Discretization of Equations

- The first step in solving any computational fluid dynamics problem is to discretize the equations
- Usually all fluid dynamics equations are in a partial differential equation format
- These differential equations must be transformed into algebraic form, so that they can become solvable
- The most straightforward discretization technique for partial differential equations is the finite difference method

$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

What is a finite difference?

Common definitions of the derivative of f(x):

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x-dx)}{2dx}$$

These are all correct definitions in the limit dx --> 0.

But we want dx to remain **FINITE**

What is a finite difference?

The equivalent ***approximations*** of the derivatives are:

$$\partial_x f^+ \approx \frac{f(x+dx)-f(x)}{dx}$$

forward difference

$$\partial_x f^- \approx \frac{f(x)-f(x-dx)}{dx}$$

backward difference

$$\partial_x f \approx \frac{f(x+dx)-f(x-dx)}{2dx}$$

centered difference

The **BIG** question

How good are the finite difference approximations?

$$\approx \neq =$$

This leads us to Taylor series....

Taylor Series

Taylor series are expansions of a function f(x) for some finite distance dx to f(x+dx)

$$f(x \pm dx) = f(x) \pm \mathrm{dx} f^{'}(x) + \frac{dx^2}{2!} f^{''}(x) \pm \frac{dx^3}{3!} f^{'''}(x) + \frac{dx^4}{4!} f^{''''}(x) \pm \ldots$$

What happens, if we use this expression for

$$\partial_x f^{+} \approx \frac{f(x+dx) - f(x)}{dx}$$

?

Taylor Series

… that leads to :

$$\frac{f(x+dx)-f(x)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^{2}}{2!}f^{''}(x)+\frac{dx^{3}}{3!}f^{'''}(x)+\ldots\right]$$
$$=f^{'}(x)+O(dx)$$

The error of the first derivative using the *forward* formulation is *of order dx*.

Is this the case for other formulations of the derivative?
Let’s check!

Taylor Series

... with the *centered* formulation we get:

$$\frac{f(x+dx/2)-f(x-dx/2)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^3}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx^2)$$

The error of the first derivative using the centered approximation is *of order* dx^2.

This is an **important** result: it DOES matter which formulation we use. The centered scheme is more accurate!

Advection Equation with Centred Scheme

Consider the advection equation

$$\frac{\partial f}{\partial t} = -u\frac{\partial f}{\partial x}$$

... with the *centered* formulation we get:

$$\frac{f_i^{(n+1)} - f_i^{(n)}}{\Delta t} = -u\left(\frac{f_{i+1}^{(n)} - f_{i-1}^{(n)}}{2\Delta x}\right)$$

Recast as

$$f_i^{(n+1)} = f_i^{(n)} - \frac{C}{2}\left(f_{i+1}^{(n)} - f_{i-1}^{(n)}\right)$$

Where C is the ***Courant number***

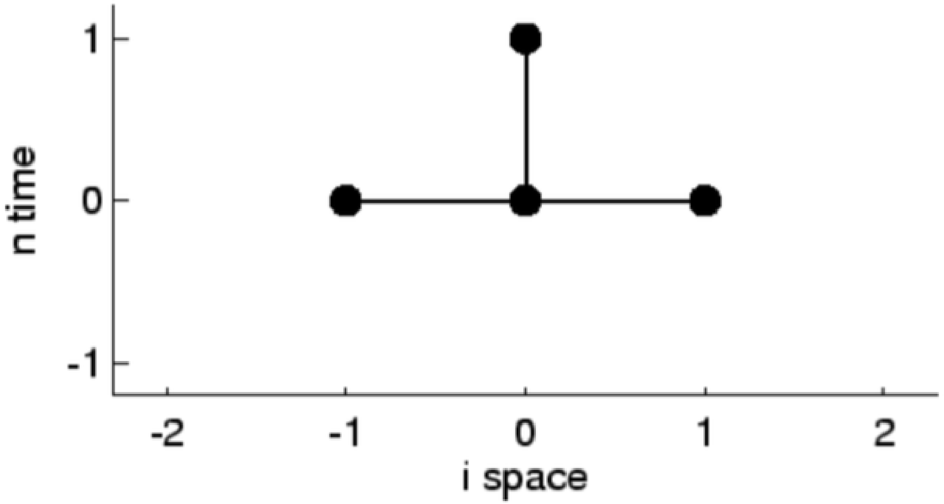
$$C \equiv \frac{u\Delta t}{\Delta x}$$

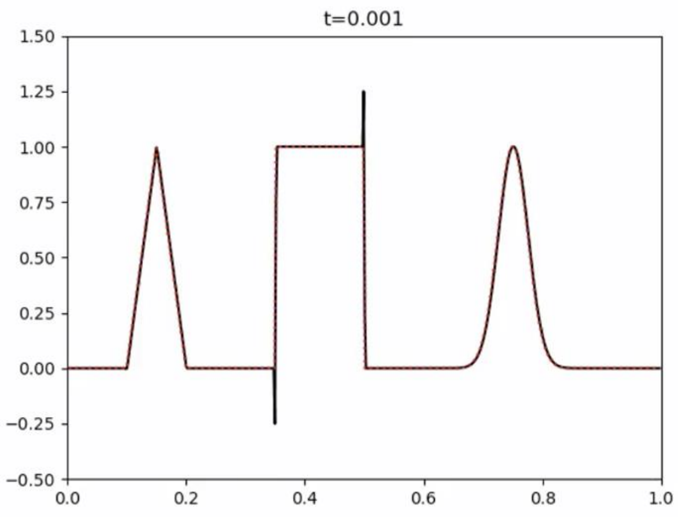
Centered Difference

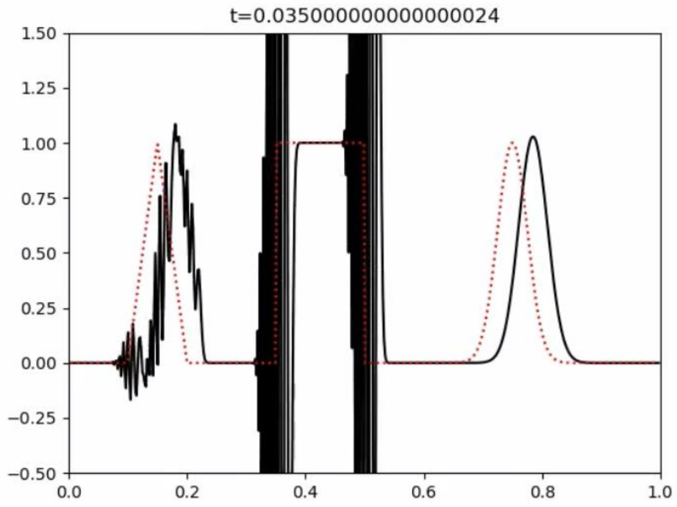
$$f_i^{(n+1)} = f_i^{(n)} - \frac{C}{2}\left(f_{i+1}^{(n)} - f_{i-1}^{(n)}\right)$$

Stencil Diagram

The field $f^{(n+1)}_i$ at grid point i and time step n + 1 depends on values at the old time step n, at center point i, plus the points downwind and upwind. This is sketched in a so-called *stencil diagram*, below.







Although in principle accurate, the scheme is ***unstable!***

Von Neumann Stability Analysis

The following analysis shows if a scheme is stable or unstable. For the centered scheme

$$f_i^{(n+1)} = f_i^{(n)} - \frac{C}{2}\left(f_{i+1}^{(n)} - f_{i-1}^{(n)}\right)$$

Consider a single Fourier mode

$$f(x,t) = A(t)e^{-ikx}$$

The scheme yields

$$A(t+\Delta t)e^{-ikx} = A(t)e^{-ikx} - \frac{C}{2}A(t)\left(e^{-ik(x+\Delta x)} - e^{-ik(x-\Delta x)}\right)$$

Multiplying by e^{ikx} and by the complex conjugate, we find the signal throughput

$$A^2(t+\Delta t) = A^2(t)\left[1 + C^2 \sin^2(k\Delta x)\right]$$

The amplitude **always grows**! That's why the scheme is unconditionally unstable.

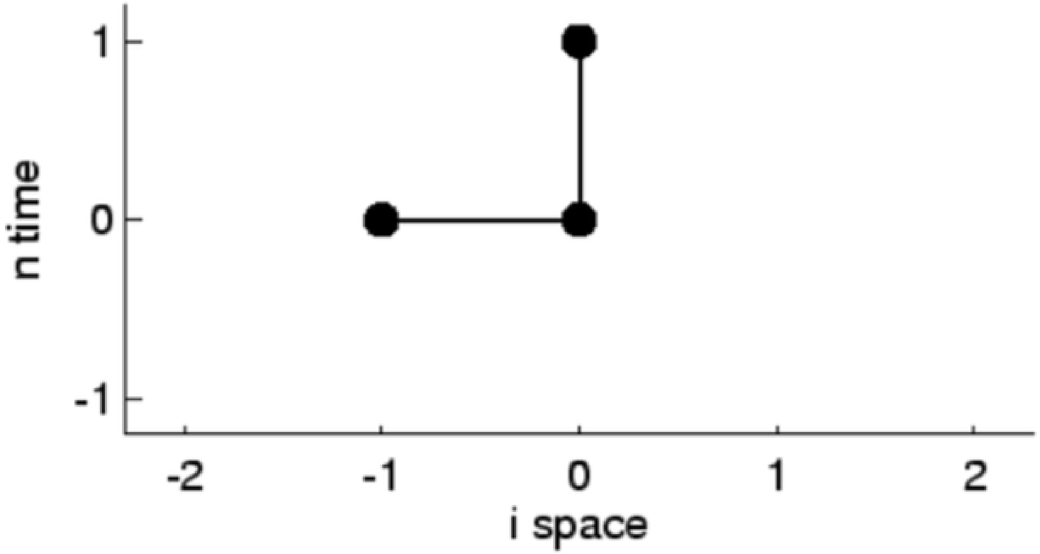
Advection Equation with Upwinding Scheme

Let's now try the advection equation

$$\frac{\partial f}{\partial t} = -u\frac{\partial f}{\partial x}$$

… with the *upwinding* formulation (i.e. using the backspace derivative)

$$\frac{\partial f}{\partial x} \approx \frac{f_i - f_{i-1}}{\Delta x}$$

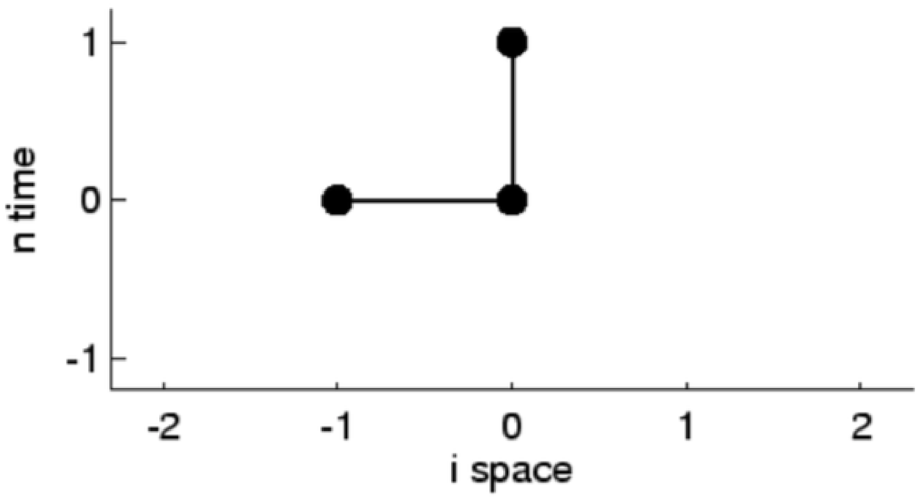


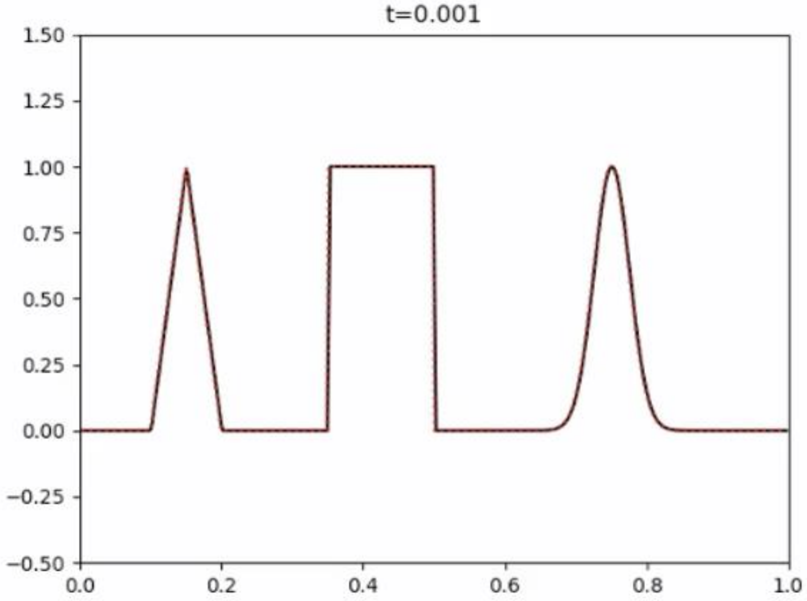
The scheme yields

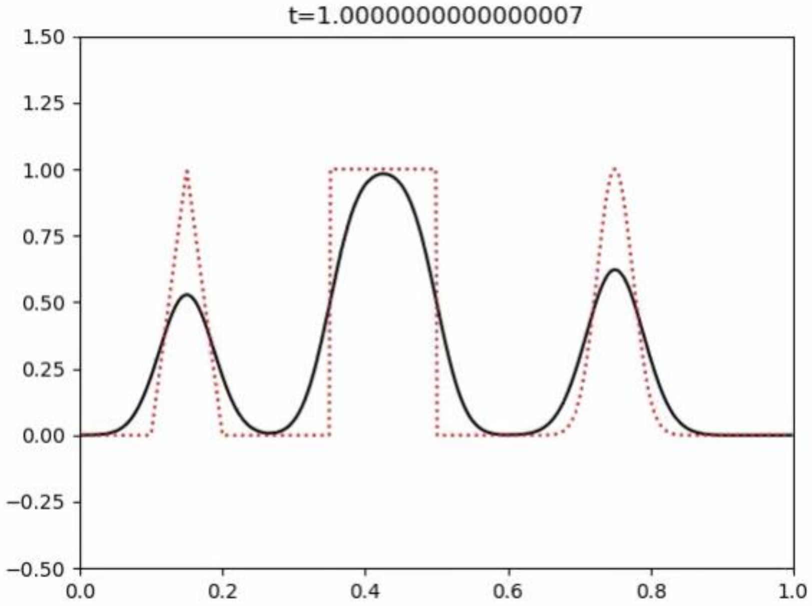
$$f_i^{(n+1)} = (1 - C)f_i^{(n)} + C f_{i-1}^{(n)}$$

Forward time back space (upwinding)

Although less accurate,
the scheme is ***stable!***







Von Neumann Stability Analysis

For the upwinding scheme

$$f_i^{(n+1)} = (1 - C) f_i^{(n)} + C f_{i-1}^{(n)}$$

Applied to a Fourier mode, the scheme yields

$$A(t + \Delta t) = A(t) \left(1 - C + C e^{ik\Delta x}\right)$$

Expanding the exponential and multiplying by the complex conjugate

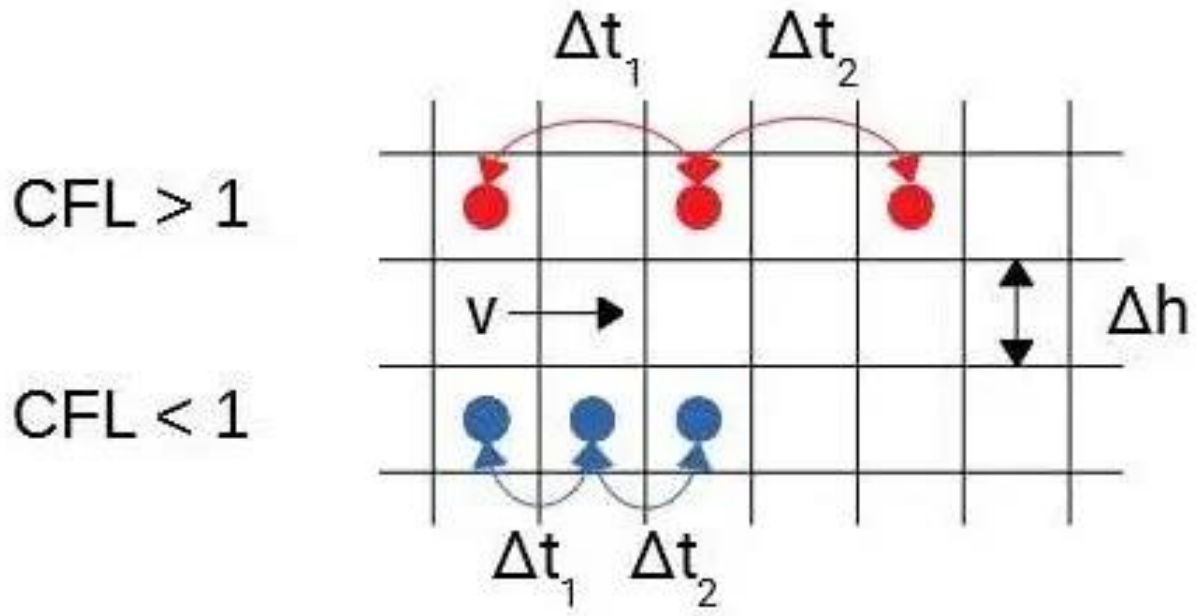
$$A^2(t + \Delta t) = A^2(t) \left[\ (1 - C)^2 + 2(1 - C) C \cos k\Delta x\ \right]$$

The amplitude is bounded if **|C| = |uΔt/Δx| <1**

This is the Courant Condition for Stability

Courant-Friedrichs-Lewy (CFL) condition

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



The Courant condition guarantees ***causality***.

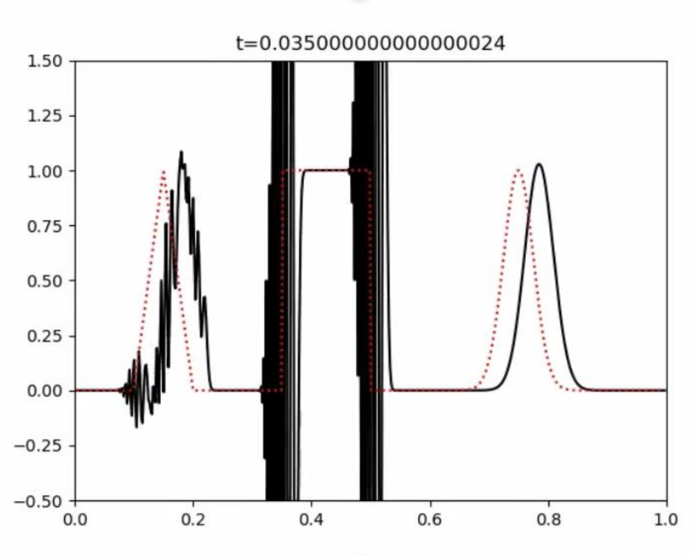
A cell has to know what happened upwind. A signal cannot jump grid cells (C > 1 in red).

$u\Delta t$ is the distance a signal travels within a timestep.

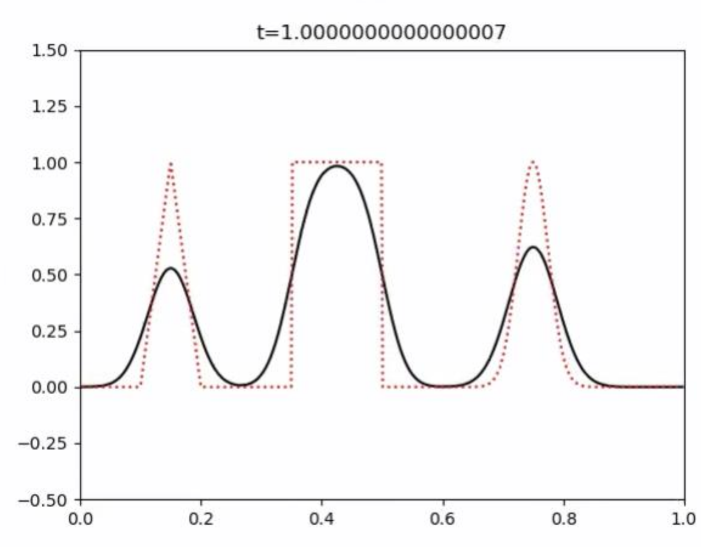
This distance cannot be bigger than a grid cell (C < 1, in blue)

Stability and Accuracy

- Accuracy and Stability do not go hand in hand.
- The centered scheme is 2nd order accurate, but unstable.
- The upwinding scheme is 1st order accurate, but stable.



Centered



Upwinding