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_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 IVP and BVP

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

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

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

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

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 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 $T_\mathrm{i} = 800°\mathrm{C}$, while the air is at temperature $T_\mathrm{a} = 20°\mathrm{C}$. We take the Newton convection coefficient $\alpha = 20\,\mathrm{W/m^2/K}$. Integrate the PDE numerically and plot the temperature profile $T(r,t)$ [not $\theta(x,\tau)$!] at 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 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:

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

where β_n is the solution to the equation

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

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.

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.

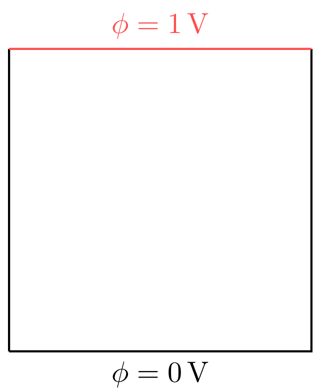

Figure 1: **Electrostatic problem in vacuum to solve.** An empty space is delimited by 4 conductors. Three of them (in black) are at zero potential, the last one (in pink) is at a potential of 1 volt.

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

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

We want to compare the speed of resolution and the accuracy of different methods.

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:

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

Compute the error between the numerical solution from the above three methods and the exact solution. 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

$$\psi(x,0) = \frac{1}{\pi^{1/4}\sqrt{\sigma}} e^{-x^2/(2\sigma^2)} e^{\mathrm{i}kx}, \tag{8}$$

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

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}, \tag{9}$$

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 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 that the recurrence relations can be recast into the linear system

$$A\Phi = B, \quad \text{with} \quad \Phi = \begin{pmatrix} \phi_0^{n+1} \\ \vdots \\ \phi_{M-1}^{n+1} \end{pmatrix}, \tag{10}$$

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

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}\varsigma(t)} e^{-x^2/\varsigma(t)^2}, \quad \varsigma(t) = \sigma\sqrt{1 + \left(\frac{\hbar t}{m\sigma^2}\right)^2} \tag{11}$$

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 $\delta = 5.10^{-12}\,\mathrm{m}$.

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

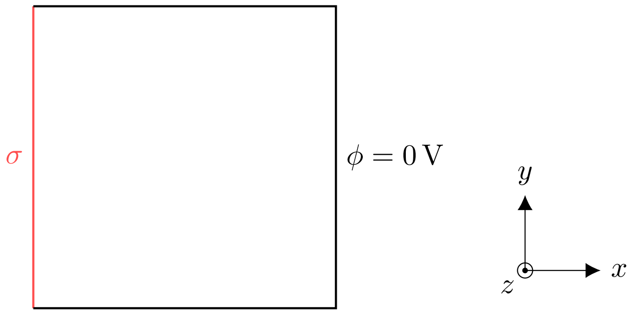

Figure 2: **Electrostatic problem in a salty solution to solve.** A solution with ions is delimited by 4 conductors. Three of them (in black) are at zero potential, the last one (in pink) is charged with a uniform charge density σ.

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

$$\Delta\phi = -\frac{\rho}{\epsilon_0\epsilon_\mathrm{r}}, \tag{12}$$

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:

$$\rho = \rho_+ + \rho_-, \quad \rho_\pm = \pm n_0 q\, e^{\mp e\phi/(k_\mathrm{B}T)}, \tag{13}$$

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:

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = \frac{2qn_0}{\epsilon_0\epsilon_\mathrm{r}}\sinh\left(\frac{q\phi}{k_\mathrm{B}T}\right), \quad \frac{\partial\phi}{\partial x}(0,y) = -\frac{\sigma}{\epsilon_0\epsilon_\mathrm{r}}, \quad \phi(1,y) = 0, \quad \phi(x,0) = 0, \quad \phi(x,1) = 0. \tag{14}$$

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

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

converges to the solution to Eq. (14) when $t \to +\infty$. Derive the recurrence relation for the FTCS scheme to solve Eq. (15) 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. (14) (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.