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

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

Diffusion interpretation of the forward difference stability criterion

- random walk in 1D
- compare to stability condition:
 - grid spacing > than diffusion distance (squared) over one integration step
 - max. allowed dt = diffusion time across one grid cell

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

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

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

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

Computational cost

- features of interest
 - length scale
 - time scale
- $au pprox rac{\lambda^2}{D}$
- number of steps needed:

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

 $\lambda \gg \Delta x$

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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Taylor expansion around split time step

(1)
$$T(x,t) = T(x,t+\frac{4t}{2}) - \frac{4t}{2} \frac{\partial T(x,t+\frac{4t}{2})}{\partial t} + o(at^2)$$

(2) $T(x,t+at) = T(x,t+\frac{4t}{2}) + \frac{4t}{2} \frac{\partial T(x,t+\frac{4t}{2})}{\partial t} + o(at^2)$

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

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

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

Previously:

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

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

Finite difference derivative for split time step

(3)
$$\frac{\partial^{2}T(x,t+\frac{4t}{2})}{\partial x^{2}} = \frac{1}{\Delta x^{2}} \left[T(x+\Delta x,t+\frac{4t}{2}) + T(x-\Delta x,t+\frac{4t}{2}) - 2T(x,t+\frac{4t}{2}) + o(4x^{3}) \right]$$

From the first order derivatives: Eq 1 + Eq 2

2
$$T(x_1t+\frac{\Delta t}{2}) = T(x_1t) + T(x_1t+\Delta t) + \sigma(\Delta t^2)$$
(4)
$$T(x_1t+\frac{\Delta t}{2}) = \frac{1}{2}(T(x_1t) + T(x_1t+\Delta t)) + \sigma(\Delta t^2)$$

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

Insert (4) into (3)

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

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

$$t = j\Delta t$$
$$x = i\Delta x$$

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

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

discretized diffusion equation (split time step)

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

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

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

Collect future terms on LHS

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

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

future

IMPLICIT SCHEME

past

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

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

$$\alpha := \frac{2}{\eta} + 2$$
Powrite as matrix equation
$$A\mathbf{x} = \mathbf{b}$$

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

Rewrite as matrix equation

$$Ax = b$$

Boundaries?

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

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

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Special equations for

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

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

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

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

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

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

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

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

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
 - 2. solve matrix equation

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

Ax = b