Partial Differential Equations

4.1 1D Heat Equation

We begin by considering a partial differential equation with only one spatial direction. This is basically a 1D boundary value once we discretise time.

Consider the one dimensional heat equation

$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial^2 f(x,t)}{\partial x^2}. \tag{4.1}$$

with boundary conditions $f(0,t) = 1$ and $\partial_x f(1,t) = 0$. This means that we keep the left end at temperature 1 and let no heat escape or enter at the right end.

The steady state of this equation is clearly $f(x,t) = 1$. We will consider the time evolution starting from $f(x,0) = e^{-5x}$.

Using implicit time discretisation we have

$$f_{t+\Delta t}(x) = f_t(x) + f''_{t+\Delta t}(x)\,\Delta t. \tag{4.2}$$

(a) Use a second order finite difference scheme to turn the above into a linear algebra problem using $N = 1000$ grid points.

(b) Solve the system using $\Delta t = 0.05$ for $t \in [0,3]$ and plot curves for $t \in \{0.0,\ 0.5,\ 1.0,\ 1.5,\ 2.0,\ 2.5,\ 3.0\}$.

(c) *(optional)* At each time step we actually have a very good guess for the solution. Namely, $x_{t+\Delta t}$ will not not be very much different from

x_t assuming Δt is small. Some solvers iterate towards a solution and they can be given an initial guess. Use `scipy.sparse.linalg.bicg` to iteratively solve for $x_{t+\Delta t}$ using `x0` $= x_t$.

4.2 2D Heat Equation

Hint: The results of exercise 1.3(d–) are useful in this exercise.

In this exercise we will consider the 2D heat equation:

$$\frac{\partial f(\boldsymbol{x})}{\partial t} = c\nabla^2 f(\boldsymbol{x}) + s(\boldsymbol{x}). \tag{4.3}$$

Here $f(\boldsymbol{x})$ is the temperature field, c is the heat conductivity, and $s(\boldsymbol{x})$ is a source (or sink, if negative) of heat. We take $c = 1$.

We will begin by taking $s(\boldsymbol{x}) = 0$ and look at the steady state. In this case the heat equation becomes Laplace's equation

$$\nabla^2 f(\boldsymbol{x}) = 0. \tag{4.4}$$

The solution to this equation is the temperature distribution after a long time. We will begin by considering a 2D square whose edges are kept at fixed temperatures:

$$f(\boldsymbol{x}) = \begin{cases} 2 & \text{on the left edge} \\ 1 & \text{on the top edge} \\ 0 & \text{on the bottom edge} \\ 1 & \text{on the right edge} \end{cases} \tag{4.5}$$

These are *Dirichlet* boundary conditions.

(a) Solve Eq. (4.4) with the above boundary conditions by forming a finite difference matrix and using `scipy.linalg.solve` or `scipy.sparse.linalg.spsolve` (faster). Use a square grid with $N = 50$ points along each direction and $\Delta x = 0.1$. Ignore issues that arise due to conflicting boundary conditions at the corners. Plot the result.
Hint: if you use the ordering defined in Exercise 1.3 you can use `x` and `y` of that exercise to locate the rows in your Laplacian matrix that correspond to boundary points.
Hint: You can use `imshow(res.reshape(N, N), origin='lower')` to plot your result.

(b) *(optional)* Change the top edge boundary condition to Neumann: $\partial_y f(\boldsymbol{x}) = 0$ and solve the equation again. Plot the result.

After this warmup (pun?) we will move on to the full heat equation. We will simulate the heating of an electrical stove. Define the field

$$s(\boldsymbol{x}) = \begin{cases} 1 & \text{if } 0.8 < r(\boldsymbol{x}) < 1.2 \\ 0 & \text{otherwise,} \end{cases} \tag{4.6}$$

where r is the distance to the center of the domain.

(c) Solve Eq. (4.3) for $t \in [0, 1.5]$ using $\Delta t = 0.01$ with the same discretisation of space as used above. Take $f(\boldsymbol{x}, t) = 0$ as the boundary conditions on all edges and initial condition $f(\boldsymbol{x}, 0) = 0$.

(d) Plot a series of images/an animation of the simulation using a suitable color mapping (e.g. `imshow(..., vmin=0, vmax=0.25, cmap='hot')`).

(e) *(optional)* What does our current boundary condition correspond to? Would it be better to use a (perhaps nonzero) Neumann boundary condition? What about a Robin boundary condition of the form $\partial_{\boldsymbol{x}} f(\boldsymbol{x}, t) = \alpha[f(\boldsymbol{x}, t) - f_0]$?

(f) *(optional)* We are modelling a stove as a 2D system, but in reality heat can also escape in the third dimension. Could we change the PDE to approximately account for this without moving to a full 3D simulation?

4.3 Shade sail

Independent exercise

We are designing a square sun sail for a Danish garden. It rains a lot in Denmark, so to ensure that water can drip off easily, we decide to hang it by four ropes tied to the following points

$$\begin{cases} A = (-1, -1, -1), \\ B = (1, 1, -1), \\ C = (-1, 1, 1), \\ D = (1, -1, 1). \end{cases} \tag{4.7}$$

Our four ropes are tightly bound between A-C, A-D, B-C, B-D.

(a) Plot the four ropes in a 3D plot.
You can use `ax = plt.figure().add_subplot(projection='3d')` to make a 3D plot followed by `ax.plot(x, y, z)`.

The sail's shape will be determined by Laplace's equation

$$\nabla^2 f(x, y) = 0, \tag{4.8}$$

where f here represents the z-coordinate, which we solve on the square $x, y \in [-1,1] \times [-1,1]$. Our boundary conditions are Dirichlet and set by the fact that the sail is tied to the ropes.

(b) Write down the boundary conditions.

(c) Solve Eq. (4.8) with the boundary conditions.

(d) Plot your solution together with the ropes.
You can use[1] `ax.plot_surface(X, Y, Z, antialiased=False)`.

4.4 2D Atoms*

The time-independent Schrodinger equation is

$$\mathcal{H}\psi = E\psi, \tag{4.9}$$

where the Hamiltonian is

$$\mathcal{H} = -\nabla^2 + V(\boldsymbol{x}) \tag{4.10}$$

in some suitable, natural units.

In this exercise we consider how orbitals would have been if atoms were two-dimensional. We intend to find the wave-function of electrons surrounding a proton ("2D hydrogen"). In suitable units we therefore have[2]

$$V(\boldsymbol{x}) = -\frac{\alpha}{|\boldsymbol{x}|}, \tag{4.11}$$

[1]Note that 3D plotting in matplotlib is a bit buggy: objects do not always appear at the correct depth.

[2]There are good arguments that in 2D the Coulomb potential should be $V(\boldsymbol{x}) = \log|\boldsymbol{x}|$, but we choose to consider $1/|\boldsymbol{x}|$.