Laboratory 3

Rules

- You can submit this assignment in groups of up to four people.
- You are free to use the programming language of your liking.
- All answers must be thoroughly justified and must be submitted in a single .pdf file.
- Due date: 1 April 2024

1 Numerical solution of the heat equation

The goal of this workshop is to compute a numerical solutions to the following problem:

$$u_t = K u_{xx}, \quad \text{for } 0 < x < L \text{ and } 0 < t < T, \tag{1}$$

$$u(x,0) = \phi(x), \tag{2}$$

$$u(0,t) = u(L,t) = 0 \tag{3}$$

The rectangular domain is discretized into grid points (t_j, x_m) with uniform time step size $\Delta t = t_{j+1} - t_j$ and space mesh size $\Delta x = x_{m+1} - x_m$, for $m = 0, 1, \ldots, M$ and $j = 0, 1, \ldots, J$. We use the following approximations for the derivatives:

$$\frac{\partial u}{\partial t}(t_j, x_m) = \frac{u_{j+1,m} - u_{j,m}}{\Delta t}. \tag{4}$$

$$\frac{\partial^2 u}{\partial x^2}(t_j, x_m) = \frac{u_{j,m+1} - 2u_{j,m} + u_{j,m-1}}{\Delta x^2}. \tag{5}$$

Substituting these approximations in the PDE yields the following explicit numerical scheme

$$\mu u_{j,m+1} + (1 - 2\mu) u_{j,m} + \mu u_{j,m-1}, \quad \text{with } \mu = K\Delta t / \Delta x^2. \tag{6}$$

Task 1: Apply the von-Neumann stability analysis to determine for which values of μ the numerical scheme is stable.

Task 2: Consider the following specific problem

$$u_t = u_{xx}, \quad \text{for } 0 < x < \pi \text{ and } 0 < t < T, \tag{7}$$

$$u(0,t) = u(\pi,t) = 0, \tag{8}$$

$$u(x,0) = \phi(x) = \begin{cases} x, & \text{for } x \in (0, \pi/2). \\ \pi - x, & \text{for } x \in (\pi/2, \pi). \end{cases} \tag{9}$$

$$\tag{10}$$

The exact solution to this problem can be written as the following series

$$u(x,t) = \sum_{k=1}^{\infty} b_k \sin(kx) e^{-k^2 t}, \tag{11}$$

where $b_k = \frac{4(-1)^{(k+1)/2}}{\pi k^2}$, for k odd and zero for k even.

Using $\Delta x = \pi/20$ choose a suitable value for Δt and compute the numerical solution. Plot the solution at different times from 0 to $T = 3\pi^2/80$.

2 The heat kernel

In this section we give a probabilistic interpretation of the heat kernel.

A random walk (of a particle initially located at $x = 0$) is simply the sum of finitely many i.i.d random variables $X_1, \ldots, X_N$. Each random variable is a step from the previous position of the particle.

The size of the step is taken to be the variance of the random variable and the duration of the walk is the variance of the sum of all the random variables involved.

For this experiment we are going to take $X_i \sim \mathcal{N}(0, \Delta t)$, so each step is taken from a mean-zero normal distribution with variance Δt, so the size of each step is Δt.

Let $T = 1$ be the total duration of the random walk and assume that the size of each step is $\Delta t = 0.01$.

Task 3: What is the probability that at $T = 1$ the particle lies in the interval (a, b)?

Task 4: What is the value of the diffusion coefficient (the constant K) corresponding c to this case?

3 Monte Carlo method for the heat equation

Use a random number generator to sample N (make a sample of the order of 10^3) numbers from the uniform distribution on the interval $|x| \leq 1/2$.
Each point now undergoes a random walk exactly as explained above (note that the initial position of the walk is no longer at $x = 0$).

Task 5: Compute the probability of finding a point inside the interval (a, b) at $T = 1$. Note: you can matlab's histogram command to compute those probabilities by bin counting.

Task 6: Find and exact expression for the probability distribution of the particles at $T = 1$ and compare your results.