

INTEGRATION OF PARTIAL DIFFERENTIAL EQUATIONS (1)

Objectives:

- ▶ Integrate a diffusion-like (first-order in time) partial differential equation numerically;
- ▶ Derive analytically the recurrence relation of a numerical solver from a partial differential equation;
- ▶ Implement the FTCS scheme;
- ▶ Implement the Crank-Nicolson scheme;
- ▶ Set up periodic boundary conditions;
- ▶ Set up boundary conditions involving the spatial derivatives of the solution.

No list manipulation is allowed in this tutorial!

I. Cooling of a ball

We consider a ball of radius R . At $t = 0$, we take it out of a oven where it was at uniform temperature T_i and we suspend it in the air at temperature T_a . We assume that the temperature field T in the ball is isotropic (*i.e.*, it only depends on r in spherical coordinates and on t). Under this assumption, the temperature profile verifies the following set of equations:

$$\begin{cases} \frac{\partial T}{\partial t} = D \Delta T = \frac{D}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right), \\ T(r, 0) = T_i, \\ -\lambda \frac{\partial T}{\partial r}(R, t) = \alpha [T(R, t) - T_a], \end{cases} \quad (1)$$

where D is the diffusion coefficient in the ball, λ its thermal conductivity, and α the Newton convection coefficient at the air/ball interface.

We define $\theta = T - T_a$, $x = r/R$, $\tau = Dt/R^2$, $\theta_i = T_i - T_a$, and $c = \alpha R/\lambda$. We can then transform Eq. (1) into a non-dimensionalized system of equations:

$$\begin{cases} \frac{\partial \theta}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x} \left(x^2 \frac{\partial \theta}{\partial x} \right), \\ \theta(x, 0) = \theta_i, \\ \frac{\partial \theta}{\partial x}(1, \tau) = -c \theta(1, \tau). \end{cases} \quad (2)$$

Question 1: We want to solve Eq. (2) using a FTCS scheme. We discretize space with a mesh size δ and time with a time step h : $x_j = j\delta$ ($j \in \llbracket 0, M \rrbracket$ with $M\delta = 1$) and $\tau_n = nh$ ($n \in \llbracket 0, N \rrbracket$).

- a. Show analytically that the discretized version of the spatial derivative reads, for $j \in \llbracket 1, M \rrbracket$,

$$\left. \frac{\partial}{\partial x} \left(x^2 \frac{\partial \theta}{\partial x} \right) \right|_j = \frac{x_{j+1/2}^2 (\theta_{j+1}^n - \theta_j^n) - x_{j-1/2}^2 (\theta_j^n - \theta_{j-1}^n)}{\delta^2}, \quad (3)$$

with $x_{j\pm 1/2} = (j \pm 1/2)\delta$.

- b. Deduce the recurrence relation, *i.e.*, the relation between θ_j^{n+1} and the $\{\theta_k^n\}_{k \leq M}$'s for $j \in \llbracket 1, M-1 \rrbracket$.

- c. We now need to set up the boundary conditions, *i.e.*, to derive the recurrence relation for $j = 0$ and $j = M$. For $j = 0$, the recurrence relation reads (the derivation of this formula is not required):

$$\theta_0^{n+1} = \theta_0^n + \frac{6h}{\delta^2} (\theta_1^n - \theta_0^n). \quad (4)$$

For $j = M$, show that the discretized version of the boundary condition at $x = 1$ reads:

$$\theta_{M+1}^n = \theta_{M-1}^n - 2c\delta\theta_M^n. \quad (5)$$

Derive eventually the recurrence relation for $j = M$ by injecting Eq. (5) into Eq. (3).

Question 2: Define a function `FTCS_step(theta, x, c, delta, h)` which takes as an input the array `theta` containing all the values $\{\theta_j^n\}_{j \leq M}$ at step n , the array `x` containing all the values $\{x_j\}_{j \leq M}$, the constant c , the mesh size δ and the time step h , and modifies in place the array `theta` such that it contains the values $\{\theta_j^{n+1}\}_{j \leq M}$ at step $n + 1$.

Hint: To avoid a loop, you can use the function `roll` of NumPy.

Question 3: We perform an experiment with a ball made of granite, for which $\lambda = 3 \text{ W/m/K}$, $D = 1.6 \cdot 10^{-6} \text{ m}^2/\text{s}$ and $R = 10 \text{ cm}$. Initially, the ball is at temperature $T_i = 800^\circ\text{C}$, while the air is at temperature $T_a = 20^\circ\text{C}$. We take the Newton convection coefficient $\alpha = 20 \text{ W/m}^2/\text{K}$.

- How should you choose h and δ for the algorithm to work? You can set δ to a reasonable value, *e.g.*, $\delta = 0.01$, and then find a value of h for which the algorithm works.
- Integrate the PDE numerically and plot the temperature profile $T(r, t)$ [not $\theta(x, \tau)$!] every 15 minutes on the same graph.
- Comment on what you see.

Question 4: We reproduce the experiment with a ball of radius $R = 5 \text{ cm}$ and another ball of radius $R = 1 \text{ m}$. Integrate the PDE numerically again and plot the temperature profile $T(r, t)$ at 15 different times between 0 and 2 hours on the same graph. Confront with the previous experiment.

II. Free quantum particle

We want to describe the evolution of a free quantum particle of mass m in 1D initially described by a Gaussian wave packet

$$\psi(x, 0) = \frac{1}{\pi^{1/4} \sqrt{\sigma}} e^{-x^2/(2\sigma^2)} e^{ikx}, \quad (6)$$

with $k = 2\pi/\lambda$, $\lambda = 5 \cdot 10^{-11} \text{ m}$, and $\sigma = 10^{-10} \text{ m}$. The evolution of the wavefunction $\psi(x, t)$ is given by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}, \quad (7)$$

where the mass of the particle is $m = 9.109 \cdot 10^{-31} \text{ kg}$. To avoid finite-size effects and to mimic the propagation of the particle in infinite space, we adopt periodic boundary conditions for the wavefunction and we integrate on a space domain $[-L/2, L/2]$ with L chosen such that $L \gg \sigma$ and such that the initial condition verifies the periodic boundary conditions. We thus choose $L = 10^{-8} \text{ m}$. We recall that $\hbar = 1.05457182 \cdot 10^{-34} \text{ kg.m}^2/\text{s}$.

Question 1: For Schrödinger equation, the FTCS scheme is unstable. We thus propose to solve the above equation using a Crank-Nicolson scheme. We discretize space and time as follows: $x_j = -L/2 + j\delta$ ($j \in \llbracket 0, M \rrbracket$) with $M\delta = L$ and $t_n = n\epsilon$ ($n \in \llbracket 0, N \rrbracket$).

- Derive analytically the recurrence relations between the $\{\psi_j^{n+1}\}_{j \leq M}$'s and the $\{\psi_j^n\}_{j \leq M}$'s.

- b. By enforcing the periodic boundary conditions, show analytically that the recurrence relations can be recast into the linear system

$$A\Psi = B, \quad \text{with} \quad \Psi = \begin{pmatrix} \psi_0^{n+1} \\ \vdots \\ \psi_{M-1}^{n+1} \end{pmatrix}, \quad (8)$$

with A a $M \times M$ matrix and B a vector column of size M to be determined.

Question 2: Use the above scheme to solve the Schrödinger equation up to $t_f = 8.10^{-16}$ s. You can take $\epsilon = 1.10^{-19}$ s and $\delta = 5.10^{-12}$ m. Plot the real part of the wavefunction for $t = 0$ s, $t = 2.10^{-16}$ s, $t = 4.10^{-16}$ s, $t = 6.10^{-16}$ s and $t = 8.10^{-16}$ s on the same graph. Comment.