Exercise 3

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1 Finite difference approximation of the second derivative

1.a fourth-order central finite-difference approximation

We derive the fourth-order central finite-difference approximation for $\frac{d^2 f}{dx^2}$ using values of f at x_i, x_{i-1}, x_{i+1}, x_{i-2}, and x_{i+2}, assuming a uniform grid spacing Δx, as provided by the text.

We then expand $f(x)$ at the neighboring points around x_i using Taylor series:

$$\begin{aligned} f(x_{i+1}) &= f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f^{(4)}(x_i)}{4!}(\Delta x)^4 + \dots, \\ f(x_{i+2}) &= f(x_i) + 2f'(x_i)\Delta x + \frac{4f''(x_i)}{2!}(\Delta x)^2 + \frac{8f'''(x_i)}{3!}(\Delta x)^3 + \frac{16f^{(4)}(x_i)}{4!}(\Delta x)^4 + \dots, \\ f(x_{i-1}) &= f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f^{(4)}(x_i)}{4!}(\Delta x)^4 - \dots, \\ f(x_{i-2}) &= f(x_i) - 2f'(x_i)\Delta x + \frac{4f''(x_i)}{2!}(\Delta x)^2 - \frac{8f'''(x_i)}{3!}(\Delta x)^3 + \frac{16f^{(4)}(x_i)}{4!}(\Delta x)^4 - \dots. \end{aligned}$$

As a further step, we add the symmetric spatial terms to cancel the odd derivatives:

$$\begin{aligned} f(x_{i+1}) + f(x_{i-1}) &= 2f(x_i) + \frac{2f''(x_i)}{2!}(\Delta x)^2 + \frac{2f^{(4)}(x_i)}{4!}(\Delta x)^4 + \dots, \\ f(x_{i+2}) + f(x_{i-2}) &= 2f(x_i) + \frac{8f''(x_i)}{2!}(\Delta x)^2 + \frac{32f^{(4)}(x_i)}{4!}(\Delta x)^4 + \dots. \end{aligned}$$

To approximate $\frac{d^2 f}{dx^2}$, we form a weighted sum of these terms:

$$\frac{d^2 f}{dx^2} = a[f(x_{i+1}) + f(x_{i-1})] + b[f(x_{i+2}) + f(x_{i-2})] + cf(x_i),$$

where a, b, c are coefficients to be determined.
We substitute the Taylor expansions into S:

$$\begin{aligned} \frac{d^2 f}{dx^2} &= 2af(x_i) + 2bf(x_i) + cf(x_i) \\ &+ \left(\frac{2a}{2!}(\Delta x)^2 + \frac{8b}{2!}(\Delta x)^2\right) f''(x_i) \\ &+ \left(\frac{2a}{4!}(\Delta x)^4 + \frac{32b}{4!}(\Delta x)^4\right) f^{(4)}(x_i) + \dots \end{aligned}$$

Match coefficients for $f(x_i), f''(x_i)$, and higher-order terms to ensure: The coefficients are determined by matching terms in the Taylor series expansions:

1. Coefficient of $f(x_i)$:

$$2a + 2b + c = 0$$

2. Coefficient of $f''(x_i)$: This should equal $\frac{1}{(\Delta x)^2}$, so:

$$a \cdot \frac{2(\Delta x)^2}{2!} + b \cdot \frac{8(\Delta x)^2}{2!} = \frac{1}{(\Delta x)^2}$$

   Simplifying:

$$a + 4b = 6$$

3. Coefficient of $f^{(4)}(x_i)$: This term should be eliminated to ensure fourth-order accuracy:

$$a \cdot \frac{2(\Delta x)^4}{4!} + b \cdot \frac{32(\Delta x)^4}{4!} = 0$$

   Simplifying:

$$a + 16b = 0$$

After solving the system of equations, the coefficients are:

$$a = 16, \quad b = -1, \quad c = -30.$$

We substitute these coefficients to get the fourth-order finite-difference approximation for $\frac{d^2 f}{dx^2}$:

$$\frac{d^2 f}{dx^2} \approx \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12(\Delta x)^2}.$$

1.b Second-order one-sided finite-difference approximation for $\frac{\partial^2 u}{\partial x^2}$

The backward second-order one-sided finite difference approximation for the second derivative $\frac{d^2 f}{dx^2}$ is derived as follows. Expand $f(x_{i-1})$ and $f(x_{i-2})$ around x_i using Taylor series:

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2}(\Delta x)^2 - \frac{f^{(3)}(x_i)}{6}(\Delta x)^3 + O((\Delta x)^4),$$

$$f(x_{i-2}) = f(x_i) - 2f'(x_i)\Delta x + 2 \cdot \frac{f''(x_i)}{2}(\Delta x)^2 - \frac{2 \cdot f^{(3)}(x_i)}{6}(\Delta x)^3 + O((\Delta x)^4).$$

We then subtract the first expansion from the second expansion:

$$f(x_{i-2}) - 2f(x_{i-1}) + f(x_i) = \left(f(x_i) - 2f'(x_i)\Delta x + \frac{2f''(x_i)}{2}(\Delta x)^2 + \dots \right) - 2\left(f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2}(\Delta x)^2 + \dots \right) + f(x_i).$$

Simplifying:

$$f(x_{i-2}) - 2f(x_{i-1}) + f(x_i) = \frac{f''(x_i)}{2}(\Delta x)^2 + O((\Delta x)^3).$$

Thus, the backward second-order one-sided finite difference approximation for the second derivative is:

$$\frac{d^2 f}{dx^2} \approx \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{(\Delta x)^2}.$$

This method is second-order accurate, with the leading error term proportional to $O((\Delta x)^2)$. It is important to note that this process can be applied to the forward difference scheme as well, with the same accuracy. In this case, the second derivative would be approximated as:

$$\frac{d^2 f}{dx^2} \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2}.$$

1.c Situations in which we need one-sided approximations

Situations in which we need one-sided approximations include the discretization of convective terms, which are challenging to approximate with CDS due to instability. Another case could be the discretization of an hyperbolic problem, such as the example we studied in the stability lecture of the hyperbolic transport equation. In that case, BDS was way more stable than CDS.

2 Finite difference approximation of the third and mixed derivatives

2.a Second-order finite-difference approximation for $\frac{\partial^3 \Psi}{\partial y^3}$

We start by recalling the central difference formula for the second derivative:

$$\frac{\partial^2 \Psi}{\partial y^2} \approx \frac{\Psi(i+1) - 2\Psi(i) + \Psi(i-1)}{\Delta y^2}. \tag{1}$$

To approximate the third derivative, we take the central difference of the second derivative:

$$\frac{\partial^3 \Psi}{\partial y^3} \approx \frac{\frac{\partial^2 \Psi}{\partial y^2}(i+1) - \frac{\partial^2 \Psi}{\partial y^2}(i-1)}{2\Delta y}. \tag{2}$$

Substitute the expression for the second derivative into this formula. First, write $\frac{\partial^2\Psi}{\partial y^2}(i+1)$ and $\frac{\partial^2\Psi}{\partial y^2}(i-1)$ as:

$$\frac{\partial^2\Psi}{\partial y^2}(i+1) \approx \frac{\Psi(i+2) - 2\Psi(i+1) + \Psi(i)}{\Delta y^2}, \tag{3}$$

$$\frac{\partial^2\Psi}{\partial y^2}(i-1) \approx \frac{\Psi(i) - 2\Psi(i-1) + \Psi(i-2)}{\Delta y^2}. \tag{4}$$

Substituting these into the expression for the third derivative:

$$\frac{\partial^3\Psi}{\partial y^3} \approx \frac{\frac{\Psi(i+2)-2\Psi(i+1)+\Psi(i)}{\Delta y^2} - \frac{\Psi(i)-2\Psi(i-1)+\Psi(i-2)}{\Delta y^2}}{2\Delta y}. \tag{5}$$

Combine the terms in the numerator:

$$\frac{\partial^3\Psi}{\partial y^3} \approx \frac{\Psi(i+2) - 2\Psi(i+1) + \Psi(i) - \Psi(i) + 2\Psi(i-1) - \Psi(i-2)}{2\Delta y^3}. \tag{6}$$

We simplify further, and we get the following result:

$$\frac{\partial^3\Psi}{\partial y^3} \approx \frac{\Psi(i+2) - 2\Psi(i+1) + 2\Psi(i-1) - \Psi(i-2)}{2\Delta y^3}. \tag{7}$$

2.b Second-order finite-difference approximation for $\frac{\partial^2\Psi}{\partial y \partial x}$

To derive the finite-difference approximation for the mixed derivative $\frac{\partial^2\Psi}{\partial x \partial y}$, we'll follow a similar step-by-step process as we did for the higher-order derivatives with respect to y. First, let's review the central difference formula for the partial derivative $\frac{\partial\Psi}{\partial y}$:

$$\frac{\partial\Psi}{\partial y} \approx \frac{\Psi(i+1,j) - \Psi(i-1,j)}{2\Delta y} \tag{8}$$

Here, i represents the grid index in the y-direction, and Δy is the grid spacing in the y-direction. Now, to get the mixed derivative $\frac{\partial^2\Psi}{\partial x \partial y}$, we need to differentiate this first derivative expression with respect to x:

$$\frac{\partial^2\Psi}{\partial x \partial y} \approx \frac{\frac{\partial\Psi}{\partial y}(i+1,j+1) - \frac{\partial\Psi}{\partial y}(i-1,j+1) - \frac{\partial\Psi}{\partial y}(i+1,j-1) + \frac{\partial\Psi}{\partial y}(i-1,j-1)}{4\Delta x \Delta y} \tag{9}$$

Substituting the central difference formula for $\frac{\partial\Psi}{\partial y}$, we get:

$$\frac{\partial^2\Psi}{\partial x \partial y} \approx \frac{(\Psi(i+1,j+1) - \Psi(i-1,j+1)) - (\Psi(i+1,j-1) - \Psi(i-1,j-1))}{4\Delta x \Delta y} \tag{10}$$

Simplifying the expression, the final second-order finite-difference approximation for the mixed derivative $\frac{\partial^2\Psi}{\partial x \partial y}$ is:

$$\frac{\partial^2\Psi}{\partial x \partial y} \approx \frac{\Psi(i+1,j+1) - \Psi(i-1,j+1) - \Psi(i+1,j-1) + \Psi(i-1,j-1)}{4\Delta x \Delta y} \tag{11}$$

3 Steady temperature distribution of an alluminium bar

3.a Non-dimensional form of the heat equation

The time-dependent heat equation in 1D is:

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2}$$

In this formulation, we have replaced the temperature T with the function $u(x,t)$.

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

where α is the thermal diffusivity defined as:

$$\alpha = \frac{\lambda}{c\rho}$$

To derive the non-dimensional form of the heat equation we have to introduce the dimensionless variables $\hat{x}$, $\hat{t}$, and $\hat{u}$, respectively, for position, time and temperature:

$$\hat{x} = \frac{x}{L^*}, \quad \hat{t} = \frac{t}{T^*}, \quad \hat{u}(\hat{x}, \hat{t}) = \frac{u(x,t)}{U^*}$$

Since the characteristic length, time, and temperature are L^*, T^*, and U^*, respectively, with dimensions:

$$[L^*] = L, \quad [T^*] = T, \quad [U^*] = U.$$

The choice for the characteristic length is $L^* = l$, the length of the rod, in this way, while x is in the range $0 < x < l$, $\hat{x}$ is in the range $0 < \hat{x} < 1$. In the following passages taken from the source [3], we have:

$$\frac{\partial u}{\partial t} = \frac{\partial \hat{u}}{\partial \hat{t}} \cdot \frac{U^*}{T^*} = \frac{U^*}{T^*} \frac{\partial \hat{u}}{\partial \hat{t}},$$
$$\frac{\partial u}{\partial x} = \frac{\partial \hat{u}}{\partial \hat{x}} \cdot \frac{U^*}{L^*} = \frac{U^*}{L^*} \frac{\partial \hat{u}}{\partial \hat{x}},$$
$$\frac{\partial^2 u}{\partial x^2} = \frac{U^*}{L^*} \cdot \frac{1}{L^*} \frac{\partial^2 \hat{u}}{\partial \hat{x}^2} = \frac{U^*}{L^2} \frac{\partial^2 \hat{u}}{\partial \hat{x}^2}.$$

Substituting these into the heat equation gives:

$$\frac{U^*}{T^*} \frac{\partial \hat{u}}{\partial \hat{t}} = \alpha \frac{U^*}{L^2} \frac{\partial^2 \hat{u}}{\partial \hat{x}^2}.$$

To make the PDE simpler, we choose for the characteristic time $T^* = \frac{L^2}{\alpha}$, so that the equation becomes:

$$\frac{\partial \hat{u}}{\partial \hat{t}} = \frac{\partial^2 \hat{u}}{\partial \hat{x}^2}$$

The most important non-dimensional number for this problem is the Fourier number wich characterizes the ratio of conductive heat transfer to thermal storage and is used to analyze heat conduction in this context.

$$Fo = \frac{\lambda t}{\rho c_p L^2}$$

3.b Dimensional form of the equation for the numerical solution

For our numerical solution we want to use the dimensional form of the equation because in this way, we can maintain physical units while controlling stability numerically. For example, the Explicit Euler method for time-stepping and central difference scheme for space gives:

$$\rho c_p \frac{T_i^{n+1} - T_i^n}{\Delta t} = \lambda \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} + q$$

The time step Δt and spatial interval Δx must satisfy the Von Neumann stability criterion:

$$\Delta t \leq \frac{\rho c_p (\Delta x)^2}{2\lambda}$$

In this way, it is possible to define a grid in terms of the effective length L and the time interval Δt, thereby maintaining physical units. The values of ρ, c_p, λ, and q can be directly substituted into the discretized equation in their dimensional form, and the boundary conditions can be applied directly. Furthermore, once the numerical solution is computed, the temperature at all nodes T_i^n is obtained directly in Kelvin, preserving dimensional consistency. While non-dimensionalization may simplify some analyses, it is not strictly necessary for straightforward numerical implementation.

3.c Discretization using a second-order central differende scheme in space

At boundaries, it is not possible to use the central difference formula directly because one or both adjacent points fall outside the domain. The loop we implemented on python skips the first and last point because the second derivative cannot be computed at the boundaries using CDS without additional information. Boundary conditions can be added separately after calculating the second derivative for the internal elements.

References

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