Diffusion Equation

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

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

diffusivity

$\underline{D > 0}$
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: $\dfrac{\partial J}{\partial t} = \dfrac{J_i^{k+1} - J_i^{k}}{\Delta t}$

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

$\boxed{\text{Crank-Nicholson method}}$

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

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

That helps us determine stability of various methods

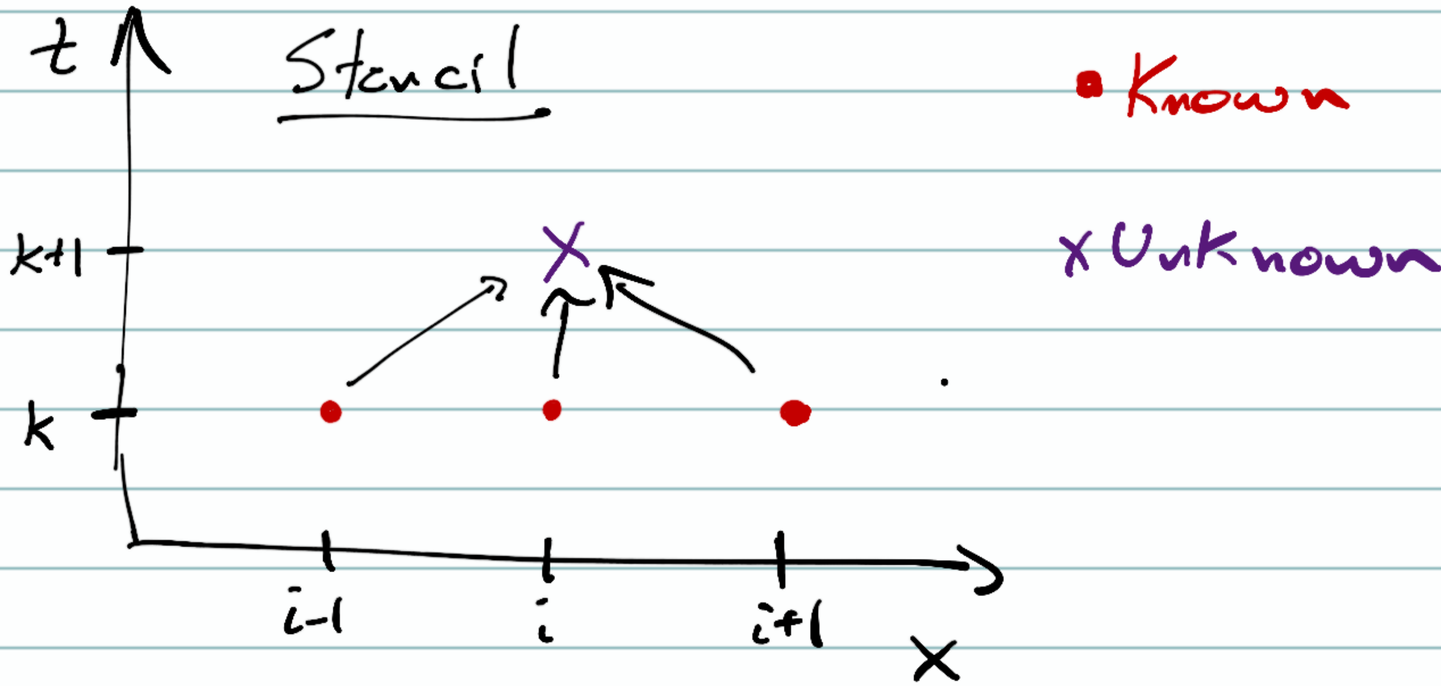
In general we write methods:

$$\boxed{\begin{aligned} &J_i^{k+1} - C_D\,\Theta\left(J_{i+1}^{k+1} - 2J_i^{k+1} + J_{i-1}^{k+1}\right) = \\ &J_i^k + C_D(1-\Theta)\left(J_{i+1}^k - 2J_i^k + J_{i-1}^k\right) \end{aligned}}$$

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 J_0 and J_{n+1} at right and left most calcs

e.g. $J_1^{k+1} = J_1^k + C_D\left(J_2^k - 2J_1^k + J_0\right)$

Neumann: $F_0 = D\frac{\partial J}{\partial x}\Big|_{x=x_0}$ imposed

$$J_1^{k+1} = J_1^k + \frac{D\Delta t}{\Delta x}\left[\frac{J_2^k - J_1^k}{\Delta x} - \underbrace{\cancel{\frac{J_1^k - J_0^k}{\Delta x}}}_{F_0/D}\right]$$

Time evolution specified through explicit matrix marching equation

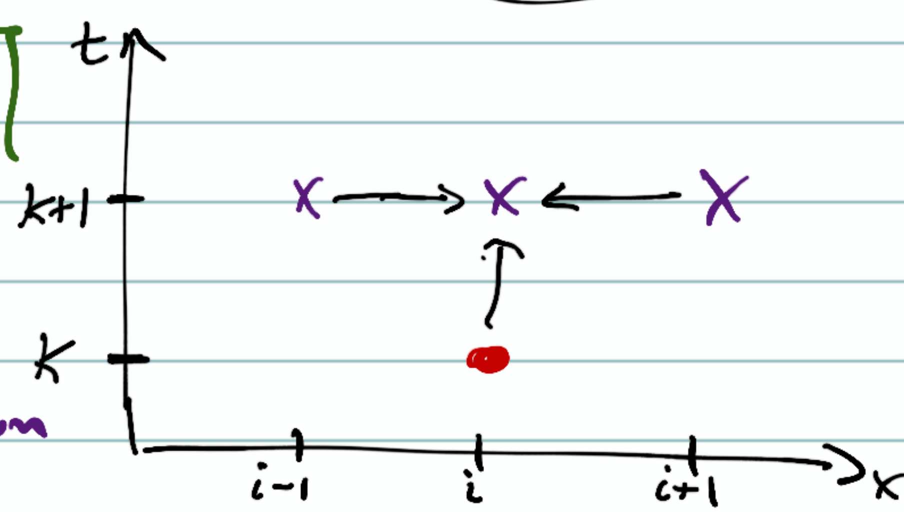
$$\left[\;\vdots\;\bar{J}_i^{k+1}\;\vdots\;\right] = \left[\;\vdots\;\bar{J}_i^{k}\;\vdots\;\right]\left[\quad M \quad\right]$$

these might be modified for BCs

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

Backward Euler

Stencil:



• Known x Unknown

$$\underbrace{J_i^{k+1}(1+2C_D) - C_D\left(J_{i+1}^{k+1} + J_{i-1}^{k+1}\right)}_{\text{unknown}} = \underbrace{J_i^{k}}_{\text{known}}$$

Matrix form

$$\begin{bmatrix} 1+2C_D & -C_D & 0 & \cdots \\ -C_D & 1+2C_D & -C_D & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ J_i^{k+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ J_i^{k} \\ \vdots \end{bmatrix}$$

$$\begin{array}{ccc} M & J_i^{k+1} & J_i^{k} \end{array}$$

To solve! $J_i^{k+1} = \underbrace{M^{-1}}_{\text{matrix inversion necessary!}} J_i^{k}$

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:

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

Neumann:

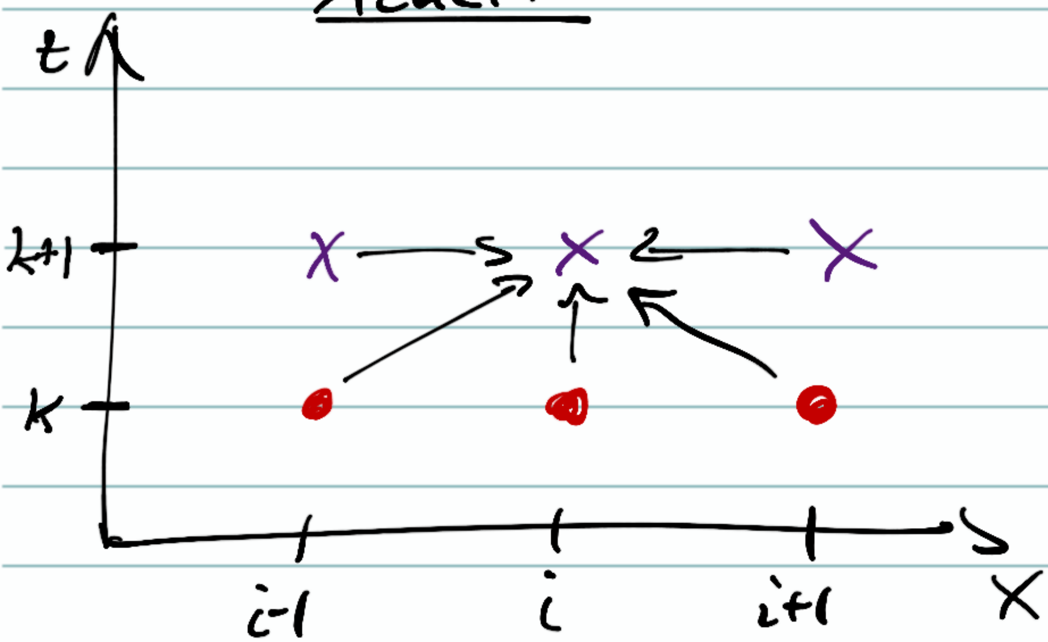
$$\bar{J}_1^{k+1} - C_D\left(\bar{J}_2^{k+1} - \bar{J}_1^{k+1}\right) + \frac{D\Delta t}{\Delta x}\left(\frac{\bar{J}_1^{k+1} - \bar{J}_0^{k+1}}{\Delta x}\right) = \ldots$$

F_0/D

This will slightly modify both M and RHS vector

Crank-Nicholson

Stencil



$$J_i^{k+1}(1+C_D) - \frac{1}{2}C_D\left(J_{i+1}^{k+1} + J_{i-1}^{k+1}\right) =$$

$$J_i^{k}(1-C_D) + \frac{1}{2}C_D\left(J_{i+1}^{k} + J_{i-1}^{k}\right)$$

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 J as Fourier series

② Stability condition requires that all wavenumbers in space decay in time

skip to final condition

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

Required for method to be stable

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

Backward Euler: Unconditionally stable (for all C_d)

Crank-Nicholson: Unconditionally stable

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