PDEs: Crank-Nicholson Method

Improve over leap-frog:

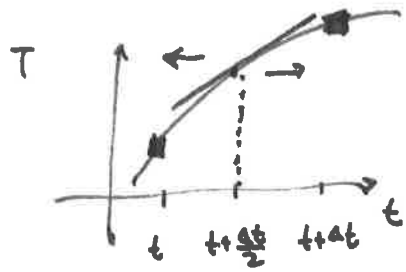
1) stability
2) accuracy

Diffusion equation (D):

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

1) Use "split time step", i.e. move from t to $t + \frac{\Delta t}{2}$.

2) Evaluate scheme at $t + \frac{\Delta t}{2}$ and derive equations for full time step



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

Taylor expansion:

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

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

Eq 2 − Eq 1:

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

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

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

lower accuracy!

4) Spatial derivatives at $t + \frac{\Delta t}{2}$

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

Insert the Taylor expansions Eq 1 and Eq 2 (averaged):

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

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

$$\hookrightarrow \Delta x^2 \frac{\partial^2 T(x, t+\frac{\Delta t}{2})}{\partial x^2} = \frac{1}{2}\Big[T(x+\Delta x, t) + T(x+\Delta x, t+\Delta t) + T(x-\Delta x, t) + T(x+\Delta x, t+\Delta t) - 2\big(T(x,t) + T(x, t+\Delta t)\big)\Big]$$

5) Discretized diffusion equation

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

, and using $t = j\Delta t$, $x = i\Delta x$

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

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

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

With $\eta := \frac{D\,\Delta t}{\Delta x^2}$ and collecting future terms on LHS:

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

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

future past implicit scheme

6) Write as matrix equation; $\alpha := \left(\frac{2}{\eta}+2\right)$, $\beta := \frac{2}{\eta} - 2$

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

Need to solve $N-2$ simultaneous equations for each timestep.
(Note: boundaries $T_{0,j}$ and $T_{N-1,j}$ are fixed.)

At boundaries: $i=0$ or $i = N-1$ $= "-1"$, so special for $T_{1,j+1}$ and $T_{N-2,j+1} \equiv T_{-2,j+1}$

$\boxed{T_1}$

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

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

$\boxed{T_{-2}}$

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

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

$\Rightarrow$ Implement Crank-Nicholson:

1) For each time step, solve matrix equation

$$\underline{\underline{A}}\,\underline{x} = \underline{b}$$

$\underline{\underline{A}} = \underline{\underline{M}}(\eta)$

$\underline{x} = (T_1, T_2, \dots, T_{N-2})$ (boundaries: $T_0 = T_{-1} = T_b$)

$\underline{b}$ = RHS from prev. page with special values for b_1 and b_{-1}

2) Improve matrix calculation:
- pre-compute inverse of constant $\underline{\underline{M}}(\eta)$
- take advantage of tridiagonal structure
  - Thomas algorithm
  - routines for banded matrices (eg. scipy.linalg.solve_banded())

Stability analysis (von Neumann)

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

Because $\sin^2\alpha \leq 1$, $|\xi(k)| \leq 1$

$\Rightarrow$ always stable (any combination of Δx and Δt!)