Introduction to finite difference method

General principles, stability, precision

Victorita Dolean

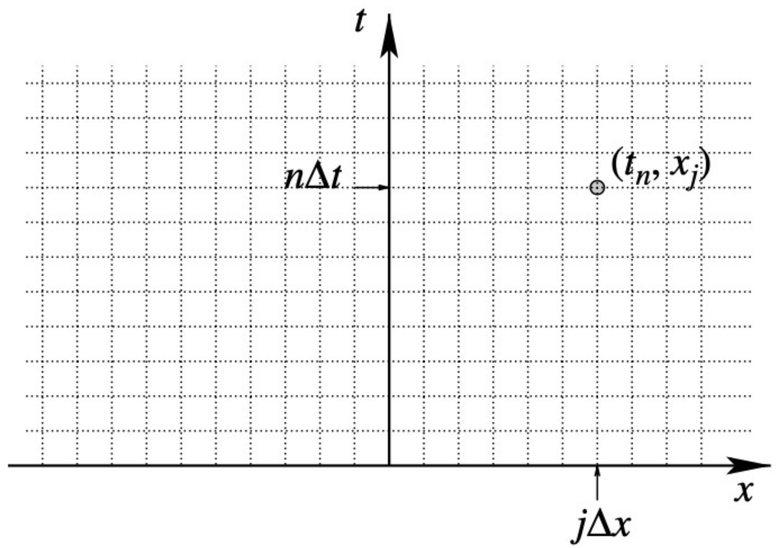
General principles

- Choose a discretisation *grid*, or a *mesh* $\left(t_n, x_j\right) = (n\Delta t, j\Delta x)$
- We approximate the solution at the grid points

$$u_j^n \sim u\left(t_n, x_j\right)$$

where $u(t, x\ )$ is the exact solution.

- *Finite difference method*: approximate the derivatives by difference operators by using only the points on the grid.



Approximation of derivatives

- In the convection diffusion equations we have 3 derivatives to approximate. (1 in time, 2 in space)

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$

- Second order derivative approximation using Taylor series

$$-\frac{\partial^2 u}{\partial x^2}(t_n, x_j) \approx \frac{-u_{j-1}^n + 2u_j^n - u_{j+1}^n}{(\Delta x)^2}$$

$$\begin{aligned} -u(t, x-\Delta x) + 2u(t,x) - u(t, x+\Delta x) = \quad & -(\Delta x)^2\frac{\partial^2 u}{\partial x^2}(t,x) \\ & -\frac{(\Delta x)^4}{12}\frac{\partial^4 u}{\partial x^4}(t,x) + \mathcal{O}\Big((\Delta x)^6\Big) \end{aligned}$$

1st order derivatives – Richardson scheme

- *Centered approximations* of first order derivatives lead to the Richardson scheme

$$V\frac{\partial u}{\partial x}(t_n, x_j) \approx V\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} \qquad \frac{\partial u}{\partial t}(t_n, x_j) \approx \frac{u^{n+1}_j - u^{n-1}_j}{2\Delta t}$$

$$\frac{u^{n+1}_j - u^{n-1}_j}{2\Delta t} + V\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} + \nu\frac{-u^n_{j-1} + 2u^n_j - u^n_{j+1}}{(\Delta x)^2} = 0.$$

- It seems a natural scheme but cannot compute solutions! Centered time approximations are not good for advection diffusion problems!

Backward Euler scheme (implicit)

- *Backward approximation* in time (we go back in time) and centered in space

$$\frac{\partial u}{\partial t}(t_n, x_j) \approx \frac{u_j^n - u_j^{n-1}}{\Delta t}$$

$$\frac{u_j^n - u_j^{n-1}}{\Delta t} + V\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \nu\frac{-u_{j-1}^n + 2u_j^n - u_{j+1}^n}{(\Delta x)^2} = 0.$$

Forward Euler scheme (explicit)

- *Forward approximation* in time (we go forward in time) and centered in space

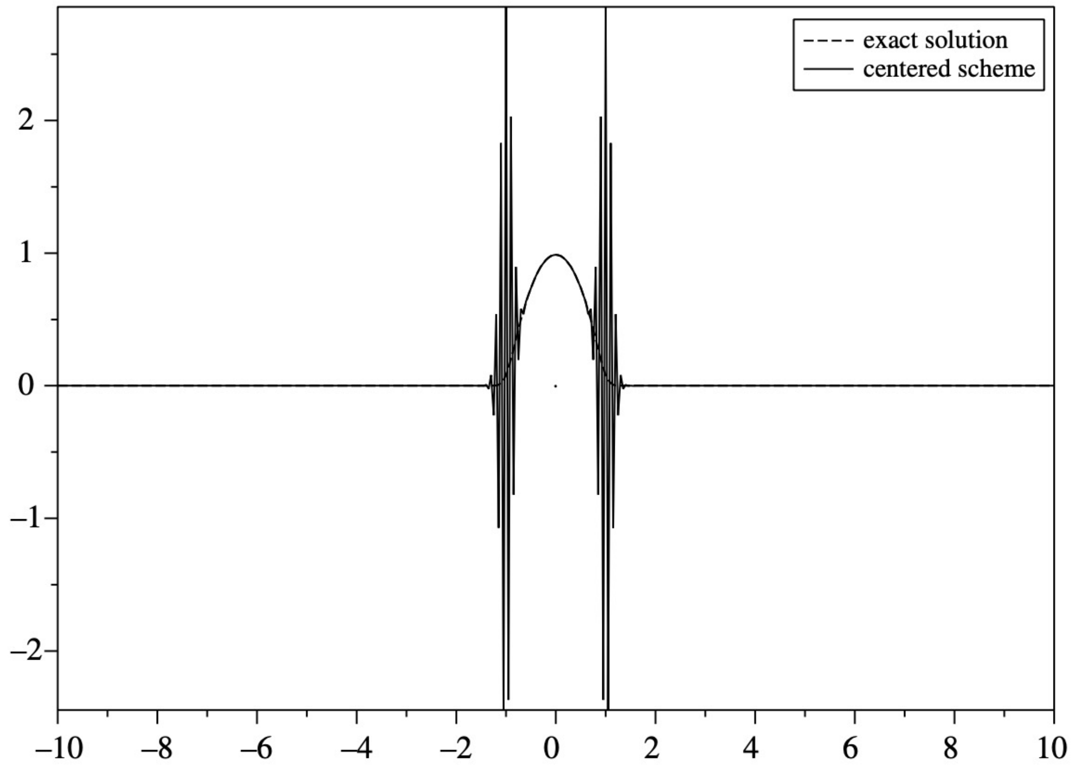
$$\frac{\partial u}{\partial t}(t_n, x_j) \approx \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + V\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \nu\frac{-u_{j-1}^n + 2u_j^n - u_{j+1}^n}{(\Delta x)^2} = 0.$$

Numerical result – centred scheme (Richardson)

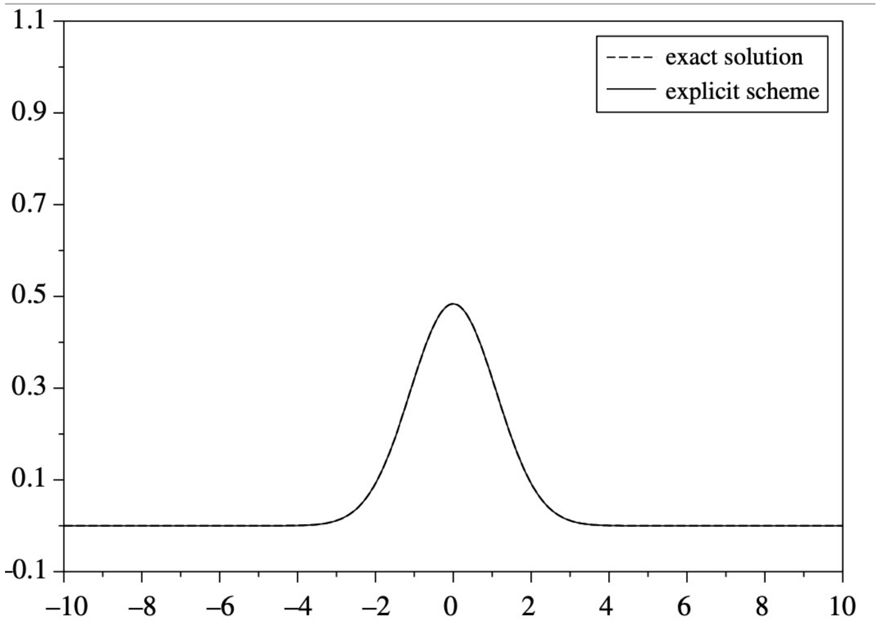
Test case

- Heat equation ($V = 0, \nu = 1$) with initial condition
  $$u_0(x) = \max(1 - x^2, 0)$$
- Computational domain
  $$\Omega = (-10,10)$$
with Dirichlet boundary conditions
- Space step
  $$\Delta x = 0.05$$
- Time step chosen such as
  $$\nu \Delta t = 0.1\, \Delta x^2$$
- The solution is not good (oscillation increasing in time) -> the scheme is *unstable*!

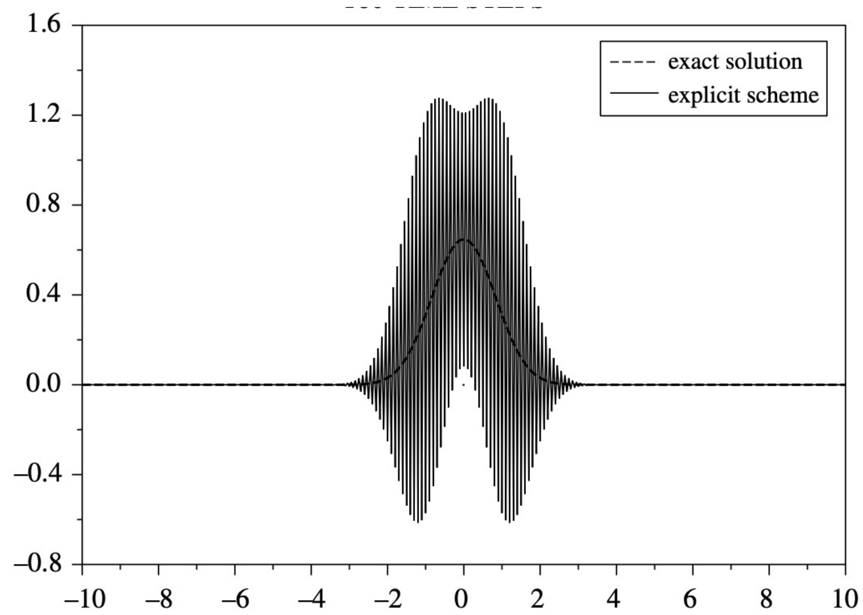


Numerical result – explicit scheme (forward Euler)

The CFL number $\frac{\nu \Delta t}{\Delta x^2}$ is a measure of stability



CFL = 0.4 (stable)



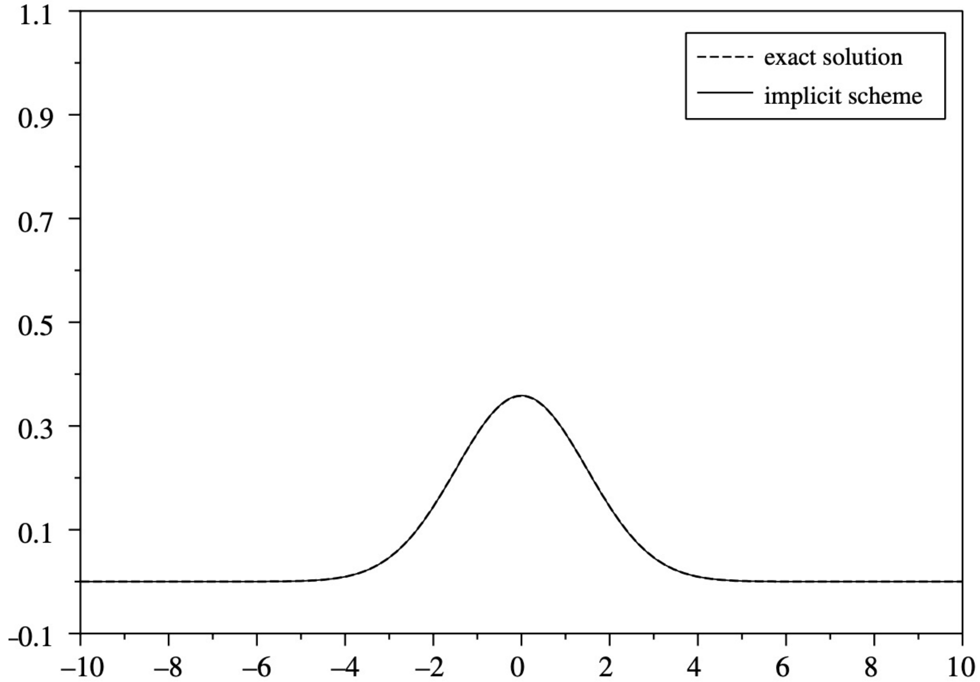
CFL = 0.51 (unstable)

Numerical result – explicit scheme (forward Euler)

The implicit scheme is always stable!

Here CFL = 2!

Unlike the centered scheme which is always unstable.



Stability and discrete maximum principle

Q: Is there a relation with the *discrete maximum principle*? Rewrite the scheme

$$u_j^{n+1} = \frac{\nu \Delta t}{(\Delta x)^2} u_{j-1}^n + \left(1 - 2\frac{\nu \Delta t}{(\Delta x)^2}\right) u_j^n + \frac{\nu \Delta t}{(\Delta x)^2} u_{j+1}^n.$$

A: Yes. By re-writing the scheme, we see that if $CFL \leq \frac{1}{2}$, u_j^{n+1} is a convex combination of $u_j^n, u_{j-1}^n, u_{j+1}^n$.

Discrete maximum principle: if the IC is bounded $m \leq u_j^0 \leq M$ then $m \leq u_j^n \leq M, \forall n \geq 0, j \in Z$

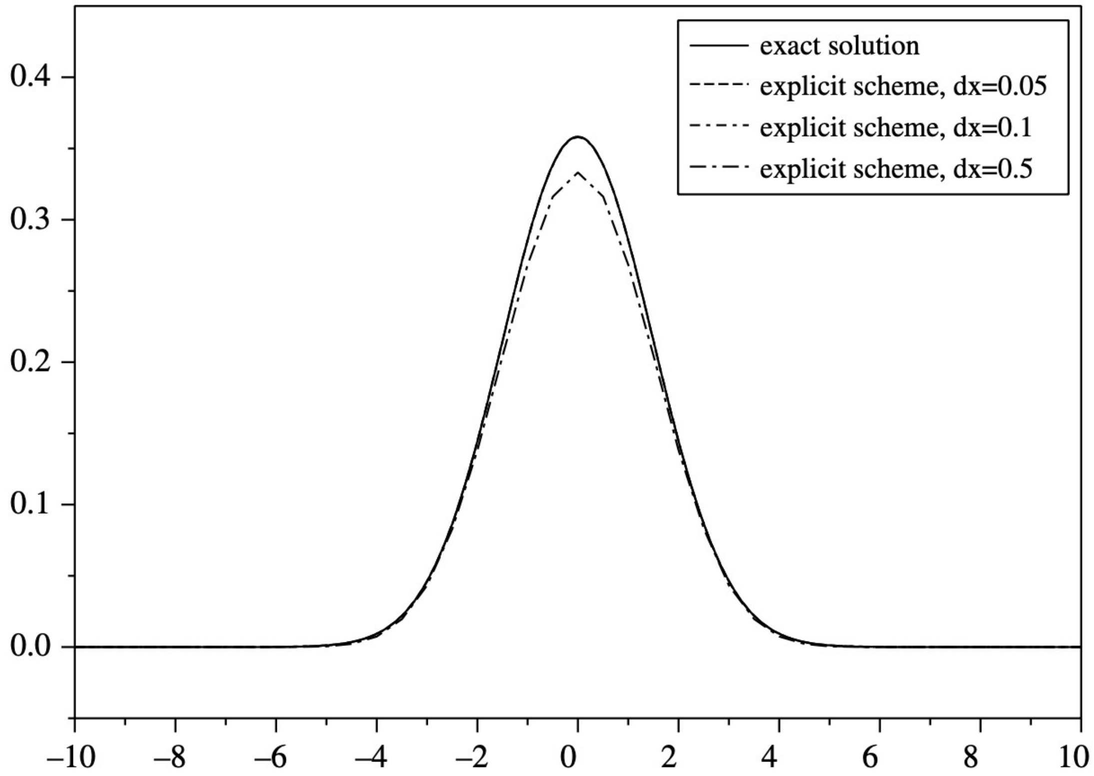
- If $CFL > \frac{1}{2}$, for $u_j^0 = (-1)^j$, the general solution below is unbounded.

$$u_j^n = (-1)^j \left(1 - 4\frac{\nu \Delta t}{(\Delta x)^2}\right)^n$$

Numerical validation - precision

- If the CFL condition is verified, we always get a solution

- We see that the solution is more accurate (i.e. closer to the exact solution) if Δx is smaller!

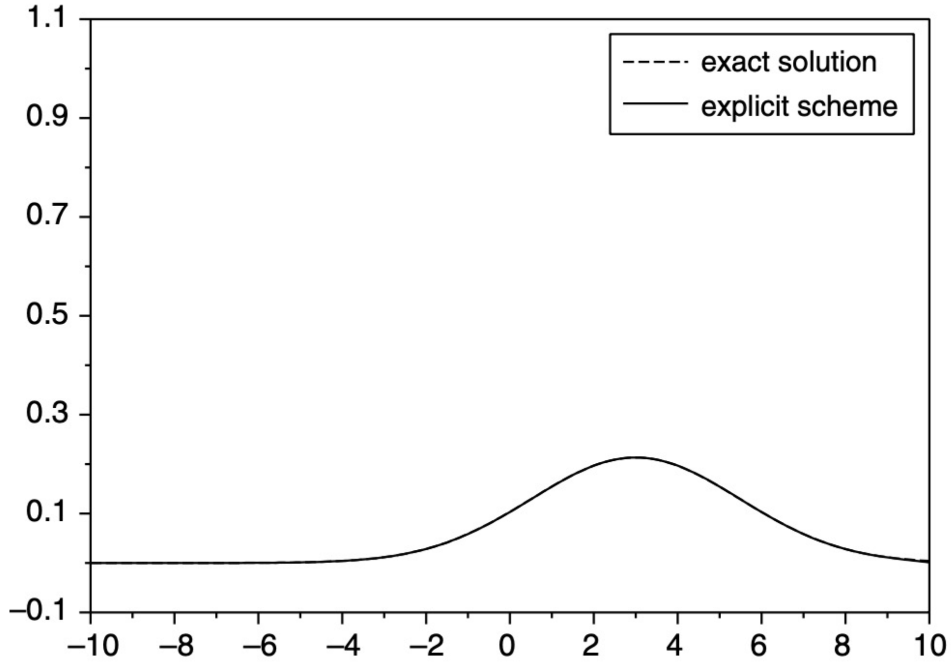


Advection-diffusion equation – test case 1

- Application of explicit scheme with CFL = 0.4

- Advection velocity : V = 1
- Test case 1: $\nu = 1 \Rightarrow Pe = 1$

- The explicit scheme works!

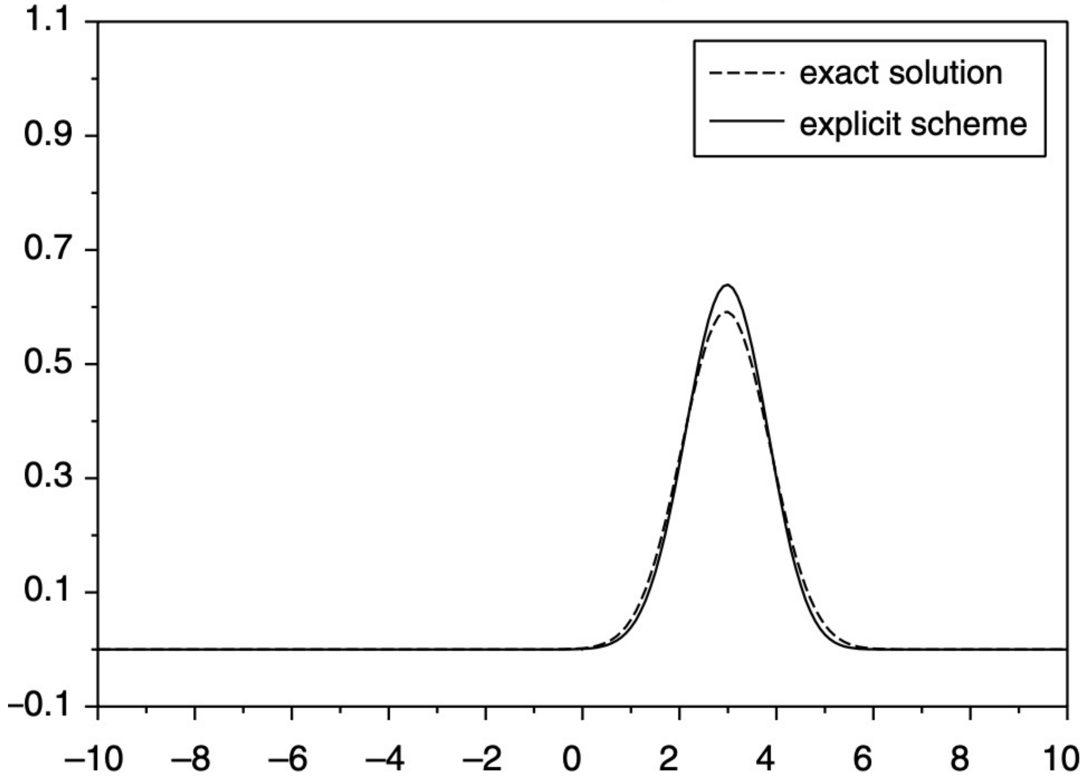


Advection-diffusion equation – test case 2

- Application of explicit scheme with
  CFL = 0.4

- Advection velocity : V = 1
- Test case 2: $\nu = 0.1 \ \Rightarrow Pe \ = \ 10$

- The explicit scheme still works but less well!

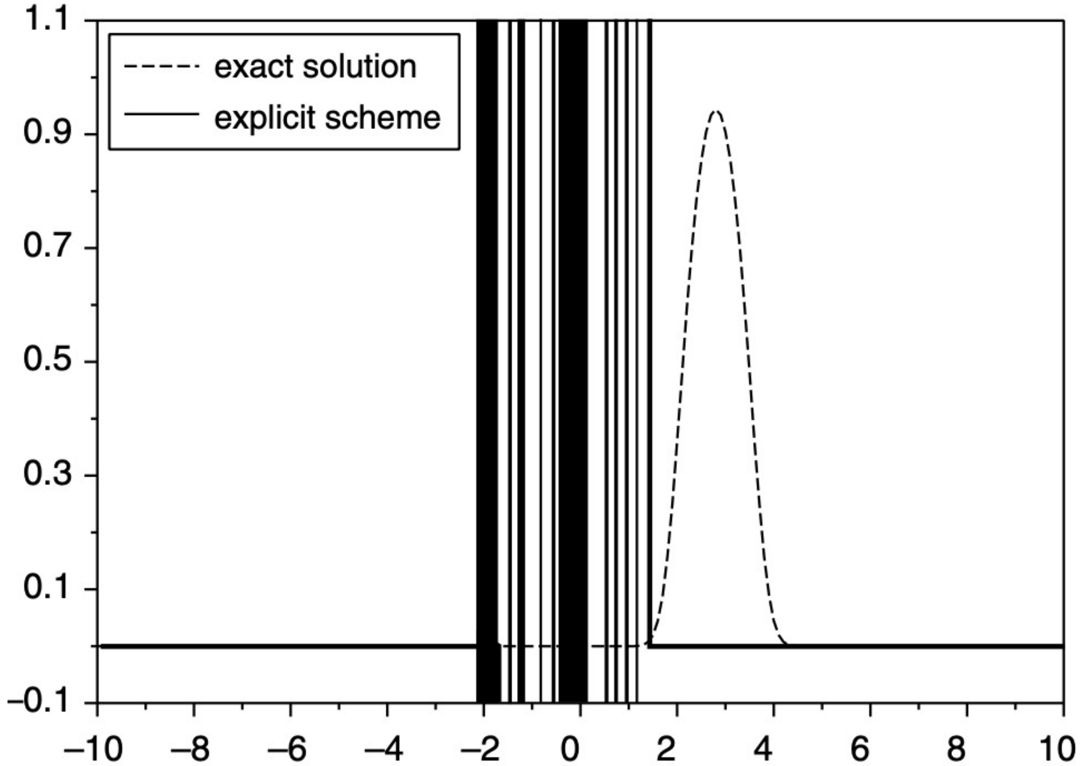


Advection-diffusion equation – test case 3

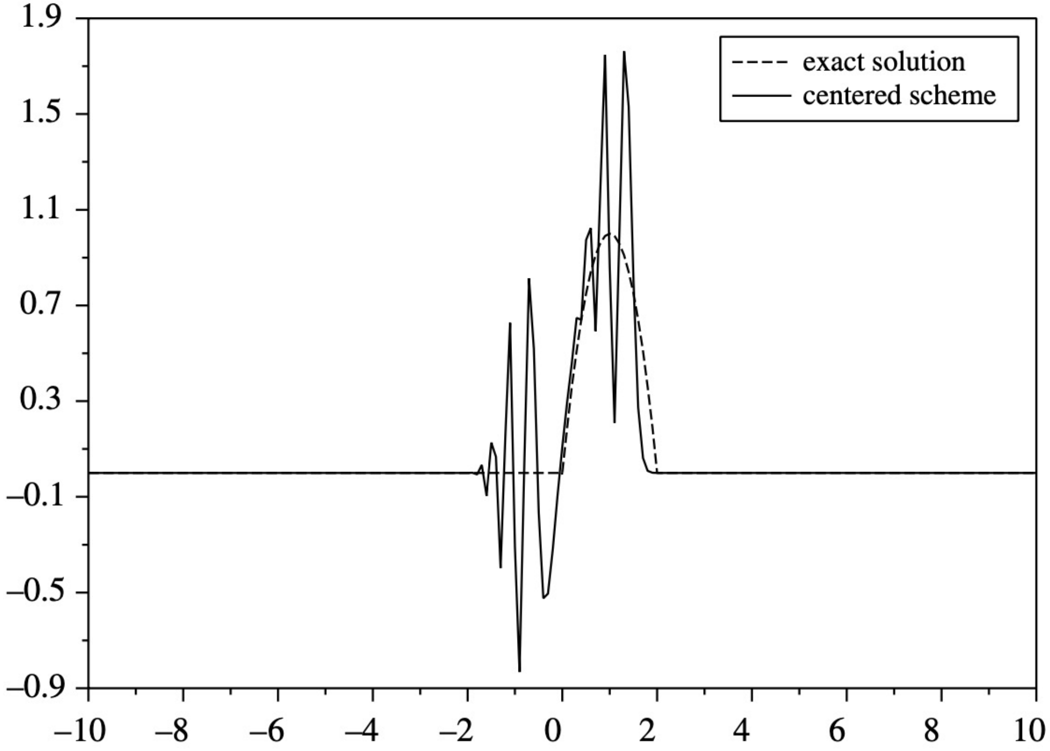
- Application of explicit scheme with CFL = 0.4

- Advection velocity : V = 1
- Test case 3: $\nu = 0.01 \Rightarrow Pe = 100$

- The explicit doesn't work anymore!



Explicit centred scheme – advection case



Pure advection: $\nu = 0 \Rightarrow Pe = \infty$

$$u_j^{n+1} = \frac{V\Delta t}{2\Delta x} u_{j-1}^n + u_j^n - \frac{V\Delta t}{2\Delta x} u_{j+1}^n.$$

We see that u_j^{n+1} cannot be a convex combination of $u_j^n, u_{j-1}^n, u_{j+1}^n$!

Downwiding vs. upwinding (V>0)

Centered schemes don't work for pure advection problems!

Downwinding: find the information (to the right) following the current!

$$V\frac{\partial u}{\partial x}(t_n, x_j) \approx V\frac{u_{j+1}^n - u_j^n}{\Delta x}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + V\frac{u_{j+1}^n - u_j^n}{\Delta x} = 0$$

BAD!

Upwinding: find the information (to the left) against the current!

$$V\frac{\partial u}{\partial x}(t_n, x_j) \approx V\frac{u_j^n - u_{j-1}^n}{\Delta x}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + V\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0$$

GOOD!

Upwind scheme - stability

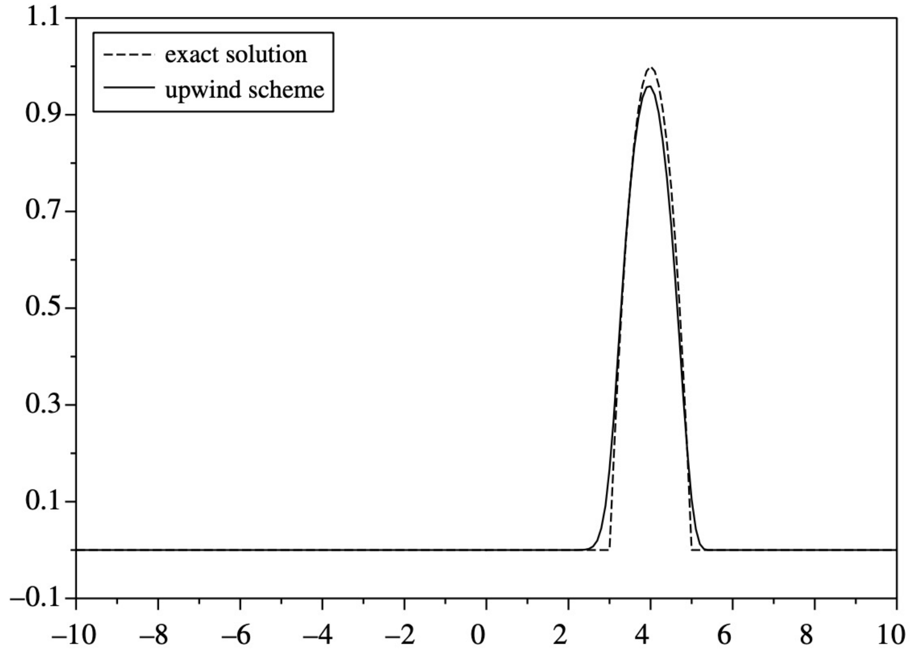
The upwind scheme

$$u_j^{n+1} = \frac{V\Delta t}{\Delta x} u_{j-1}^n + \left(1 - \frac{V\Delta t}{\Delta x}\right) u_j^n,$$

Is a convex combination if

$$\text{CFL} = \frac{V\Delta t}{\Delta x} \leq 1$$

Test case with CFL = 0.9



Classification of second order PDEs

General form of a second order partial differential equation (PDE)

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu = g.$$

The second order PDE is *elliptic* if $b^2 - 4ac < 0$, *hyperbolic* if $b^2 - 4ac > 0$ and *parabolic* if $b^2 - 4ac < 0$.

Origin of the term: classification of the conic section, the underlying quadratic equation defines and ellipse, hyperbola or parabola.

$$ax^2 + bxy + cy^2 + dx + ey + f = 0$$

Elliptic problem – Poisson equation

- The simplest elliptic problem

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

- If $f = 0$, we call it Laplace problem.
- Different applications: it can be seen as a steady heat problem, mathematical model for electrostatic potential,…
- Maybe the most popular and studied PDE model.

Hyperbolic problem – wave equation

- Second order equation: we need 2 initial conditions!

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \Delta u = f & \text{in } \Omega \times \mathbb{R}_*^+ \\ u = 0 & \text{on } \partial\Omega \times \mathbb{R}_*^+ \\ u(t=0) = u_0 & \text{in } \Omega \\ \dfrac{\partial u}{\partial t}(t=0) = u_1 & \text{in } \Omega \end{cases}$$

An elliptic indefinite problem: Helmholtz equation

Hermann von Helmholtz (1821-1894)

$$-\Delta u - k^2 u = f$$

a.k.a. the *reduced wave equation* or time-harmonic wave equation.

Scalar wave equation ($c(x)$ local speed of propagation

$$\partial_{tt} v - c^2(x)\Delta v = F(x,t)$$

If $F(x,t) = f(x)e^{-i\omega t}$ (mono-chromatic) we can assume

$$v(x,t) = u(x)e^{-i\omega t}$$

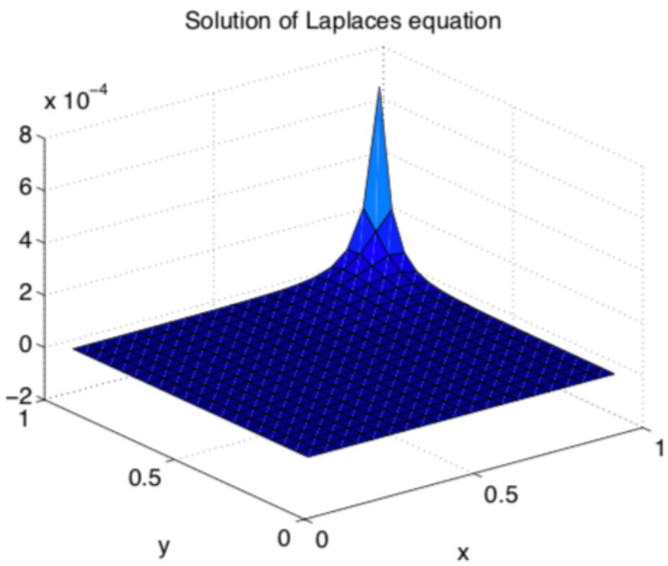
which leads to

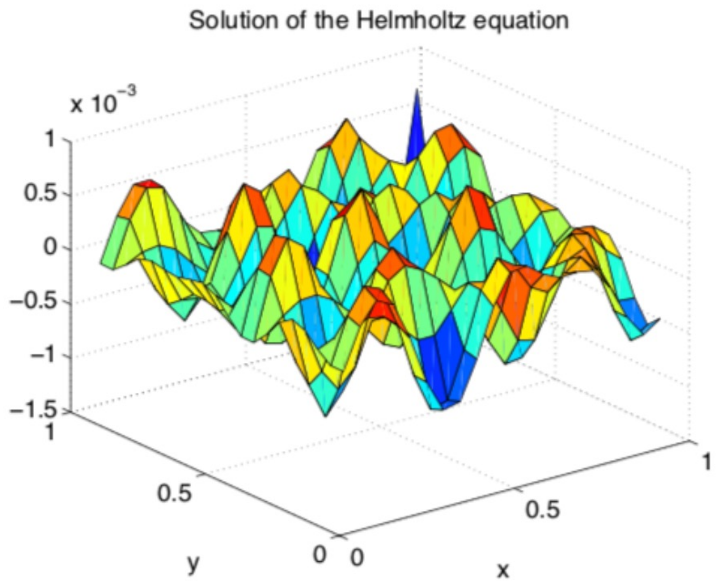
$$-\Delta u - n(x)^2\omega^2 u = f,$$

where $n(x) = \frac{1}{c(x)}$ is the **index of refraction**, $k^2 = n^2\omega^2$ is called **wave number**.

Laplace vs. Helmholtz equation

- Elliptic problems can be very different in nature (positive definite or indefinite)





Parabolic problem – Black-Scholes equation

- Very similar to the heat equation: Black-Scholes models the option pricing in finance

$$\begin{cases} \dfrac{\partial u}{\partial t} - ru + 1/2rx\dfrac{\partial u}{\partial x} + 1/2\sigma^2 x^2 \dfrac{\partial^2 u}{\partial x^2} = 0 & \text{for } (x,t) \in \mathbb{R} \times (0,T) \\ u(t=T,x) = \max(x-k,0) & \text{for } x \in \mathbb{R} \end{cases}$$

- Parabolic equation with a final condition (instead of initial condition)

Other examples: advection, Euler, Navier-Stokes

- Linear elasticity (Lamé system)

$$\begin{cases} -\mu\Delta u - (\mu+\lambda)\nabla(\mathrm{div} u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

- Schrodinger equation

$$\begin{cases} i\dfrac{\partial u}{\partial t} + \Delta u - Vu = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}_*^+ \\ u(t=0) = u_0 & \text{in } \mathbb{R}^N \end{cases}$$

- (incompressible) Stokes equations

$$\begin{cases} \nabla p - \mu\Delta u = f & \text{in } \Omega \\ \mathrm{div} u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$