TUTORIAL: INTEGRATION OF PARTIAL DIFFERENTIAL EQUATIONS

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 $T_{\rm i}$ and we suspend it in the air at temperature $T_{\rm a}$. 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 IVP and BVP

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

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

Question 1: We define $\theta = T - T_{\rm a}$, $x = r/R$, $\tau = Dt/R^2$ and $c = \alpha R/\lambda$. Show analytically that Eq. (1) becomes

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

Question 2: We want to solve the above IVP and BVP using a FTCS scheme. We discretize space and time as follows: $x_j = j\delta$ ($j \in [\![0,\, M]\!]$ with $M\delta = 1$) and $\tau_n = nh$ ($n \in [\![0,\, N]\!]$).

a. Derive analytically the recurrence relation between θ_j^{n+1} and the θ_j^n's for $j \geq 1$. Do not forget to enforce the boundary condition.

b. For $j = 0$, the recurrence relation reads (the derivation of this formula is not required):

$$\theta_0^{n+1} = \theta_0^n + \frac{6h}{\delta^2}\left(\theta_1^n - \theta_0^n\right). \tag{3}$$

Implement the FTCS scheme.

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 $T_{\rm i} = 800^\circ\mathrm{C}$, while the air is at temperature $T_{\rm a} = 20^\circ\mathrm{C}$. We take the Newton convection coefficient $\alpha = 20\,\mathrm{W/m^2/K}$. Integrate the PDE numerically and plot the temperature profile $T(r,t)$ [not $\theta(x,\tau)$!] at 15 different times between 0 and 2 hours on the same graph. Comment.

Question 4: We reproduce the experiment with a ball made of gold, for which $\lambda = 315\,\mathrm{W/m/K}$, $D = 1.3.10^{-4}\,\mathrm{m^2/s}$ and $R = 10\,\mathrm{cm}$. Integrate the PDE numerically, plot the temperature profile $T(r,t)$ at 15 different times between 0 and 2 hours on the same graph, and confront with the previous experiment.

Question 5 (bonus): The exact analytic solution to Eq. (1) can be derived:

$$T(r,t) = T_\mathrm{a} + \frac{2\alpha R^2 (T_\mathrm{i} - T_\mathrm{a})}{\lambda r} \sum_{n=1}^{+\infty} (-1)^{n+1} \frac{\sqrt{\beta_n^2 + \left(\frac{\alpha R}{\lambda} - 1\right)^2}}{\beta_n \left[\beta_n^2 + \frac{\alpha R}{\lambda}\left(\frac{\alpha R}{\lambda} - 1\right)\right]} \sin\left(\frac{\beta_n r}{R}\right) e^{-\beta_n^2 D t / R^2}, \tag{4}$$

where β_n is the solution to the equation

$$\left(\frac{\alpha R}{\lambda} - 1\right) \tan\beta + \beta = 0 \tag{5}$$

in the range $[(n-1)\pi,\, (n-1/2)\pi]$ if $\alpha R/\lambda < 1$, and in the range $[(n-1/2)\pi,\, n\pi]$ if $\alpha R/\lambda > 1$. Compare the results of the two previous questions with this exact solution by plotting on the same graph the numerical solution and the exact solution at 15 different times between 0 and 2 hours.

II. Electrostatic potential between conductors

We want to determine the electrostatic potential in a square of 1 meter long delimited by 4 conductors at fixed electrostatic potential, see Fig. 1. We assume that the space between the conductors is empty.

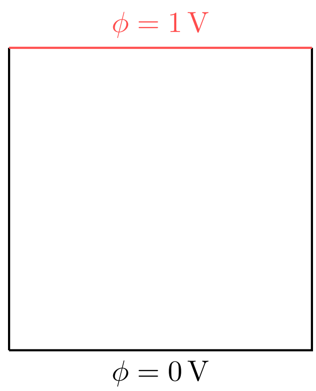

Figure 1: **Electrostatic problem in vacuum to solve.** An empty space is delimited by 4 conductors. Three of them (in black) are at zero potential, the last one (in pink) is at a potential of 1 volt.

The BVP to solve is thus (with distances expressed in meters, and the potential expressed in volt):

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0, \quad \phi(0,y) = 0, \quad \phi(1,y) = 0, \quad \phi(x,0) = 0, \quad \phi(x,1) = 1. \tag{6}$$

We want to compare the speed of resolution and the accuracy of different methods. For all methods, we describe space as follows: $x_j = j\delta$, $y_k = k\delta$, with δ the discretization step size, $j,k \in [\![1,\, M-1]\!]$, and $M\delta = 1$.

Question 1: Solve Eq. (6) using the Jacobi method, and plot a heat map of the solution. How long does it take for the method to converge?

Question 2: Solve Eq. (6) using the Gauss-Seidel method, and plot a heat map of the solution. How long does it take for the method to converge?

Question 3: Solve Eq. (6) using the overrelaxation method, and plot a heat map of the solution. How long does it take for the method to converge?

Question 4: The exact solution to Eq. (6) is known and reads:

$$\phi(x,y) = \frac{4}{\pi} \sum_{m=0}^{+\infty} \frac{\sin[(2m+1)\pi x] \sinh[(2m+1)\pi y]}{(2m+1)\sinh[(2m+1)\pi]}. \tag{7}$$

We define the relative error between the numerical solution and the exact solution as

$$e = \frac{\sum_{j,k} |\phi_{jk} - \phi(x_j, y_k)|}{\sum_{j,k} |\phi(x_j, y_k)|}, \tag{8}$$

with .

a. For the three methods implemented above, compute e.

b. Which solution is a good compromise between computation time and accuracy?

III. 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

$$\psi(x, 0) = \frac{1}{\pi^{1/4}\sqrt{\sigma}} e^{-x^2/(2\sigma^2)} e^{\mathrm{i}kx}, \tag{9}$$

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

$$\mathrm{i}\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}, \tag{10}$$

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: We want to solve the above IVP and BVP 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 $t_n = nh$ ($n \in [\![0,\, N]\!]$).

a. Derive analytically the recurrence relations between the ϕ_j^{n+1}'s and the ϕ_j^n's. Do not forget to enforce the boundary condition.

b. Show analytically that the recurrence relations can be recast into the linear system

$$A\Phi = B, \quad \text{with} \quad \Phi = \begin{pmatrix} \phi_0^{n+1} \\ \vdots \\ \phi_{M-1}^{n+1} \end{pmatrix}, \tag{11}$$

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 $h = 2.10^{-18}\,\mathrm{s}$ and $\delta = 5.10^{-12}\,\mathrm{m}$. Plot the real part of the wavefunction for $t = 2.10^{-16}\,\mathrm{s}$, $t = 4.10^{-16}\,\mathrm{s}$, $t = 6.10^{-16}\,\mathrm{s}$ and $t = 8.10^{-16}\,\mathrm{s}$ on the same graph. Comment.

Question 3 (bonus): Solve Schrödinger equation for $L = 5.10^{-9}\,\mathrm{m}$ up to $t_\mathrm{f} = 1.10^{-16}\,\mathrm{s}$ and plot the probability density $|\psi(x, t_\mathrm{f})|^2$ at the end of the simulation. Confront with the exact solution

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}\varsigma(t)} e^{-x^2/\varsigma(t)^2}, \quad \varsigma(t) = \sigma\sqrt{1 + \left(\frac{\hbar t}{m\sigma^2}\right)^2}, \tag{12}$$

and comment. You can do this for the following values of parameters:

- $h = 2.10^{-20}\,\mathrm{s}$ and $\delta = 2.10^{-12}\,\mathrm{m}$;
- $h = 2.10^{-19}\,\mathrm{s}$ and $\delta = 2.10^{-12}\,\mathrm{m}$;
- $h = 2.10^{-19}\,\mathrm{s}$ and $\delta = 5.10^{-12}\,\mathrm{m}$;
- $h = 2.10^{-18}\,\mathrm{s}$ and $\delta = 5.10^{-12}\,\mathrm{m}$.

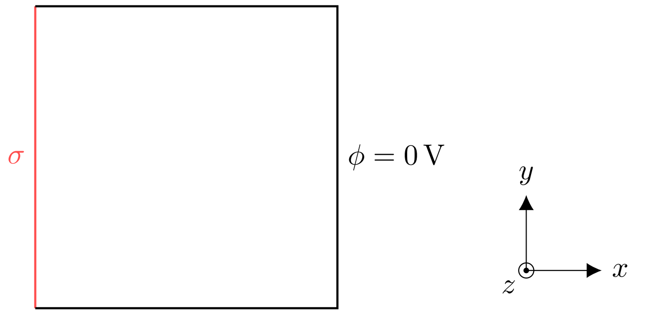

Figure 2: **Electrostatic problem in a salty solution to solve.** A solution with ions is delimited by 4 conductors. Three of them (in black) are at zero potential, the last one (in pink) is charged with a uniform charge density σ.

IV. Electrostatic potential in a salty solution

We want to determine the electrostatic potential in a solution in the vicinity of a charged wall of uniform charge density σ, see Fig. 2. We assume that the problem is translationally invariant in the z-direction and that the system is closed by three conducting walls of length 1 meter maintained at zero electrostatic potential. The solution is a salty water solution containing positive ions of charge $+q$ and negative ions of charge $-q$, with $q = 1.602176634.10^{-19}\,\mathrm{C}$ the elementary charge. The electrostatic potential now verifies a Poisson equation

$$\Delta\phi = -\frac{\rho}{\epsilon_0\epsilon_\mathrm{r}}, \tag{13}$$

with $\epsilon_0 = 8.85418782.10^{-12}\,\mathrm{F/m}$ the vacuum permittivity and $\epsilon_\mathrm{r} = 80.10$ the relative permittivity of water. The charge density ρ depends on the potential itself via the Boltzmann distribution at temperature T:

$$\rho = \rho_+ + \rho_-, \quad \rho_\pm = \pm n_0 q\, e^{\mp e\phi/(k_\mathrm{B}T)}, \tag{14}$$

with $k_\mathrm{B} = 1.380649.10^{-23}\,\mathrm{J/s}$ the Boltzmann constant and n_0 the number of ions per unit volume. We are thus left with the following BVP to solve:

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = \frac{2qn_0}{\epsilon_0\epsilon_\mathrm{r}}\sinh\left(\frac{q\phi}{k_\mathrm{B}T}\right), \quad \frac{\partial\phi}{\partial x}(0,y) = -\frac{\sigma}{\epsilon_0\epsilon_\mathrm{r}}, \quad \phi(1,y) = 0, \quad \phi(x,0) = 0, \quad \phi(x,1) = 0. \tag{15}$$

The above BVP is non-linear and we thus go step by step to find its solution numerically.

Question 1: We proceed similarly as in the lecture notes and we assume that the solution to the IVP and BVP

$$\frac{\partial\phi}{\partial t} = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} - \frac{2qn_0}{\epsilon_0\epsilon_\mathrm{r}}\sinh\left(\frac{q\phi}{k_\mathrm{B}T}\right) \tag{16}$$

converges to the solution to Eq. (15) when $t \to +\infty$. Derive analytically the recurrence relation for the FTCS scheme to solve Eq. (16) by discretizing space with a step size δ in the x-direction and in the y-direction, and by discretizing time with a step size h. Do not forget to enforce the boundary conditions.

Question 2: Implement the above FTCS scheme for $n_0 = 10^{10}\,\mathrm{m}^{-3}$, $\sigma = 10^{-9}\,\mathrm{C/m}^2$, and $T = 350\,\mathrm{K}$ (you are generalizing the Jacobi method to a non-linear PDE!). You can take $\delta = 5.10^{-3}\,\mathrm{m}$ and you must choose a small-enough time step h for the scheme to be stable. Integrate for N time steps until the solution converges to the stationary solution to Eq. (15) (you should give yourself a quantitative criterion to stop the iteration).

Question 3: Plot the heat map of the potential ϕ, and of the absolute value of the charge densities $|\rho_\pm|$. Comment.

Question 4: Repeat the resolution for $n_0 = 10^8\,\mathrm{m}^{-3}$ and plot the heat maps of ϕ and $|\rho_\pm|$. Confront with the result of the previous question and comment.