Diffusion Equation and Numerical Stability

22 November 2021 11:37

Parabolic PDEs

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

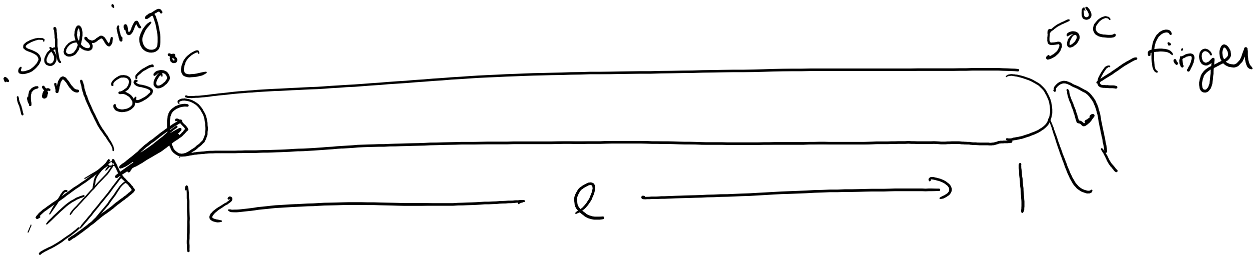
— Diffusion Equation

D — Diffusion Coefficient

Steel : $11 \ \frac{mm^2}{s}$

Silver : $\sim 100 \ \frac{mm^2}{s}$

Graphite : ~ 1000



Property: Over time "quantity will smooth out" <u>not</u> amplify.

On the Computer: ??

$x \in [0, L] \quad t \geq 0$

Boundary conditions as well as Initial conditions

Given

$$u(t=0, x) = u^{(0)}(x)$$
$$u(t, x=0) = u_1(t)$$
$$u(t, x=L) = u_2(t)$$

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

+1 −2 +1

OPTION 1

option 1

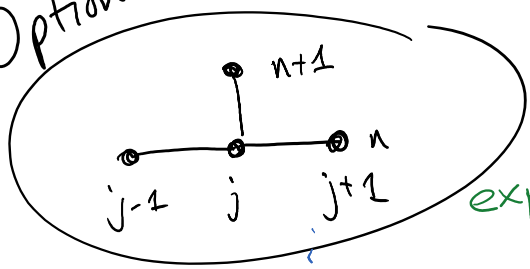
$$\left.\frac{\partial u}{\partial t}\right|_j \cong \frac{u_j^{(n+1)} - u_j^{(n)}}{\Delta t} = D\,\frac{u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}}{\Delta x^2}$$

$$\boxed{\alpha = \frac{D\,\Delta t}{\Delta x^2}}$$

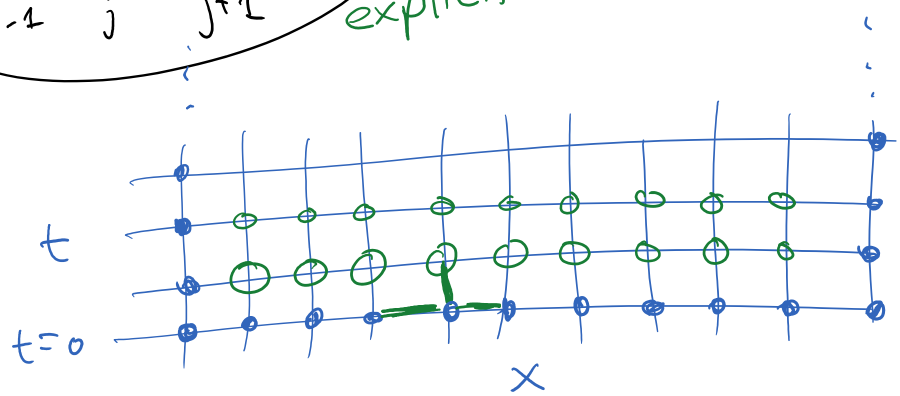
Option 1

$$u_j^{(n+1)} = \underbrace{u_j^{(n)} + \alpha\left(\overset{+1\quad -2\quad +1}{\bullet\!-\!\!-\!\bullet\!-\!\!-\!\bullet}\right)}_{\text{everything is given}}$$

: explicit method



explicit

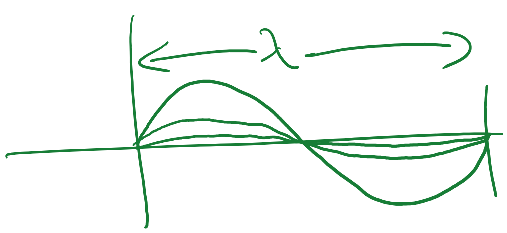


von Neumann Stability Analysis

Propose wave:

$$\boxed{u_j^{(n)} = A^n e^{ikj\Delta x}}$$

$$Ae^{i\Theta} = A(\cos\Theta + i\sin\Theta)$$



$$\lambda = \frac{2\pi}{k}$$

$|A| < 1$: Stable — the wave gets smoothed out

over time
$A^n \to 0$

$|A| > 1$: Unstable
└ Amplification!

$$u_j^{(n+1)} = u_j^{(n)} + \alpha\left(u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}\right)$$

$$A^{n+1}\cancel{e^{ikj\Delta x}} = \cancel{A^n e^{ikj\Delta x}} + \alpha \cancel{A^n}\left(\cancel{e^{ik(j+1)\Delta x}} - 2\cancel{e^{ikj\Delta x}} + e^{ik(j-1)\Delta x}\right)$$

$$A = 1 + \alpha\left(e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right)$$

$$\cos(k\Delta x) = \frac{e^{ik\Delta x} + e^{-ik\Delta x}}{2}$$

$$A = 1 + \alpha\left(2\cos(k\Delta x) - 2\right)$$

$$\sin^2\left(\frac{x}{2}\right) = \frac{1}{2}\left[1 - \cos(x)\right]$$ use this identity

$$\boxed{A = 1 - 4\alpha\sin^2\left(\frac{k\Delta x}{2}\right)}$$

We want $|A| < 1$ for all possible k!

$$\sin^2(\;) \in [0, 1]$$

$$A \in 1 - 4\alpha[0, 1]$$

$$A \in [1 - 4\alpha, 1]$$ ✓

$$|A| < 1 \Rightarrow A^2 < 1$$

$$\Rightarrow A \in (-1, 1)$$

lower bound is the critical one...

$$-1 < 1 - 4\alpha$$

$$-2 < -4\alpha$$

$$\boxed{\alpha < \frac{1}{2}}$$

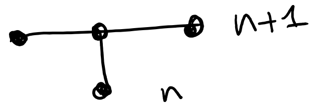
$$\boxed{\frac{D\,\Delta t}{\Delta x^2} < \frac{1}{2}}$$

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

Numerical Time step, Physical Timescale is typically much longer!

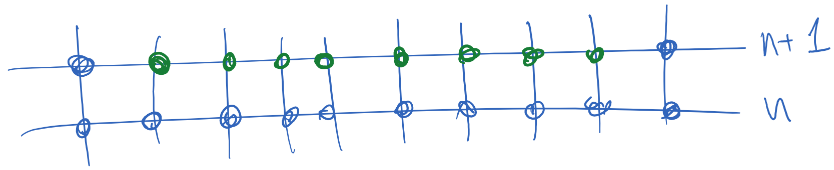
Option 2 Always Stable? Can we make a method that is unconditionally stable?

Yes.

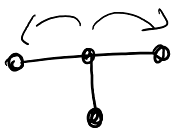


$$u_j^{(n+1)} = u_j^{(n)} + \alpha\left(u_{j+1}^{(n+1)} - 2u_j^{(n+1)} + u_{j-1}^{(n+1)}\right)$$

Implicit method



$$A = \frac{1}{1 + 4\alpha \sin^2\left(\frac{k\Delta x}{2}\right)}$$



$|A| < 1 \quad \forall k$ Always Stable!

$$\underline{\underline{M}}\,\underline{x} = \underline{b} \qquad \underbrace{\begin{pmatrix} \ddots & \ddots & \emptyset \\ \ddots & \ddots & \ddots \\ \emptyset & \ddots & \ddots \end{pmatrix}}_{\mathcal{O}(N) \text{ solution}} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-1} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{N-1} \end{pmatrix}$$

tri-diagonal Matrix Solution.

Error of the methods

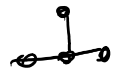
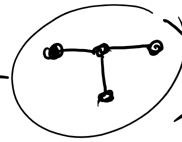
$\mathcal{O}(\Delta x^2)$ resolution

$\mathcal{O}(\Delta t)$ in time

For higher accuracy I need to take many small timesteps due to the truncation error of the methods $\underset{\text{error}}{\mathcal{O}(\Delta t)}$

Crank-Nicholson Method

"Average" options 1 & 2:

$\frac{1}{2}\Big($  $+$  $\Big)$ Implicit, Stable $\mathcal{O}(\Delta t^2)$!

$$\boxed{u_j^{(n+1)} - u_j^{(n)} = \frac{\alpha}{2}\left(u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)} + u_{j+1}^{(n+1)} - 2u_j^{(n+1)} + u_{j-1}^{(n+1)}\right)}$$

$$M\underline{x} = \underline{b} \qquad M = \begin{pmatrix} \ddots & \ddots & \emptyset \\ \ddots & \ddots & \ddots \\ \emptyset & \ddots & \ddots \end{pmatrix} \checkmark$$

Tridiagonal Solution