FYS3150

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Numerical solution to diffusion equation

1+1 dimensional problem, analytical solution

1+1 dimensional, numerical notes

In this project I will solve the 1+1 dimensional diffusion equation by Monte Carlo methods using Markov Chains. I will simulate the diffusion equation by programming the following random walk steps:

1. Set initial number of particles, N_0, that start at $x = 0$. This number will be conserved for $x = 0$ throughout the whole simulation.
2. Set up a vector, u, that contain positions of each individual particle. The positions will be split up into Nx different bins with width dx.
3. For each particle, draw a random number, r. If $r < 0.5$ then $pos_{new} = pos_{old} - l_0$ else $pos_{new} = pos_old + l_0$.
4. If a particle moves beyond $x = 1$, remove particle.
5. If a particle moves from $x = 0$, add a new at $x = 0$ to maintain N_0. In addition: If the move is negative, remove particle from vector.
6. Repeat 2-5 for all time steps until final time is reached.

I will implement two different algorithms. The first algorithm will have constant steplength

$$l_0 = \sqrt{2\Delta t}$$

and the other will have

$$l_0 = \sqrt{2\Delta t}\xi$$

Where ξ is a random number generated by a Gaussian distribution with mean value 0 and standard deviation $\frac{1}{\sqrt{2}}$

Analytical solution of 2+1 dimensional problem

We have seen before that the solution of a 1+1 dimensional problem is

$$u(x,t) = \sum_{n=1}^{\infty} \frac{-2}{\pi n} sin(n\pi x)e^{-n^2\pi^2 t} + x - 1$$

To find the solution for the 2+1 dimensional problem, I will use separation of variables for both $X(x)$, $Y(y)$ and $T(t)$. I need boundary conditions for X and Y and initial condition for T. The boundary conditions for X are given as

$$u(0,y,t) = 1, \quad u(1,y,t) = 0$$

The initial condition is given as

$$u(x,y,0) = 0, \quad 0 < x < 1$$

The boundary conditions for the Y-direction is not given, so I have to set them for myself. Since the synaptic cleft is finite, the concentration of ions must be reduced in the y-direction, so a guess for boundary conditions might be

$$u(x, 0, t) = u(x, 1, t) = 0$$