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:

$$\begin{cases} \dfrac{\partial T}{\partial t} = D\Delta T = \dfrac{D}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial T}{\partial r}\right), \\ T(r,0) = T_\mathrm{i}, \\ -\lambda\dfrac{\partial T}{\partial r}(R,t) = \alpha\left[T(R,t) - T_\mathrm{a}\right], \end{cases} \tag{1}$$

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 $\theta = T - T_\mathrm{a}$, $x = r/R$, $\tau = Dt/R^2$, $\theta_\mathrm{i} = T_\mathrm{i} - T_\mathrm{a}$, and $c = \alpha R/\lambda$. We can then transform Eq. (1) into a non-dimensionalized system of equations:

$$\begin{cases} \dfrac{\partial \theta}{\partial \tau} = \dfrac{1}{x^2}\dfrac{\partial}{\partial x}\left(x^2\dfrac{\partial \theta}{\partial x}\right), \\ \theta(x,0) = \theta_\mathrm{i}, \\ \dfrac{\partial \theta}{\partial x}(1,\tau) = -c\,\theta(1,\tau). \end{cases} \tag{2}$$

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: $x_j = j\delta$ ($j \in [\![0,\, M]\!]$ with $M\delta = 1$) and $\tau_n = nh$ ($n \in [\![0,\, N]\!]$).

a. Show analytically that the discretized version of the spatial derivative reads, for $j \in [\![1,\, M]\!]$,

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

with $x_{j\pm1/2} = (j \pm 1/2)\delta$.

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

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):

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

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 $\lambda = 3\,\mathrm{W/m/K}$, $D = 1.6.10^{-6}\,\mathrm{m^2/s}$ and $R = 10\,\mathrm{cm}$. Initially, the ball is at temperature $T_\mathrm{i} = 800°\mathrm{C}$, while the air is at temperature $T_\mathrm{a} = 20°\mathrm{C}$. We take the Newton convection coefficient $\alpha = 20\,\mathrm{W/m^2/K}$.

a. 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.

b. Integrate the PDE numerically and plot the temperature profile $T(r,t)$ [not $\theta(x,\tau)$!] every 15 minutes on the same graph.

c. Comment on what you see.

Question 4: We reproduce the experiment with a ball of radius $R = 5\,\mathrm{cm}$ and another ball of radius $R = 1\,rmm$. 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

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

with $k = 2\pi/\lambda$, $\lambda = 5.10^{-11}\,\mathrm{m}$, and $\sigma = 10^{-10}\,\mathrm{m}$. The evolution of the wavefunction $\psi(x,t)$ is given by the time-dependent Schrödinger equation

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

where the mass of the particle is $m = 9.109.10^{-31}\,\mathrm{kg}$. 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 $L = 10^{-8}\,\mathrm{m}$. We recall that $\hbar = 1.05457182.10^{-34}\,\mathrm{kg.m^2/s}$.

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: $x_j = -L/2 + j\delta$ ($j \in [\![0,\, M]\!]$ with $M\delta = L$) and $t_n = n\epsilon$ ($n \in [\![0,\, N]\!]$).

a. 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

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

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 $t_\mathrm{f} = 8.10^{-16}\,\mathrm{s}$. You can take $\epsilon = 1.10^{-19}\,\mathrm{s}$ and $\delta = 5.10^{-12}\,\mathrm{m}$. Plot the real part of the wavefunction for $t = 0\,\mathrm{s}$, $t = 2.10^{-16}\,\mathrm{s}$, $t = 4.10^{-16}\,\mathrm{s}$, $t = 6.10^{-16}\,\mathrm{s}$ and $t = 8.10^{-16}\,\mathrm{s}$ on the same graph. Comment.