# Foundations of Multiscale Modelling: Kinetics. Homework 2. Diffusion and the first passage. Due 23:59 17 Feb.

February 8, 2022

## 1. Diffusion on a semi-infinite interval (7 points)

One of the most developed and useful frameworks for studying diffusion processes is based on the overdamped Fokker-Planck equation description,

$$\frac{\partial P(x,t)}{\partial t} = \frac{1}{\gamma}\frac{\partial}{\partial x}\left(\frac{\partial U(x)}{\partial x}P(x,t)\right) + \frac{\partial^2}{\partial x^2}\left(D(x)P(x,t)\right), \tag{1}$$

where $\gamma$ is the friction coefficient, $-\partial U(x)/\partial x = F(x)$ is the force produced by the potential $U(x)$, $D(x)$ is the diffusion coefficient and $P(x,t)$ is the particle density distribution.

(a) Find an analytic solution of the 1D Fokker-Planck equation on a semi-infinite interval $x \in [0,\infty)$ with the origin $x = 0$ being an adsorbing boundary, i.e. $P(0,t) = 0$ ($P(\infty,t) = 0$ as well. This is a so-called natural boundary condition). Assume that the initial condition is given by $P(x, t = 0) = \delta(x - x_0)$, the diffusion coefficient is $D = \text{const}$ and the constant drift $u$ is present in the system (i.e. $U(x) = u \cdot x$).

(b) Calculate the survival probability $S(t) = \int_0^\infty P(x,t)\,dx$, i.e. the probability that a boundary was not reached, and first-passage probability $\varphi_{FP}(t) = -\frac{dS(t)}{dt}$.

(c) Find asymptotic expressions for the quantities $S(t)$ and $\varphi_{FP}(t)$ for small and large times $t$. Expressions should be obtained in terms of elementary functions.

(d) Find the probability of being trapped (adsorbed) at the origin for the cases of $x_0 = 1$, $u = 0, \pm 1$ using the problem parameters described in (a).

(e) Simulate the overdamped Langevin equation which corresponds to Fokker-Planck equation (1) with the parameters given in (a). Compute the first-passage time density, survival probability, mean first-passage time and absorption probability. Assume that $x_0 = 1$ and $u = 1$ for your simulations.

*Hint* 1. The overdamped Langevin equation neglects any inertia effects and, thus, the acceleration of a particle is zero, $m\frac{dv}{dt} = 0$. The forces left are the random force, viscous friction and

potential forces. The velocity of a particle can be expressed as a time derivative of the position. For the system with a constant drift the overdamped Langevin equation reads,

$$\frac{dx}{dt} = -\frac{1}{\gamma}u + \frac{1}{\gamma}F_{rand}(t). \tag{2}$$

*Hint 2.* The simulation procedure is identical to the numerics from the problem 2 in the first homework, i.e. you need to implement a finite-difference scheme for the Langevin equation and use a generator of Gaussian distributed random variables.

*Hint 3.* The Langevin equation simulations require proper boundary conditions as a set of rules. In this problem the rule for an absorbing boundary condition is as follows. During the simulation you should stop any run once the position $x = 0$ is reached. Then update the first-passage time density and start a new run.

*Hint 4.* In this simulation all of the quantities can be obtained using the computed first-passage time density normalized to the number of runs.

## 2. Kramers formula (5 points)

(a) Consider a diffusion on an interval [0,1] with a reflecting boundary on the left and an adsorbing boundary on the right. Assume that the initial condition is given by $P(x, t = 0) = \delta(x - 0.25)$ and the potential has the following form,

$$U(x) = \begin{cases} \omega(x - 0.25)^2, & \text{if } 0 \leq x \leq 0.5. \\ \omega/8 - \omega(x - 0.75)^2, & \text{if } 0.5 \leq x \leq 1. \end{cases} \tag{3}$$

Find an estimation for the mean first-passage time (MFPT) from the Kramers formula.

(b) Write a program which computes the mean first-passage time by simulating a discrete jump process on a lattice. Keep in mind that the left boundary of the interval is reflecting while the right one is absorbing. The period of a lattice $\delta x$ should be relatively small. Use the Monte Carlo algorithm from the paper uploaded into the assignments folder as Doering.pdf (Eqs. 12-17 in the paper) for making decisions about jump directions according to values of the potential. Assume that the system is kept at constant temperature $k_B T = 1$. Compare the results with (a) for $\omega = 10, 20, 30$. Does the Kramers formula work well? Discuss an agreement between the simulation results and Kramers formula.

## 3. Numerical methods for Fokker-Planck equation* (2 points)

Write a program which implements a finite-difference scheme for solving the Fokker-Planck equation with the harmonic potential $U(x) = a(x - 0.5)^2$. Assume that the diffusion happens on an interval [0,1], the ends are absorbing boundaries ($P(0, t) = P(1, t) = 0$) and the initial

condition is given by $P(x, t = 0) = \delta(x - 0.25)$. Take both the friction $\gamma$ and diffusion $D$ coefficients equal to unity. Plot the computed values of $P(x, t)$.

(a) Find the steady-state solution analytically. Rescale the steady-state probability distribution to unity.

(b) Implement the forward Euler method (often called as FTCS).

(c) Implement the Cranck-Nicolson method. This method is often used for solving the diffusion equation numerically. It is an implicit method and second-order accurate in time. The finite-difference scheme of the Cranck-Nicolson method is given by

$$\begin{aligned}\frac{P_i^{n+1} - P_i^n}{\Delta t} = \frac{1}{2}\Bigg[ & 2aP_i^{n+1} \quad + \quad V_i \frac{P_{i+1}^{n+1} - P_{i-1}^{n+1}}{2\Delta x} + \frac{P_{i+1}^{n+1} - 2P_i^{n+1} + P_{i-1}^{n+1}}{\Delta x^2} \\ & + 2aP_i^n \quad + \quad V_i \frac{P_{i+1}^n - P_{i-1}^n}{2\Delta x} + \frac{P_{i+1}^n - 2P_i^n + P_{i-1}^n}{\Delta x^2} \Bigg],\end{aligned}$$

where $V_i = V(x_i) = \frac{\partial U}{\partial x}|_{x=x_i}$. On each time step you need to solve a system of linear equations given above. This can be done by implementing the Thomas algorithm for tridiagonal systems of equations or by using the command scipy.linalg.solve in Python.

(d) What can you say about the stability of these methods? How many time steps does it take to reach the steady-state solution in both cases? Plot the numerical solution and compare it to the plot of the scaled steady-state solution.

*Hint 1.* The initial condition $P(x, t = 0) = \delta(x - 0.25)$ can be approximated by the smooth Gaussian probability density function

$$P(x, t = 0) \approx \frac{1}{\sqrt{2\pi\sigma}} \mathrm{e}^{-(x-0.25)^2/2\sigma^2}$$

with a strong narrow peak at $x = 0.25$ (take small $\sigma \ll 1$).

*Hint 2.* The numerical solution of the Fokker-Planck equation should reach the steady-state solution.

*Hint 3.* Try to avoid nested loops as much as possible. Use the *vectorization*.