Writing a PDE in matrix form (for optimal initial conditions, transient growth, and stochastic optimals, also demonstrating grid choice depending on type of boundary conditions)

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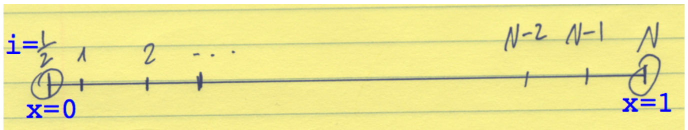
Consider for example,

$$T_t + uT_x = \kappa T_{xx}, \tag{1}$$

with constant velocity u and diffusivity κ, and b.c. of prescribed flux on one side and prescribed temperature on the other,

$$(uT - \kappa T_x)|_{x=0} = 0, \quad T|_{x=1} = A.$$

Given the two different boundary conditions at the two ends (prescribed flux at $x = 0$ vs fixed value at $x = 1$), it is convenient to let $x = 0$ be at a half grid location (that is, between two grid points), and $x = 1$ at a grid point location,



Define $T_{i+\frac{1}{2}} = (T_i + T_{i+1})/2$, $dT/dx|_{i+1/2} = (T_{i+1} - T_i)/\Delta x$, and write the b.c. as,

$$uT_{i=\frac{1}{2}} - \kappa \left.\frac{dT}{dx}\right|_{i=\frac{1}{2}} = 0$$
$$T_{i=N} = A.$$

The equation in finite difference is then,

$$
\begin{aligned}
\frac{d}{dt}T_1 &= -(uT_{1\frac{1}{2}} - 0)/\Delta x + \kappa \left(\left.\frac{dT}{dx}\right|_{1\frac{1}{2}} - 0 \right) /\Delta x \\
\frac{d}{dt}T_i &= -(uT_{i+\frac{1}{2}} - uT_{i-\frac{1}{2}})/\Delta x + \kappa \left(\left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} - \left.\frac{dT}{dx}\right|_{i-\frac{1}{2}} \right) /\Delta x \\
\frac{d}{dt}T_{N-1} &= -(uT_{N-\frac{1}{2}} - uT_{N-1\frac{1}{2}})/\Delta x + \kappa \left(\left.\frac{dT}{dx}\right|_{N-\frac{1}{2}} - \left.\frac{dT}{dx}\right|_{N-1\frac{1}{2}} \right) /\Delta x
\end{aligned}
$$

These translate into

$$
\begin{aligned}
\frac{d}{dt}T_1 &= -u(T_1 + T_2)/(2\Delta x) + \kappa(T_2 - T_1)/(\Delta x)^2 \\
\frac{d}{dt}T_i &= -u(T_{i+1} - T_{i-1})/(2\Delta x) + \kappa(T_{i+1} - 2T_i + T_{i-1})/(\Delta x)^2 \\
\frac{d}{dt}T_{N-1} &= -u(A - T_{N-2})/(2\Delta x) + \kappa(A - 2T_{N-1} + T_{N-2})/(\Delta x)^2
\end{aligned}
$$

which may be written as a set of equations for $T_1, \ldots, T_{N-1}$,

$$
\begin{aligned}
\frac{d}{dt}T_1 &= T_1 \left(-\frac{u}{2\Delta x} - \frac{\kappa}{\Delta x^2} \right) + T_2 \left(-\frac{u}{2\Delta x} + \frac{\kappa}{\Delta x^2} \right) \\
&= T_1 a_{11} + T_2 a_{12} \\
\frac{d}{dt}T_i &= T_{i-1} \left(\frac{u}{2\Delta x} + \frac{\kappa}{\Delta x^2} \right) + T_i \left(-2\frac{\kappa}{\Delta x^2} \right) + T_{i+1} \left(-\frac{u}{2\Delta x} + \frac{\kappa}{\Delta x^2} \right) \\
&= T_{i-1} a_{i,i-1} + T_i a_{ii} + T_{i+1} a_{i,i+1} \\
\frac{d}{dt}T_{N-1} &= T_{N-2} \left(\frac{u}{2\Delta x} + \frac{\kappa}{\Delta x^2} \right) + T_{N-1} \left(-2\frac{\kappa}{\Delta x^2} \right) + A \left(-\frac{u}{2\Delta x} + \frac{\kappa}{\Delta x^2} \right) \\
&= T_{N-2} a_{N-1,N-2} + T_{N-1} a_{N-1,N-1} + b_{N-1},
\end{aligned}
$$

or,

$$
\frac{d}{dt} \begin{pmatrix} T_1 \\ \vdots \\ T_i \\ \vdots \\ T_{N-1} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \ldots & & & & 0 \\ & & & & & & \\ 0 & \ldots & a_{i,i-1} & a_{i,i} & a_{i,i+1} & \ldots & 0 \\ & & & & & & \\ 0 & \ldots & & & & a_{N-1,N-2} & a_{N-1,N-1} \end{pmatrix} \begin{pmatrix} T_1 \\ \vdots \\ T_i \\ \vdots \\ T_{N-1} \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ b_{N-1} \end{pmatrix}.
$$