Problem Set 3

Submission deadline: February 23, 2022

Submission type: Report (soft or hard copy) and source code (soft copy)

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:

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

Heat Equation

The 1-D expression of the conservation of heat energy is written 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 position x at instant t, $\rho(x)$ the density, $c_p(x)$ the specific heat at constant pressure, and $q(x,t)$ the heat flux. The heat flux is related to the temperature through Fourier's law of heat conduction:

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

where $k(x)$ is the thermal conductivity. Fourier's law expresses the fact that the rate of heat flow is driven by the negative gradient of temperature.

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 can be rewritten 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.

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

$$\begin{aligned} T(x,0) &= 0 \quad (x \neq 50) \\ T(x,0) &= 1 \quad (x = 50) \quad . \end{aligned}$$

The boundary conditions are:

$$\begin{aligned} T(0,t) &= 0 \quad (t \in [0,+\infty)) \\ T(L,t) &= 0 \quad (t \in [0,+\infty)) \quad . \end{aligned}$$

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.

1 Finite Difference solution

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.

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

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

2 Explicit versus Implicit Schemes

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 time marching is straightforward, 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 has to be solved in order to march from $T^{n-1} = T(x,t-\Delta t)$ to $T^n = T(x,t)$.

Write the heat equation using a backward time scheme and a centered space discretization, and show that you end up with a matrix-vector 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 the direct 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 $L\,U$ factorization. Thus, $A\,v = d$ is equivalent to $(L\,U)\,v = d$ or $L\,(U\,v) = d$, so we solve $L\,w = d$ & $U\,v = w$.

Implement the heat equation using the implicit scheme. Plot the temperature field evolution for the same Δt s previously given and compare the results with the explicit scheme.

3 Crank-Nicolson Scheme

Thus far we have seen forward and 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 schemes. But contrary to the backward scheme, it offers a second-order accuracy in time.

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