

Diffusion Equation

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

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

$\overbrace{D > 0}^{\text{diffusivity}}$
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: $\frac{\partial T}{\partial t} = \frac{T_i^{k+1} - T_i^k}{\Delta t}$

In space (most general form):

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

θ is a parameter we can use to choose between methods

- a) $\theta = 0 \rightarrow$ first term vanishes \rightarrow Forward Euler method
- b) $\theta = 1 \rightarrow$ second term vanishes \rightarrow Backward Euler - need to do matrix inversion

c) $\theta = 0.5 \rightarrow$ 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

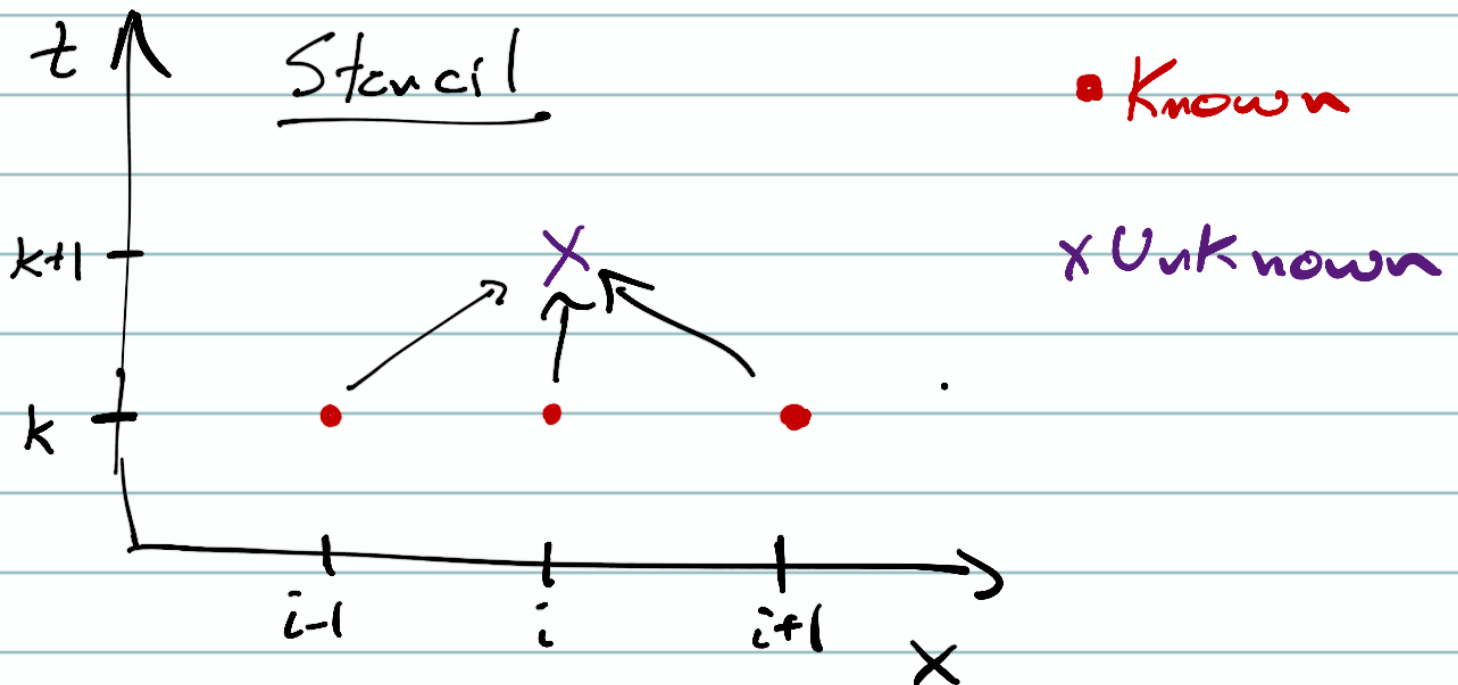
In general we write methods:

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

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. $J_1^{k+1} = J_1^k + C_D (J_2^k - 2J_1^k + \bar{J}_0)$

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

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

F_0/D

Time evolution specified through explicit matrix marching equation

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

these might be modified for BCs

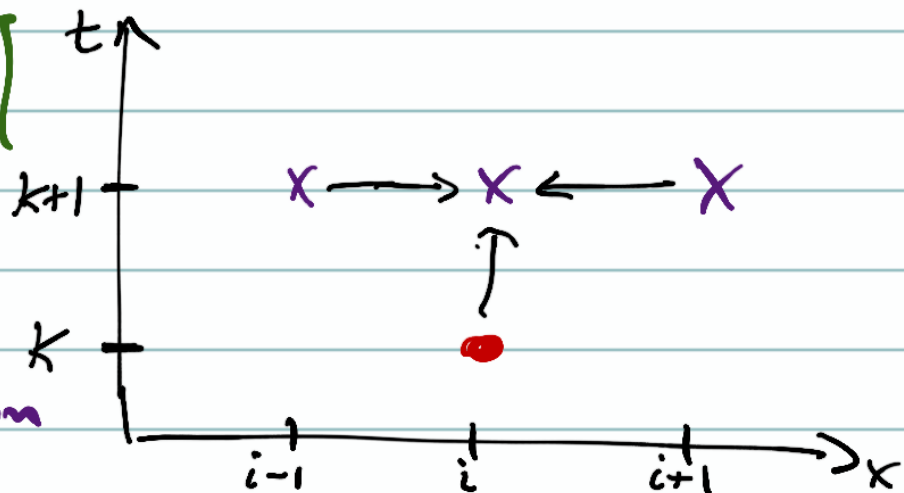
$$M = \begin{bmatrix} 1-2C_D & C_D & 0 & \dots \\ C_D & 1-2C_D & C_D & 0 \\ 0 & C_D & 1-2C_D & 0 \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Backward Euler

Stencil:

• Known

x Unknown



$$\underbrace{\bar{J}_i^{k+1}(1+2C_0) - C_0(\bar{J}_{i+1}^{k+1} + \bar{J}_{i-1}^{k+1})}_{\text{LHS}} = \bar{J}_i^k \quad \text{RHS}$$

known

Matrix form

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

To solve: $J_i^{k+1} = M^{-1} J_i^k$
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:

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

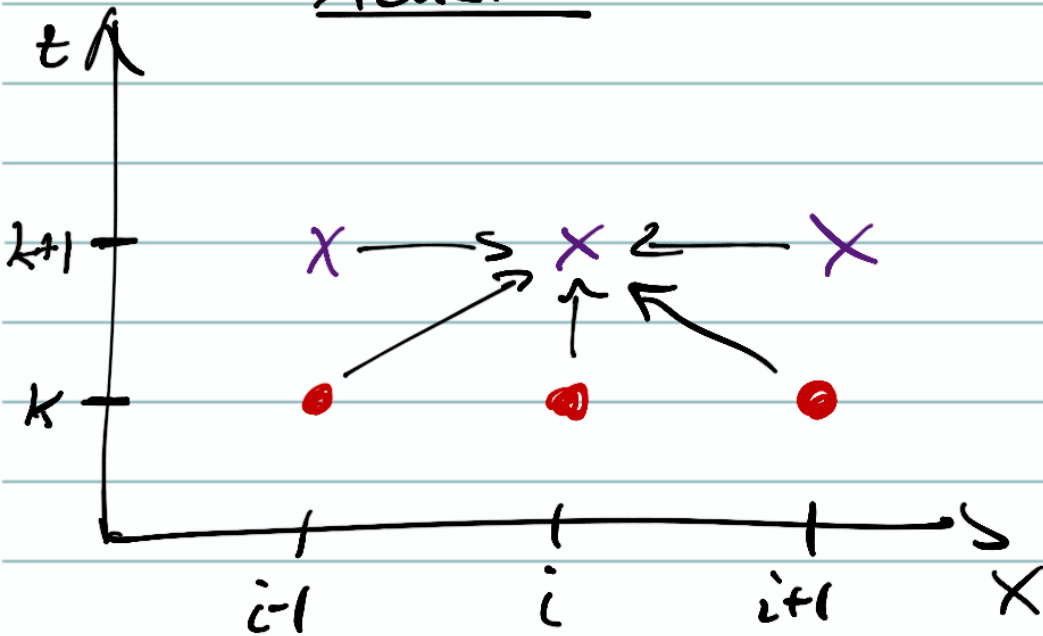
Neumann:

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

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

Crank-Nicholson

Stencil



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

Matrix inversion necessary - similar to BE \rightarrow 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{u} 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