Diffusion Equation

→ Typically represents the action of small-scale processes to "mix" a quantity down-gradient (i.e. moving from greater to lower)

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

D ← diffusivity

$D > 0$

important

This is the time-dependent version of the 1D diffusion in the Earth we considered before

- Often use to describe heat conduction
- Can also model spreading / diffusion of material in a porous matrix (i.e. contaminant in an aquifer)

How to discretize?

In time: $\frac{\partial J}{\partial t} = \frac{J_i^{k+1} - J_i^k}{\Delta t}$

In space (most general form):

$$D\frac{\partial^2 J}{\partial x^2} = D\,\theta\,\frac{J_{i+1}^{k+1} - 2J_i^{k+1} + J_{i-1}^{k+1}}{(\Delta x)^2} + D(1-\theta)\,\frac{J_{i+1}^{k} - 2J_i^{k} + J_{i-1}^{k}}{(\Delta x)^2}$$

θ is a parameter we can use to choose between methods

a) $\theta = 0$ → first term vanishes → Forward Euler method

b) $\theta = 1$ → second term vanishes → Backward Euler - need to do matrix inversion

c) $\theta = 0.5$ → mix of two methods

Crank-Nicholson method

Much like the Courant number in advection eqn, we can define a diffusion number:

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

that helps us determine stability of various methods

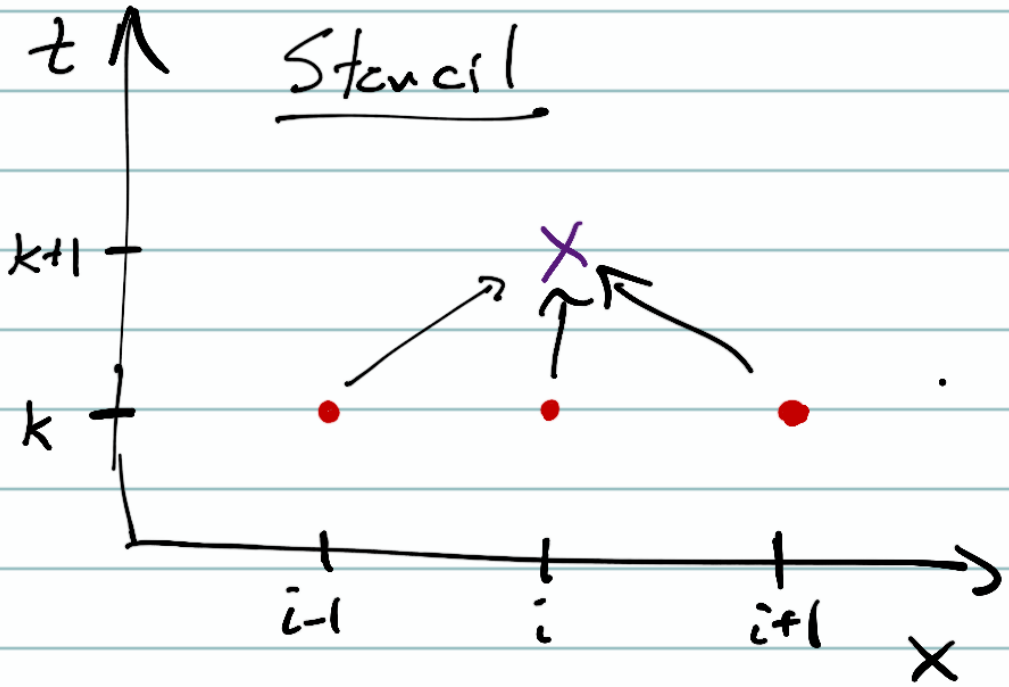
In general we write methods:

$$\bar{J}_i^{k+1} - C_D\theta\left(\bar{J}_{i+1}^{k+1} - 2\bar{J}_i^{k+1} + \bar{J}_{i-1}^{k+1}\right) = \bar{J}_i^{k} + C_D(1-\theta)\left(\bar{J}_{i+1}^{k} - 2\bar{J}_i^{k} + \bar{J}_{i-1}^{k}\right)$$

How to implement?

→ for each method, we consider the stencil, matrix form, how to specify BCs and stability condition

Forward Euler



Boundary conditions (same as when we did BVP)

Dirichlet: Simply sub in $\bar{J}_0$ and $\bar{J}_{n+1}$ at right and left most calcs

e.g. $\bar{J}_1^{k+1} = \bar{J}_1^k + C_D(\bar{J}_2^k - 2\bar{J}_1^k + \bar{J}_0)$

Neumann: $F_0 = D\left.\frac{\partial \bar{J}}{\partial x}\right|_{x=x_0}$ imposed

$$\bar{J}_1^{k+1} = \bar{J}_1^k + \frac{D\Delta t}{\Delta t}\left[\frac{\bar{J}_2^k - \bar{J}_1^k}{\Delta x} - \frac{\bar{J}_1^k - \bar{J}_0^k}{\Delta x}\right]$$

$\bar{F}_0/D$

Time evolution specified through explicit matrix marching equation

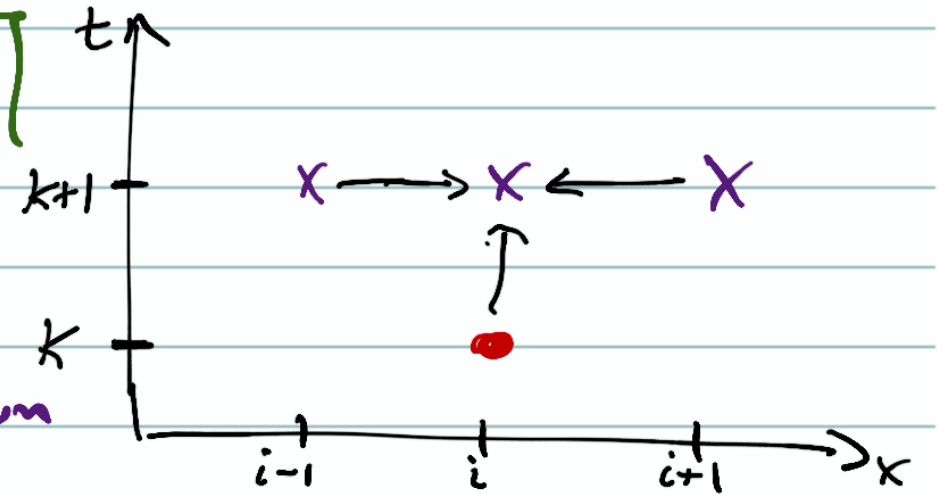
$$\begin{bmatrix} \\ \vdots \\ \overline{J}_i^{k+1} \\ \vdots \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \vdots \\ \overline{J}_i^{k} \\ \vdots \\ \\ \end{bmatrix} \begin{bmatrix} \\ \\ M \\ \\ \\ \end{bmatrix}$$

$$M = C_D \begin{bmatrix} -2 & 1 & 0 & & & \\ 1 & -2 & 1 & 0 & & \\ 0 & 1 & -2 & 1 & 0 & \\ & & & & & \end{bmatrix}$$

← these might be modified for BCs

Backward Euler

Stencil:



● Known x Unknown

$$\bar{J}_i^{k+1}(1+2C_D) - C_D\left(\bar{J}_{i+1}^{k+1} + \bar{J}_{i-1}^{k+1}\right) = \bar{J}_i^{k}$$

unknown — known

Matrix form

$$\begin{bmatrix} 1+2C_D & -C_D & 0 & \cdots \\ -C_D & 1+2C_D & -C_D & 0 \cdots \\ 0 & & & \end{bmatrix} \begin{bmatrix} \\ \bar{J}_i^{k+1} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \bar{J}_i^{k} \\ \\ \end{bmatrix}$$

M $\quad \bar{J}_i^{k+1}$ $\quad \bar{J}_i^{k}$

To solve: $\bar{J}_i^{k+1} = M^{-1}\bar{J}_i^{k}$

matrix inversion necessary!

But... M doesn't change, so only need to invert once. And... M is tridiagonal

Boundary conditions

Mainly specified by moving terms from the unknown side to known side

Dirichlet: $\bar{J}_1^{k+1}(1+2C_D) - C_D\bar{J}_2^{k+1} - C_D\bar{J}_0 = \bar{J}_1^k$

$$\bar{J}_1^{k+1}(1+2C_D) - C_D\bar{J}_2^{k+1} = \bar{J}_1^k + C_D\bar{J}_0$$

M doesn't change, but first element of RHS vector does:

$$\begin{bmatrix} \bar{J}_1^k + C_D\bar{J}_0 \\ \bar{J}_2^k \\ \vdots \end{bmatrix}$$

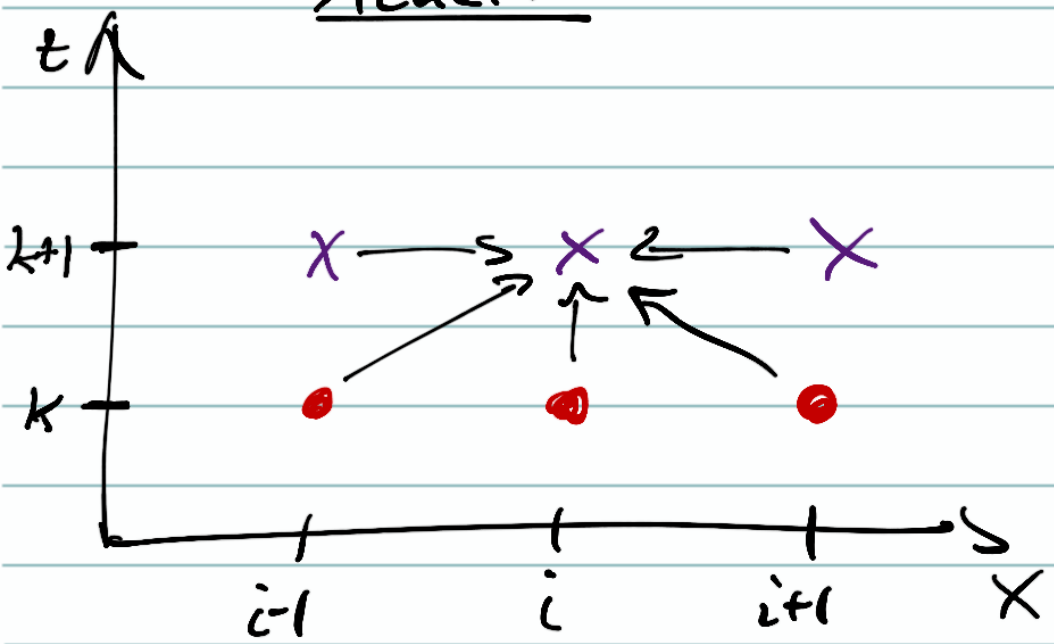
Neumann:

$$\bar{J}_1^{k+1} - C_D(\bar{J}_2^{k+1} - \bar{J}_1^{k+1}) + \frac{D\theta t}{\Delta x}\left(\frac{\bar{J}_1^{k+1} - \bar{J}_0^{k+1}}{\Delta x}\right) = \ldots$$

This will slightly modify both M and RHS vector F_0/D

Crank-Nicholson

Stencil



$$\bar{J}_i^{k+1}\left(1+C_D\right)-\frac{1}{2}C_D\left(\bar{J}_{i+1}^{k+1}+\bar{J}_{i-1}^{k+1}\right)=$$

$$\bar{J}_i^{k}\left(1-C_D\right)+\frac{1}{2}C_D\left(\bar{J}_{i+1}^{k}+\bar{J}_{i-1}^{k}\right)$$

Matrix inversion necessary - similar to BE → small diffs in terms and RHS vector is a little more complicated.

To determine stability of different methods, use Von-Neumann method:

1. Expand $\bar{J}$ as Fourier series
2. Stability condition requires that all wavenumbers in space decay in time

skip to final condition

$$\left| \frac{1 - 4C_d(1-\Theta)}{1 + 4C_d\Theta} \right| \leq 1$$

Required for method to be stable

Forward Euler: $\boxed{C_D \leq \frac{1}{2}}$

Backward Euler: Unconditionally stable (for all C_d)

Crank-Nicholson: Unconditionally stable

↳ C-N method usually preferred bc its more accurate than BE