Crank-Nicholson Method

15 PDEs

Diffusion equation: stability

$$\frac{\partial u}{\partial t} = D\nabla^2 u(x,t)$$

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho}\nabla^2 T(x,t)$$

- leap frog **(forward difference)** : only stable for

$$\eta = \frac{D\Delta t}{\Delta x^2} < \frac{1}{2}$$

$$\eta = \frac{K\Delta t}{C\rho\Delta x^2} < \frac{1}{2}$$

Diffusion interpretation of the forward difference stability criterion

- random walk in 1D

$$2D\Delta t = \Delta x^2$$

- compare to **stability condition:**

$$\eta = \frac{D\Delta t}{\Delta x^2} < \frac{1}{2}$$

  - grid spacing > than *diffusion distance (squared)* over one integration step

$$\Delta x^2 > 2D\Delta t$$

  - max. allowed dt = *diffusion time* across one grid cell

$$\Delta t < \frac{\Delta x^2}{2D}$$

Computational cost

- features of interest
  - length scale
  - time scale

$$\lambda \gg \Delta x$$

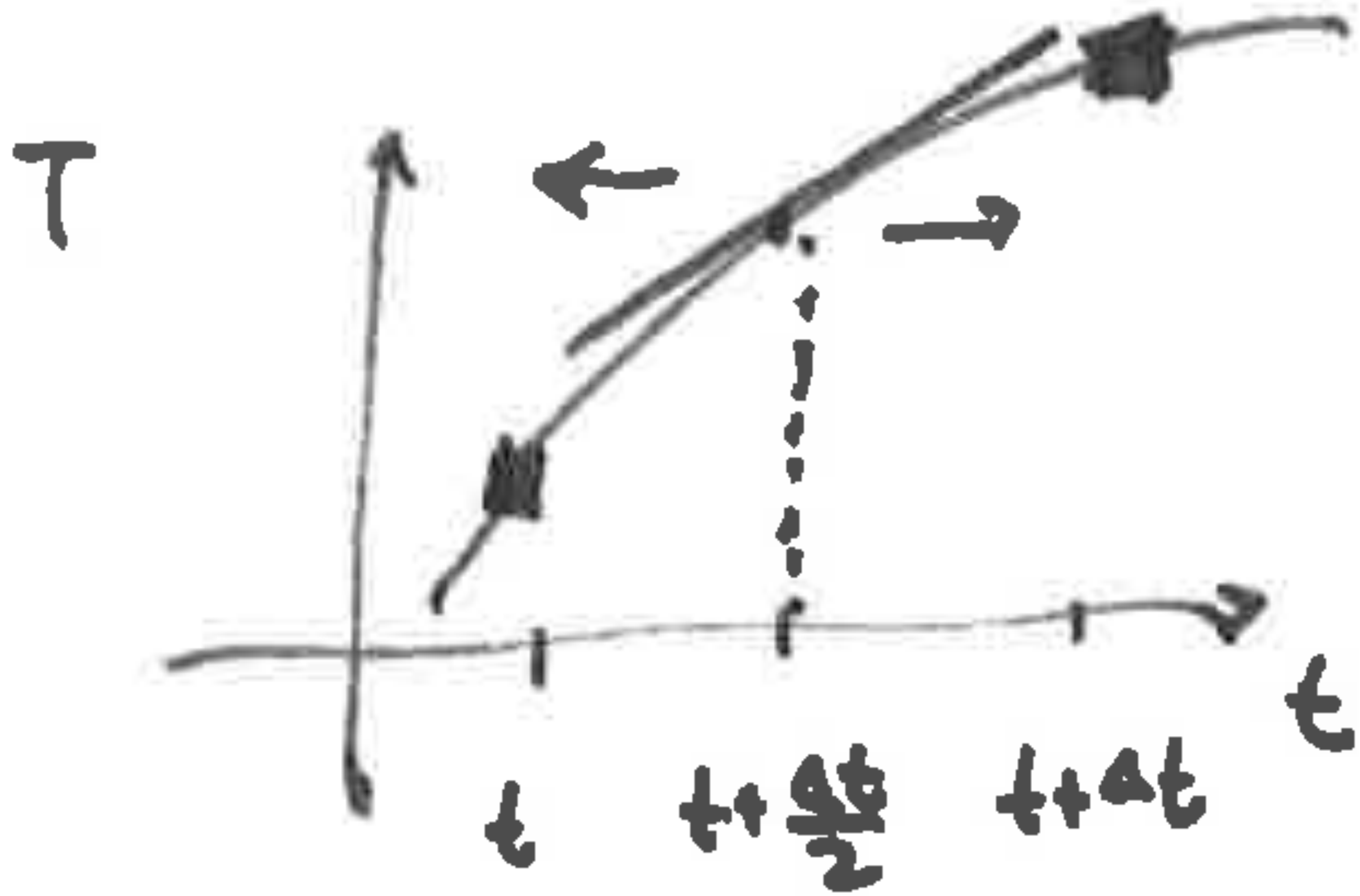
$$\tau \approx \frac{\lambda^2}{D}$$

- number of steps needed:

$$\frac{\tau}{\Delta t} \approx \frac{\lambda^2}{D} \frac{2D}{\Delta x^2} \approx \frac{\lambda^2}{\Delta x^2}$$

Crank-Nicholson algorithm

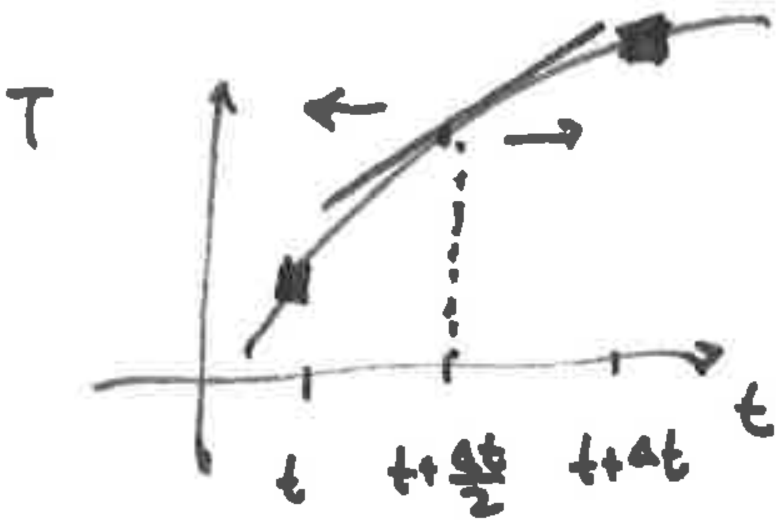
- Goals:
  - better stability (larger time steps)
  - higher accuracy (than forward difference 1st order)
- Key ideas:
  - use “split time steps” as intermediate
  - implicit scheme (coupled equation, matrix problem)



$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

$$\frac{\partial T(x, t+\frac{\Delta t}{2})}{\partial t} = \dots$$

$$\frac{\partial^2 T(x, t+\frac{\Delta t}{2})}{\partial x^2} = \dots$$



$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

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

Taylor expansion around split time step

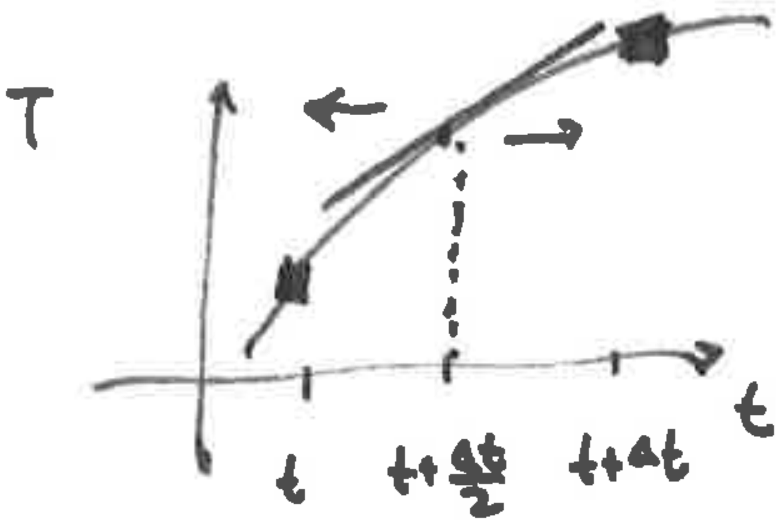
$$(1) \quad T(x,t) = T\left(x, t + \frac{\Delta t}{2}\right) - \frac{\Delta t}{2}\frac{\partial T(x, t+\frac{\Delta t}{2})}{\partial t} + O(\Delta t^2)$$

$$(2) \quad T(x,t+\Delta t) = T\left(x, t + \frac{\Delta t}{2}\right) + \frac{\Delta t}{2}\frac{\partial T(x, t+\frac{\Delta t}{2})}{\partial t} + O(\Delta t^2)$$

Eq 2 – Eq 1

$$\Delta t \frac{\partial T(x, t+\frac{\Delta t}{2})}{\partial t} = T(x, t+\Delta t) - T(x,t) + O(\Delta t^3)$$

$$\boxed{\frac{\partial T(x, t+\frac{\Delta t}{2})}{\partial t} = \frac{T(x, t+\Delta t) - T(x,t)}{\Delta t} + O(\Delta t^2)}$$



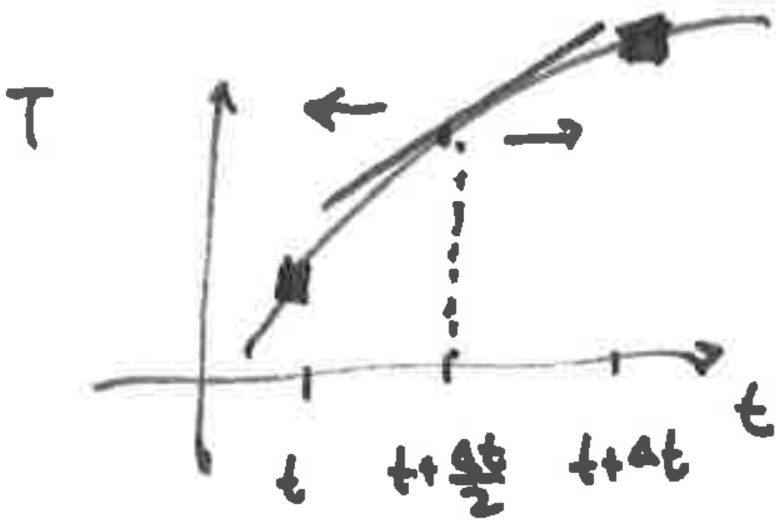
$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

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

$$\boxed{\frac{\partial T(x,t+\frac{\Delta t}{2})}{\partial t} = \frac{T(x,t+\Delta t) - T(x,t)}{\Delta t} + \mathcal{O}(\Delta t^2)}$$

Previously:

$$\frac{\partial T(x,t)}{\partial t} = \frac{T(x,t+\Delta t) - T(x,t)}{\Delta t} + \mathcal{O}(\Delta t)$$



$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

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

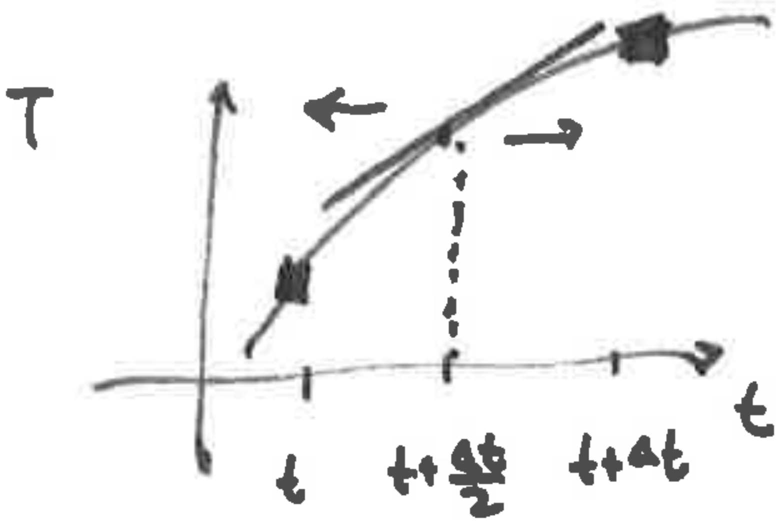
Finite difference derivative for split time step

(3) $$\frac{\partial^2 T(x, t+\frac{\Delta t}{2})}{\partial x^2} = \frac{1}{\Delta x^2}\left[T(x+\Delta x, t+\frac{\Delta t}{2}) + T(x-\Delta x, t+\frac{\Delta t}{2}) - 2\,T(x, t+\frac{\Delta t}{2}) + O(\Delta x^3)\right]$$

From the first order derivatives: Eq 1 + Eq 2

$$2\,T(x, t+\frac{\Delta t}{2}) = T(x,t) + T(x, t+\Delta t) + O(\Delta t^2)$$

(4) $$\boxed{T(x, t+\frac{\Delta t}{2}) = \frac{1}{2}\Big(T(x,t) + T(x, t+\Delta t)\Big) + O(\Delta t^2)}$$

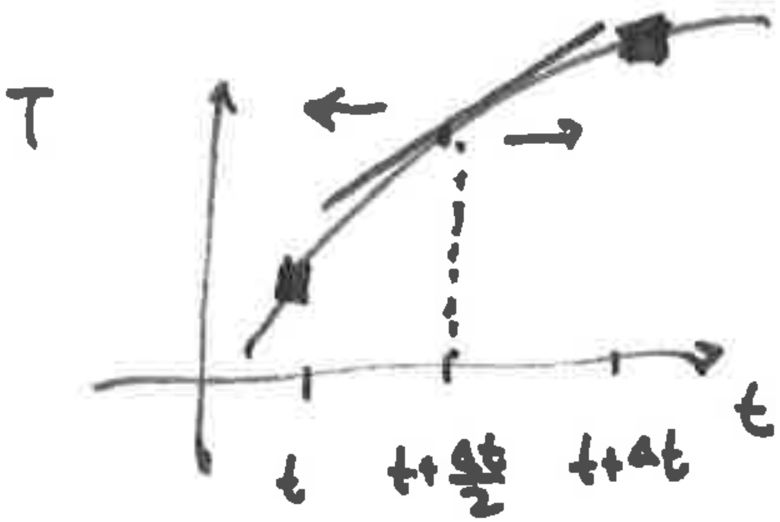


$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

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

Insert (4) into (3)

$$\boxed{\begin{aligned} \Delta x^2 \frac{\partial^2 T(x, t + \frac{\Delta t}{2})}{\partial x^2} = \frac{1}{2}\Big[& T(x+\Delta x, t) + T(x+\Delta x, t+\Delta t) \\ & + T(x-\Delta x, t) + T(x-\Delta x, t+\Delta t) \\ & - 2\big(T(x,t) + T(x, t+\Delta t)\big)\Big] \end{aligned}}$$



$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T(x,t)}{\partial x^2}$$

$$t = j\Delta t \qquad T(x,t) \equiv T_{ij}$$

$$x = i\Delta x \qquad T(x+\Delta x, t+\Delta t) \equiv T_{i+1,j+1}$$

$$\boxed{\begin{aligned} \frac{1}{\Delta t}\left(T_{i,j+1} - T_{i,j}\right) = \frac{D}{2\Delta x^2}\Big[& T_{i+1,j} + T_{i+1,j+1} \\ & + T_{i-1,j} + T_{i-1,j+1} \\ & - 2\left(T_{i,j} + T_{i,j+1}\right)\Big] \end{aligned}}$$

discretized diffusion equation (split time step)

$$\mathcal{O}(\Delta t^2)$$

$$\frac{1}{\Delta t}\left(T_{i,j+1} - T_{i,j}\right) = \frac{D}{2\Delta x^2}\Big[T_{i+1,j} + T_{i+1,j+1} + T_{i-1,j} + T_{i-1,j+1} - 2\left(T_{ij} + T_{i,j+1}\right)\Big]$$

$$\eta := \frac{D\Delta t}{\Delta x^2}$$

Collect future terms on LHS

$$\frac{2}{\eta}\left(T_{i,j+1} - T_{ij}\right) = \left(T_{i-1,j} - 2T_{ij} + T_{i+1,j}\right) + \left(T_{i-1,j+1} - 2T_{i,j+1} + T_{i+1,j+1}\right)$$

$$\boxed{-T_{i-1,j+1} + \left(\frac{2}{\eta}+2\right)T_{i,j+1} - T_{i+1,j+1} = T_{i-1,j} + \left(\frac{2}{\eta}-2\right)T_{ij} + T_{i-1,j}}$$

implicit scheme

LHS = **future**

$j+1$

RHS = **present**

j

$$-T_{i-1,j+1} + \left(\frac{2}{\eta}+2\right)T_{i,j+1} - T_{i+1,j+1} = T_{i-1,j} + \left(\frac{2}{\eta}-2\right)T_{ij} + T_{i-1,j}$$

$$-T_{i-1,j+1} + \alpha T_{i,j+1} - T_{i+1,j+1} = T_{i-1,j} + \beta T_{ij} + T_{i-1,j}$$

$$\alpha := \frac{2}{\eta} + 2$$

$$\beta := \frac{2}{\eta} - 2$$

Rewrite as matrix equation $\mathrm{A}\mathbf{x} = \mathbf{b}$

$$\begin{pmatrix} \alpha & -1 & & & 0 \\ -1 & \alpha & -1 & & \\ & -1 & \alpha & -1 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & -1 & \alpha \end{pmatrix} \begin{pmatrix} T_{1,j+1} \\ \vdots \\ T_{i-1,j+1} \\ T_{i,j+1} \\ T_{i+1,j+1} \\ \vdots \\ T_{N-2,j+1} \end{pmatrix} = \begin{pmatrix} (*) \\ \vdots \\ T_{i-1,j} + \beta T_{ij} + T_{i+1,j} \\ \vdots \\ (**) \end{pmatrix}$$

N-2 unknowns

Boundaries?

$$T_{0,j} = \text{const}$$

$$T_{N-1,j} = \text{const} \equiv T_{-1,j}$$

$$\begin{pmatrix} \alpha & -1 & & & 0 \\ -1 & \alpha & -1 & & \\ & -1 & \alpha & -1 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & -1 & \alpha \end{pmatrix} \begin{pmatrix} T_{1,j+1} \\ \vdots \\ T_{i-1,j+1} \\ T_{i,j+1} \\ T_{i+1,j+1} \\ \vdots \\ T_{N-2,j+1} \end{pmatrix} = \begin{pmatrix} \boxed{(*)} \\ \vdots \\ T_{i-1,j} + \beta T_{ij} + T_{i+1,j} \\ \vdots \\ \boxed{(**)} \end{pmatrix}$$

Special equations for

$$T_{1,j+1}$$

$$\boxed{-T_{0,j+1}} + \alpha T_{1,j+1} - T_{2,j+1} = T_{0j} + \beta T_{1j} + T_{2j}$$

$$\alpha T_{1,j+1} - T_{2,j+1} = T_{0j} + \beta T_{1j} + T_{2j} + \boxed{T_{0,j+1}} \qquad (*)$$

$$T_{-2,j+1}$$

$$-T_{-3,j+1} + \alpha T_{-2,j+1} - \boxed{T_{-1,j+1}} = T_{-3j} + \beta T_{-2j} + T_{-1j}$$

$$-T_{-3,j+1} + \alpha T_{-2,j+1} = T_{-3j} + \beta T_{-2j} + T_{-1j} + \boxed{T_{-1,j+1}} \qquad (**)$$

Crank-Nicholson

1. Set-up matrix A (N-2,N-2)
2. For each time step
    1. Set-up RHS vector
    2. solve matrix equation

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

$$\mathsf{A} = \mathsf{M}(\eta) = \begin{pmatrix} \alpha & -1 & & & \\ -1 & \alpha & -1 & & \\ & -1 & \alpha & -1 & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & \alpha \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} T_1 \\ \vdots \\ T_i \\ \vdots \\ T_{-2} \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} T_{0,j+1} + T_{0,j} + \beta T_{1,j} + T_{2,j} \\ \vdots \\ T_{i-1,j} + \beta T_{i,j} + T_{i+1,j} \\ \vdots \\ T_{-3,j} + \beta T_{-2,j} + T_{-1,j} + T_{-1,j+1} \end{pmatrix}$$

Crank-Nicholson: Performance Improvements

- pre-compute inverse of **constant** matrix **A**=**M**(η) and solve matrix problem as $\mathbf{x} = \mathrm{A}^{-1}\mathbf{b}$
- take advantage of the *tridiagonal* structure
    - *Thomas* algorithm
    - routines for banded matrices (`scipy.linalg.solve_banded()`)

Crank-Nicholson: Stability

- von Neumann stability analysis yields

$$|\xi(k)| = \left| \frac{1 - 2\eta \sin^2 \frac{k\Delta x}{2}}{1 + 2\eta \sin^2 \frac{k\Delta x}{2}} \right|$$

- because $\sin^2 \alpha \leq 1$, we *always* have $|\xi(k)| \leq 1$
- **always stable** (*any* combination of Δx and Δt)