Problem Set 1

Finite Difference Method

The finite difference approximation of derivatives may be obtained by Taylor's expansion. The following is what you need in order to solve this problem set:

$$\begin{aligned}
\partial_t T(x,t) &\approx \frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} \\
\partial_x^2 T(x,t) &\approx \frac{T(x+\Delta x,t)-2T(x,t)+T(x-\Delta x,t)}{\Delta x^2}
\end{aligned}$$

Heat Equation

The 1-D expression of the conservation of heat energy writes as:

$$\rho(x)\ c_p(x)\ \partial_t T(x,t) = -\partial_x q(x,t)\,, \qquad x\in[0,L], \quad t\in[0,+\infty)\,,$$

where $T(x,t)$ is the temperature field at the position x at the instant t, $\rho(x)$ is the density, $c_p(x)$ is the specific heat at constant pressure, and $q(x,t)$ is the heat flux. The heat flux is related to the temperature through the Fourier's law of heat conduction:

$$q(x,t) = -k(x)\ \partial_x T(x,t)\,,$$

where $k(x)$ is the thermal conductivity. The Fourier's law expresses the fact that the flow rate of heat energy is driven by the negative gradient of temperature across a surface.
The heat equation can thus be expressed as:

$$\rho(x)\ c_p(x)\ \partial_t T(x,t) = \partial_x\left[k(x)\ \partial_x T(x,t)\right]\,.$$

If we further assume constant thermal properties, this equation rewrites as:

$$\partial_t T(x,t) = D\ \partial_x^2 T(x,t)\,,$$

where we have introduced $D \equiv k/(\rho c_p)$, the thermal diffusivity.

Problem:

Use the finite difference approximation given above to solve the 1-D heat flow equation. You are strongly encouraged to write your code without the constant thermal properties assumption, keeping it general and allowing for heterogeneous material properties.

Consider a string of length $L = 100$ with a spike of temperature at $x = 50$. The initial conditions are:

$$T(x,0) = 0 \quad (x \neq 50)$$
$$T(x,0) = 1 \quad (x = 50)$$

The boundary conditions are:

$$T(0,t) \quad = 0 \quad (t \in [0, +\infty))$$
$$T(L,t) \quad = 0 \quad (t \in [0, +\infty))$$

The grid size is defined by $\Delta x = L/(N-1)$, where N is the number of nodes in the x-direction. In this problem, Δx is chosen to be 1.

Plot the temperature field at different times, and experiment with four different time steps Δt:

$$\Delta t = 0.4\frac{\Delta x^2}{D}, \quad 0.45\frac{\Delta x^2}{D}, \quad 0.55\frac{\Delta x^2}{D}, \quad 0.6\frac{\Delta x^2}{D}$$

Extra Question – Explicit versus Implicit Scheme

The finite difference approximation $\partial_t T(x,t) \approx \frac{T(x,t+\Delta t)-T(x,t)}{\Delta t}$ we used above is named *forward* finite difference. The corresponding algorithm is an 'Explicit Scheme', since it's straightforward for time marching, i.e., from $T^n = T(x,t)$ to $T^{n+1} = T(x,t+\Delta t)$.

In contrast, $\partial_t T(x,t) \approx \frac{T(x,t)-T(x,t-\Delta t)}{\Delta t}$ is called a *backward* finite difference, and the algorithm is referred to as an 'Implicit Scheme', where a set of equations have to be solved in order to march from $T^{n-1} = T(x,t-\Delta t)$ to $T^n = T(x,t)$.

Problem:

Write the heat equation using a backward time scheme and a centered space discretization, and show that you end up with a matricial expression of the form:

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 & 0 \\ 0 & 0 & ... & ... & ... & 0 \\ 0 & 0 & 0 & a_{N-1} & b_{N-1} & c_{N-1} \\ 0 & 0 & 0 & 0 & a_N & b_N \end{bmatrix} \begin{bmatrix} T_1^n \\ T_2^n \\ T_3^n \\ ... \\ T_{N-1}^n \\ T_N^n \end{bmatrix} = \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{N-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_N \end{bmatrix} \begin{bmatrix} T_1^{n-1} \\ T_2^{n-1} \\ T_3^{n-1} \\ ... \\ T_{N-1}^{n-1} \\ T_N^{n-1} \end{bmatrix}$$

Identify the coefficients a_i, b_i, c_i, and d_i, for $i = 1,..,N$. Notice that inversion of a matrix A can be expensive. One way to solve the problem is to recognize that this system can be efficiently solved using LU factorization. Thus, $Av = d$ is equivalent to $(LU)v = d$ or $L(Uv) = d$, so we solve $Lw = d$ and $Uv = w$.

Implement the heat equation using the implicit scheme. Plot the temperature field evolution for the same Δt than previously and compare the results.

Extra Question – Crank-Nicolson Scheme

Thus far we have seen forward & backward time schemes, which are both first-order accurate in time. If accuracy is important, one uses a *Crank-Nicolson* scheme, which relies on a backward time difference and an average of the central space difference scheme applied to the current and the previous time step.

The Crank-Nicolson scheme, depending on the previous time step like the backward scheme, belongs to the category of *implicit* time scheme. But contrary to the backward scheme, it offers a second-order accuracy in time.

Problem:

Write the heat equation using a Crank-Nicolson scheme. Show the corresponding matricial form.