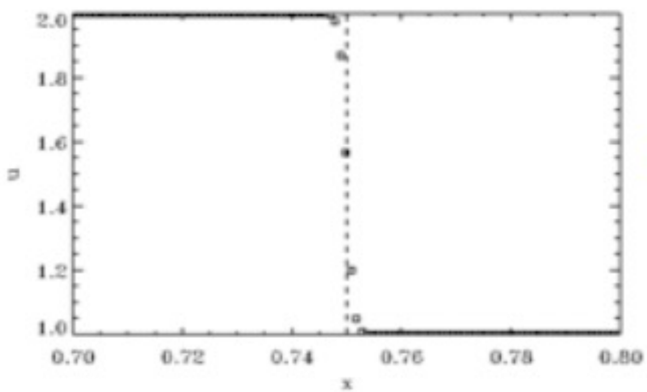
first order

`slope_type=0`



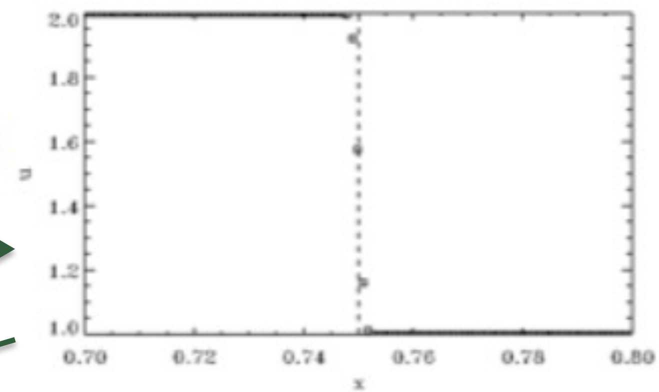
minmod

`slope_type=1`

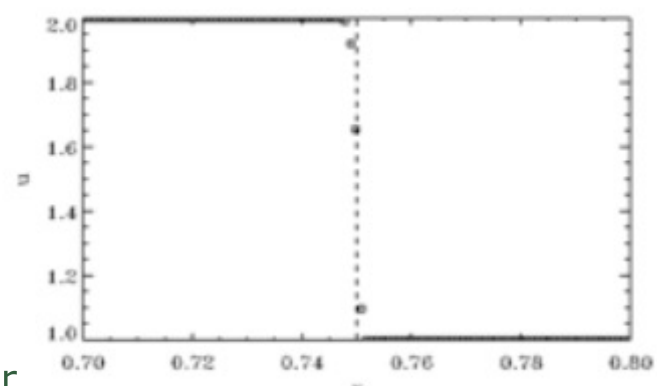


moncen

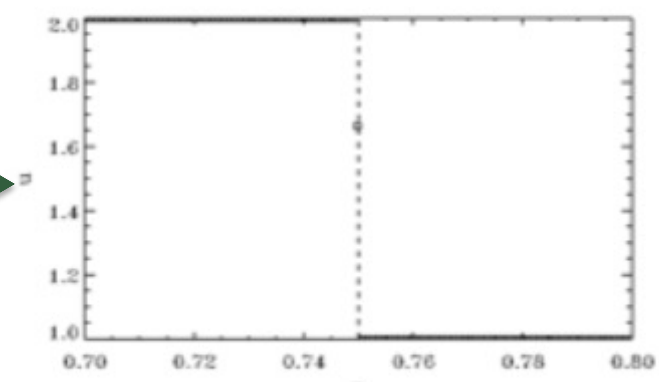
`slope_type=2`



superbee



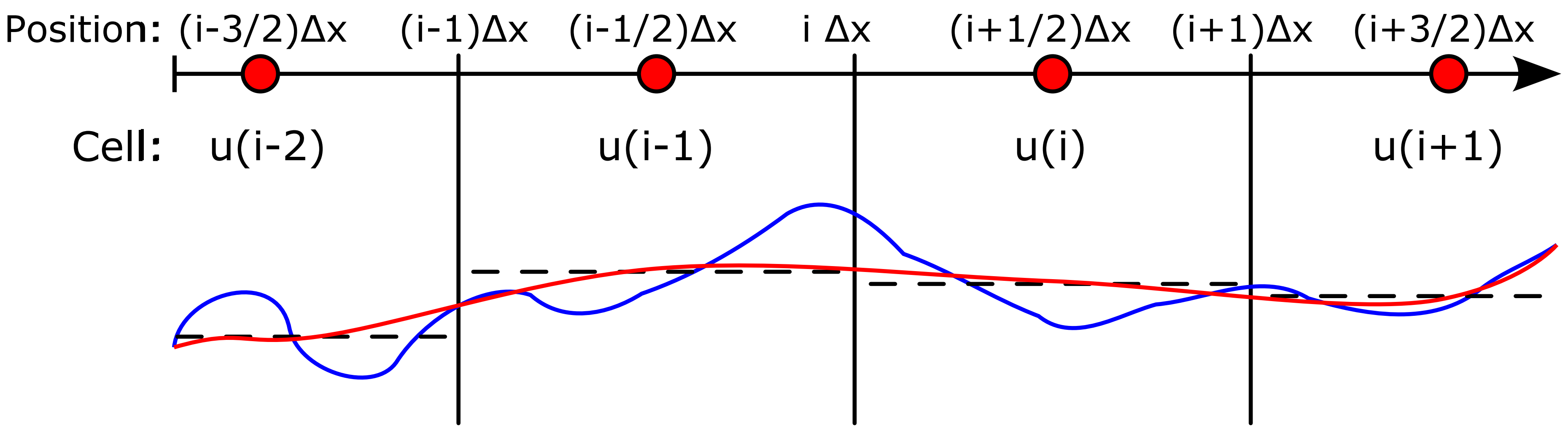
ultrabee



Made with RAMSES by R. Teyssier

Higher Order in Space – Slope reconstruction

- As we have seen the Upwind method is very diffusive. Van Leer got the idea (1979) to also use spatial reconstruction for the Flux



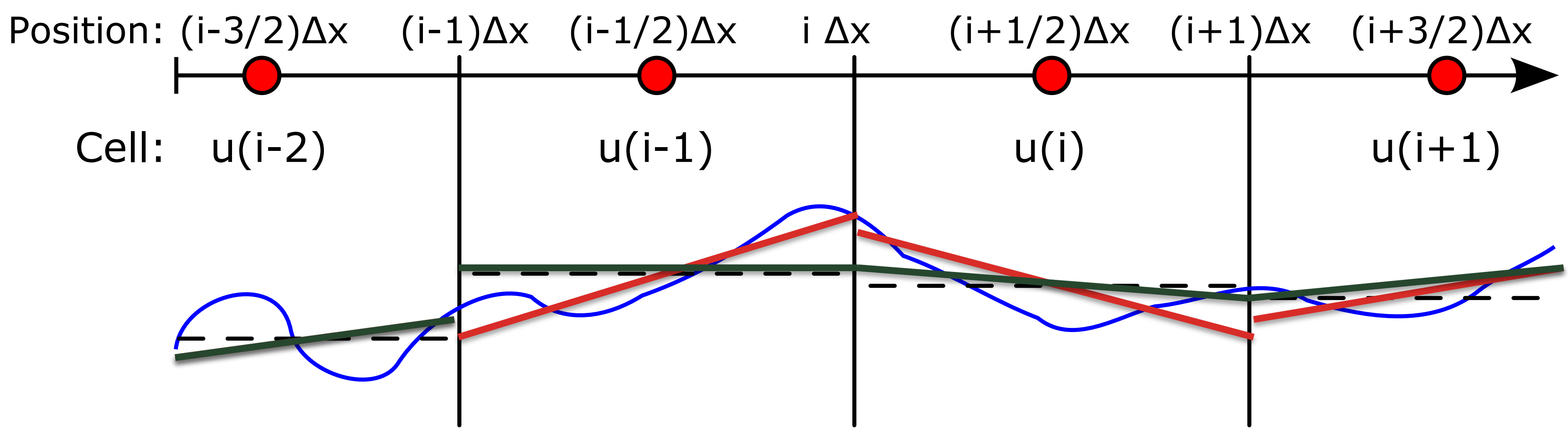
- Even higher order methods uses piece-wise parabolic reconstruction (PPM) or higher order polynomials (WENO).

Summary Finite Volume Methods for PDE's

1. Start with the average values in a cell u(x,t).

2. Find the fastest signal speed and adjust the timestep size Δt

3. Reconstruct the interface values through slope reconstruction+limiter



4. Calculate the time averaged flux.

5. Evolve using the equation: $u_i(t+\Delta t) - u_i(t) = -\frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+1/2} - \tilde{F}_{i-1/2}\right)$