Exercise 6

FY8503 Advanced theoretical physics
Transport modelling with Stochastic differential equations

October 16, 2023

Problem 1

In this exercise, we will consider the "well-mixed condition" for a diffusion problem with variable diffusivity and reflecting boundaries. The diffusion equation for variable diffusivity is

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(K(x)\frac{\partial p}{\partial x}\right). \tag{1}$$

The well-mixed condition says that if the density is uniform (p = const), then the density should remain uniform, since $\frac{\partial p}{\partial x} = 0 \Rightarrow \frac{\partial p}{\partial t} = 0$. If an SDE model is to be equivalent with solving the diffusion PDE, then it must of course also satisfy this condition.

Task a

Find the SDE corresponding to Eq. (1).

Task b

Implement a solver for the SDE found above, with a reflecting boundaries at $x = 0$ and $x = 1$. Solve the SDE for a large number of particles, with initial uniform distribution between 0 and 1. Try with constant diffusivity, and with variable diffusivity $K(x) = K_0 + xK_1$, for some suitable values of K_0 and K_1. Run the model for sufficiently long time t to reach a "steady state" distribution (up to random fluctuations).

Ways of identifying the steady state can for example be to plot average particle position as a function of time, or to create a histogram of particle positions and take the RMS error relative to the theoretical uniform distribution, and plot this as a function of time.

Task c

With the linear diffusivity, run the simulation until steady state for a few different timesteps. Plot the error in the steady-state average particle position as a function of timestep.

Task d

Modify the diffusivity to make the derivative of the diffusivity zero at the boundary at $x = 0$. For example like this:

$$K(x) = \begin{cases} K_0 + xK_1 & \text{if} \quad x \geq h, \\ K_0 + \frac{K_1}{2}\left(h + \frac{x^2}{h}\right) & \text{if} \quad x < h. \end{cases} \tag{2}$$

Run the simulation until steady state with different timesteps, like in Task c, and see if the modified diffusivity makes a difference.

You can also try other modifications if you prefer, just make sure that $K(x) > 0$ everywhere, and that $\partial K/\partial x$ is continuous.