

Crank-Nicolson scheme for 1D diffusive transport

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Assuming zero-flux boundary conditions, variable diffusivity and variable area over depth, we start with the one-dimensional diffusion equation:

$$\frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial z} (K(z) A(z) \frac{\partial T}{\partial z}) \quad (1)$$

Expanding this we get:

$$\frac{\partial T}{\partial t} = \frac{1}{A} \left(\frac{\partial K}{\partial z} A(z) \frac{\partial T}{\partial z} + K(z) \frac{\partial A}{\partial z} \frac{\partial T}{\partial z} + K(z) A(z) \frac{\partial^2 T}{\partial z^2} \right) \quad (2)$$

We discretise the expanded form using central second-order finite differences for both the first and second derivatives, as well as implicit midpoint method in time to derive:

$$\begin{aligned} \frac{T_n^{i+1} - T_n^i}{\Delta t} = & \frac{1}{2} \frac{1}{A} \left(\frac{K_{n+1} - K_{n-1}}{2\Delta z} A_n \frac{T_{n+1}^{i+1} - T_{n-1}^{i+1}}{2\Delta z} + K_n \frac{A_{n+1} - A_{n-1}}{2\Delta z} \frac{T_{n+1}^{i+1} - T_{n-1}^{i+1}}{2\Delta z} + \right. \\ & K_n A_n \frac{T_{n+1}^{i+1} - 2T_n^{i+1} + T_{n-1}^{i+1}}{\Delta z^2} + \frac{K_{n+1} - K_{n-1}}{2\Delta z} A_n \frac{T_{n+1}^i - T_{n-1}^i}{2\Delta z} + K_n \frac{A_{n+1} - A_{n-1}}{2\Delta z} \frac{T_{n+1}^i - T_{n-1}^i}{2\Delta z} + \\ & \left. K_n A_n \frac{T_{n+1}^i - 2T_n^i + T_{n-1}^i}{\Delta z^2} \right) \end{aligned} \quad (3)$$

We can set $\alpha = \frac{\Delta t}{2A_n \Delta z^2}$, $K'_n = K_{n+1} - K_{n-1}$, and $A'_n = A_{n+1} - A_{n-1}$ to get a tridiagonal system of equations:

$$\begin{aligned} T_{n-1}^{i+1} \left(\frac{\alpha K'_n A_n}{4} + \frac{\alpha K_n A'_n}{4} - \alpha K_n A_n \right) + T_n^{i+1} (1 + 2\alpha K_n A_n) + T_{n+1}^{i+1} \left(-\frac{\alpha K'_n A_n}{4} - \frac{\alpha K_n A'_n}{4} - \alpha K_n A_n \right) = \\ T_{n-1}^i \left(-\frac{\alpha K'_n A_n}{4} - \frac{\alpha K_n A'_n}{4} + \alpha K_n A_n \right) + T_n^i (1 - 2\alpha K_n A_n) + T_{n+1}^i \left(\frac{\alpha K'_n A_n}{4} + \frac{\alpha K_n A'_n}{4} + \alpha K_n A_n \right) \end{aligned} \quad (4)$$

We can set up the tridiagonal matrix using $a = \frac{\alpha K'_n A_n}{4} + \frac{\alpha K_n A'_n}{4} - \alpha K_n A_n$, $b = 1 + 2\alpha K_n A_n$, and $c = -\frac{\alpha K'_n A_n}{4} - \frac{\alpha K_n A'_n}{4} + \alpha K_n A_n$ (here exemplary shown for a 4x4 problem):

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 \\ 0 & a_3 & b_3 & c_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} T_1^{i+1} \\ T_2^{i+1} \\ T_3^{i+1} \\ T_4^{i+1} \end{pmatrix} = \begin{pmatrix} T_1^i \\ -a_2 T_1^i + T_2^i (1 - 2\alpha K_2 A_2) - c T_3^i \\ -a_2 T_2^i + T_3^i (1 - 2\alpha K_2 A_2) - c T_4^i \\ T_4^i \end{pmatrix} \quad (5)$$

where the first and last equations are just boundary conditions that are equal to the simulated temperatures at both ends.

We also need to treat the boundaries for A'_n as well as K'_n at 1 and N (surface and bottom, respectively) as

$$A'_1 = 2(A_2 - A_1) \tag{6}$$

and

$$A'_N = 2(A_N - A_{N-1}) \tag{7}$$

(and similarly for K').