

# Crank-Nicholson Method

16 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  $\Delta t$  = *diffusion time across one grid cell*

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

# Computational cost

- features of interest

$$\lambda \gg \Delta x$$

- length scale

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

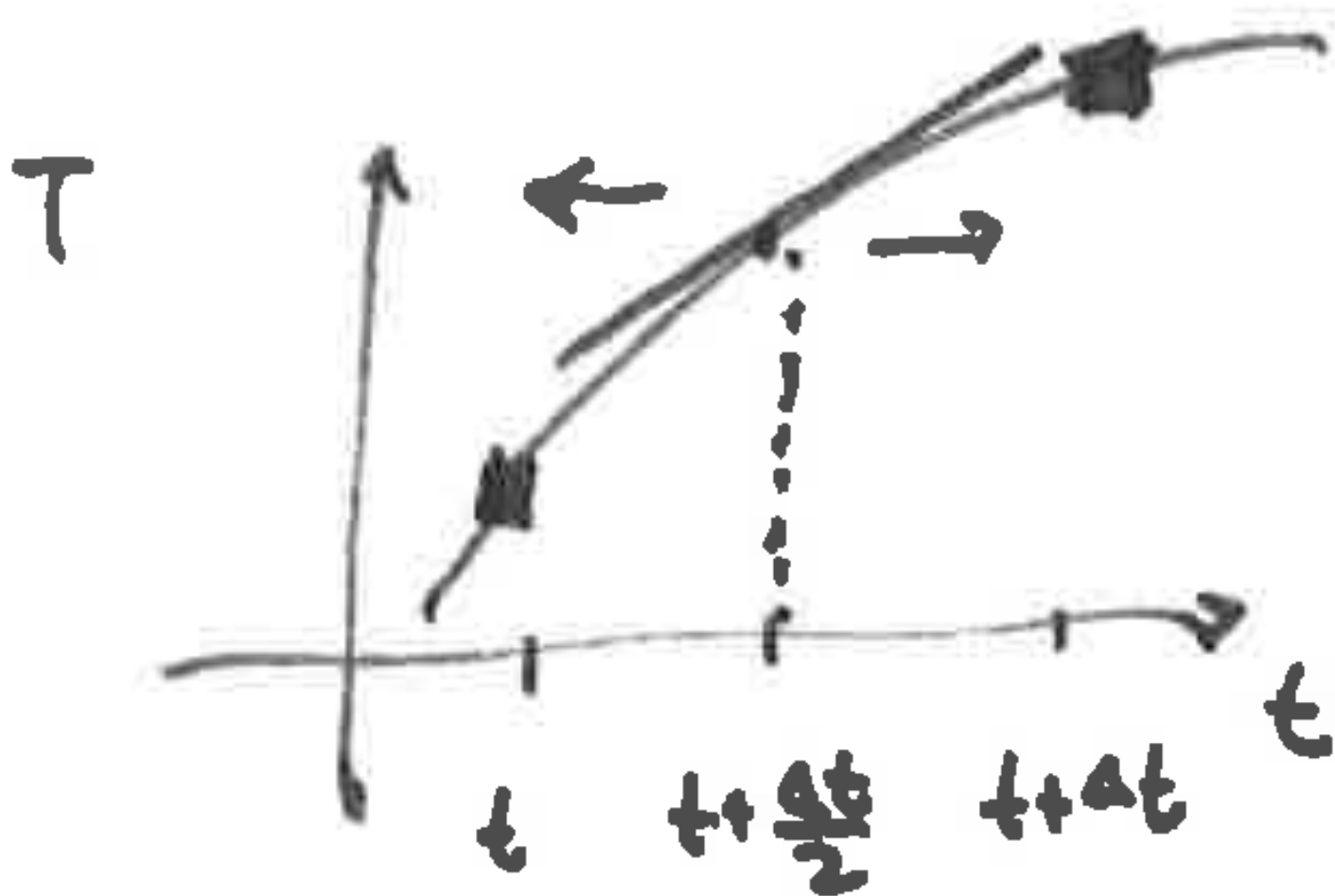
- time scale

- 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

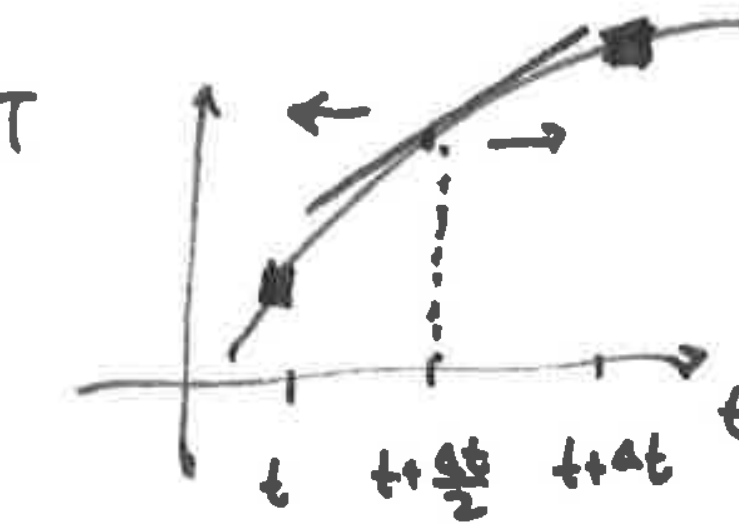
- Goals:
  - better stability (larger time steps)
  - higher accuracy (than forward difference 1st order)
- Key ideas:
  - use “split time steps” as intermediate
  - implicit scheme (coupled equation, matrix problem)



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

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

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

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

Taylor expansion around **split time step**

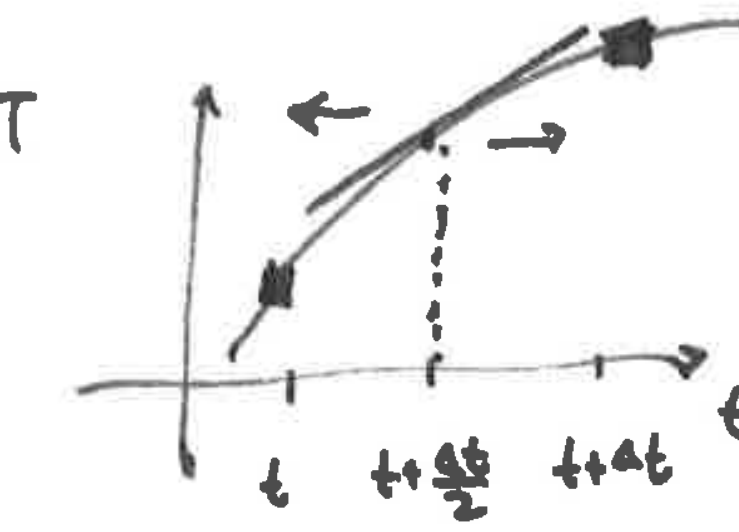
$$(1) \quad T(x, t) = T(x, t + \frac{\Delta t}{2}) - \frac{\Delta t}{2} \frac{\partial T(x, t + \frac{\Delta t}{2})}{\partial t} + O(\Delta t^2)$$

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

Eq 2 – Eq 1

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

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



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

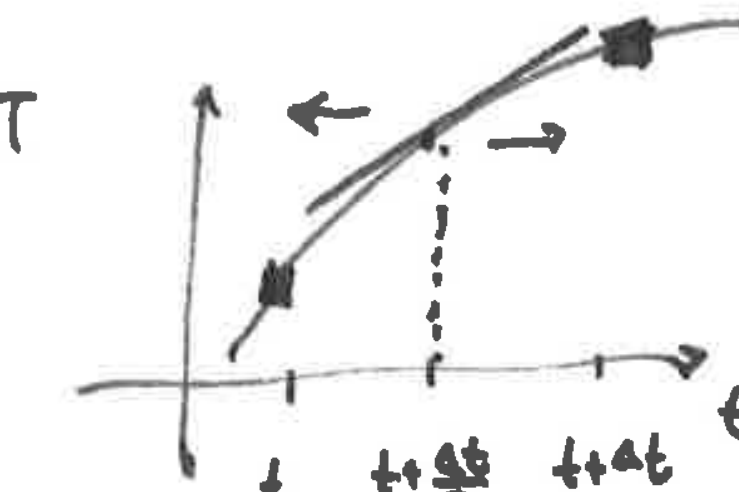
$$\frac{\partial T(x, t + \frac{\Delta t}{2})}{\partial t} = \dots$$

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

Previously:

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





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

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

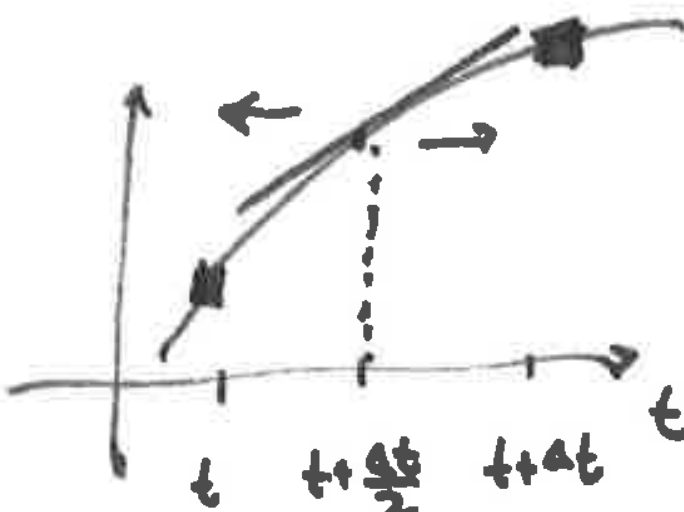
Finite difference derivative for **split time step**

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

From the first order derivatives: Eq 1 + Eq 2

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

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

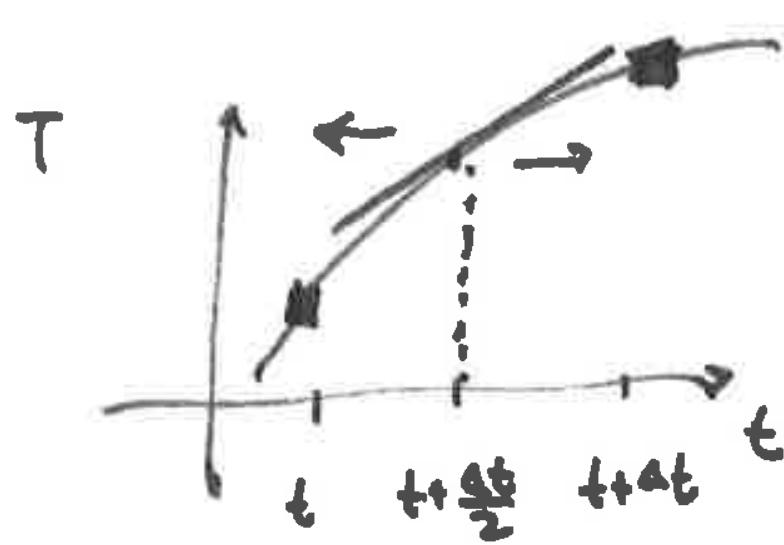


$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T(x, t)}{\partial x^2}$$

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

Insert (4) into (3)

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



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

$$t = j\Delta t$$

$$T(x, t) \equiv T_{ij}$$

$$x = i\Delta x$$

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

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

discretized  
diffusion equation  
(split time step)

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

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

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

Collect **future terms** on LHS

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

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

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

$$-T_{i-1,j+1} + \alpha T_{i,j+1} - T_{i+1,j+1} = T_{i-1,j} + \beta T_{ij} + T_{i+1,j} \quad \alpha := \frac{2}{\eta} + 2$$

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

Rewrite as matrix equation  $\mathbf{Ax} = \mathbf{b}$

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

Boundaries?

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

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

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

Special equations for

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

$$\begin{aligned} -T_{0,j+1} + \alpha T_{1,j+1} - T_{2,j+1} &= T_{0j} + \beta T_{1j} + T_{2j} \\ \alpha T_{1,j+1} - T_{2,j+1} &= T_{0j} + \beta T_{1j} + T_{2j} + T_{0,j+1} \quad (*) \end{aligned}$$

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

$$\begin{aligned} -T_{-3,j+1} + \alpha T_{-2,j+1} - T_{-1,j+1} &= T_{-3j} + \beta T_{-2j} + T_{-1j} \\ -T_{-3,j+1} + \alpha T_{-2,j+1} &= T_{-3j} + \beta T_{-2j} + T_{-1j} + T_{-1,j+1} \quad (**') \end{aligned}$$

# Crank-Nicholson

1. Set-up matrix A (N-2,N-2)

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

2. For each time step

1. Set-up RHS vector

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

2. solve matrix equation

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

# Crank-Nicholson: Performance Improvements

- pre-compute inverse of **constant** matrix  $\mathbf{A}=\mathbf{M}(\eta)$  and solve matrix problem as  $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$
- 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  $\Delta x$  and  $\Delta t$ )