CHEM-LV03 Analysis and Simulation of Stochastic Reaction-diffusion Systems
Department of Chemical and Metallurgical Engineering
Aalto University
Summer 2022 Exercise 5

Classroom problem

(System with multiple favourable states, revisited)
Consider a chemical species $\mathcal{A}$ being subjected to four reactions in a container of volume $V = 0.5$:

R1) $3\mathcal{A} \xrightarrow{\kappa_1} 2\mathcal{A}$

R2) $2\mathcal{A} \xrightarrow{\kappa_2} 3\mathcal{A}$

R3) $\mathcal{A} \xrightarrow{\kappa_3} \emptyset$

R4) $\emptyset \xrightarrow{\kappa_4} \mathcal{A}$.

The following ODE approximates the evolution of the average number $\overline{n_\mathcal{A}}$ of molecules of $\mathcal{A}$:

$$d\overline{n_\mathcal{A}}(t) = -\frac{\kappa_1}{6V^2}\overline{n_\mathcal{A}}^3(t) + \frac{\kappa_2}{2V}\overline{n_\mathcal{A}}^2(t) - \kappa_3\overline{n_\mathcal{A}}(t) + \kappa_4 V, \quad \overline{n_\mathcal{A}}(0) = 0,$$

where the equation rates are in the time scale of minutes. Consider the first **5 minutes** of the reaction and the following rate constants:

$$\kappa_1 = 1.5 \times 10^{-3}, \quad \kappa_2 = 0.36, \quad \kappa_3 = 37.5, \quad \kappa_4 = 2200.$$

(a) plot the time evolution of the copy number by solving the SDE corresponding to the scenario above. Compare it with the deterministic solution. Are there any significant differences between the stochastic and deterministic solutions?

(b) change V to $20V$ and solve the corresponding ODE and SDE. What is the effect of changing the volume V?

(c) back to the original volume $V = 0.5$, prepare a routine to compute the empirical distribution of the copy number given the initial condition. You may follow the procedure bellow:

1. choose a number N_r of realisations ($N_r < 10^4$ will suffice).
2. solve the corresponding SDE N_r times. You may use the same time discretisation as in (a) and (b) and any method for solving SDEs, e.g. Euler-Maruyama. *Hint*: you might need to impose some boundary conditions at $N_\mathcal{A}(t) = 0$, for the sake of simplicity, you may impose a reflective boundary. For details, check the end of this document.
3. for instants $0 = t_0, t_1, \ldots, t_i, \ldots, t_{I-1}, t_I = T$, count the number of realisations which fall into the interval $[(j-1)\Delta n_\mathcal{A}, j\Delta n_\mathcal{A})$, with $j = 1, \ldots, J$. Here, we set a computational upper bound $B > 0$, and divide the computational domain $[0, B]$ into J volumes of length $\Delta n_\mathcal{A}$. You may decide on a value for B based on your result from (a).
4. at each time step, normalise the counts by the total amount of realisations N_r
5. check the evolution of the density $p^{SDE}(n_\mathcal{A}, t)$ of the empirical distribution for some selected time steps.

(d) Let $p^{FP}(n_\mathcal{A}, t)$ denote the solution to the Fokker-Planck equation given the stochastic model and some initial condition. Solve it for the same space-time discretisation used for the empirical probability density function $p^{SDE}(n_\mathcal{A}, t)$. *Hint*: propagate the density $p^{FP}(n_\mathcal{A}, t)$ for the centroids of the space discretisation.

(e) compare the evolution of the density $p^{SDE}(n_\mathcal{A}, t)$ with $p^{FP}(n_\mathcal{A}, t)$. Ideally, the two densities should match as $N_r \to \infty$.

Homework

In this section, we work with the experiments carried out by [1] to observe and analyse the trajectories of swimming microorganisms. Algae, for instance, have their random movement influenced by the balance between gravitational and viscous torques, as algae are bottom-heavy. Their random movement is also influenced by a light source.

Let us work on the random walk of a swimming microorganism fixed on a two dimensional space. Initially, the organism is placed on the point $x_0 = (x_0^{(1)}, x_0^{(2)}) = (0, 0)$, with an orientation θ_0 with respect to the $x_0^{(1)}$-axis. Assume that the organism, currently at time t, will change its direction at a random time $t + \tau$, changing its original orientation θ_t to $\theta_t + \delta_{\theta_t}$. The turning angle δ_θ can be model by a distribution whose probability density function satisfies

$$p(\delta_\theta) \geq 0, \quad -\pi \leq \delta_\theta \leq \pi, \tag{1}$$

under the condition that

$$\int_{-\pi}^{\pi} p(\delta_\theta)\, d\delta_\theta = 1. \tag{2}$$

This is the case for the von Mises distribution, which has the following probability density function:

$$p(\delta_\theta) = \frac{1}{2\pi I_0(\kappa)} \exp\left(\kappa \cos\left(\delta_\theta - \mu_\delta\right)\right), \quad -\pi \leq \delta_\theta \leq \pi, \tag{3}$$

where I_m denotes the modified Bessel function of the first kind and order m. When $\kappa = 0$, the von Mises distribution equals the uniform distribution, and as $\kappa \to \infty$ the distribution becomes sharply peaked around the mean turning angle μ_δ.

Based on their experiments, [1] suggested the following form for the mean turning angle μ_δ:

$$\mu_\delta(\theta, \tau) = \begin{cases} -d_\tau \sin\theta, & -\pi \leq \theta \leq \pi, \\ 0, & \theta = \pm\pi, \end{cases} \tag{4}$$

where d_τ is a dimensionless parameter.

Problem 1. *Simulate a two dimensional random walk using a velocity-jump process where the organism moves at a constant velocity $s = 1$ and changes direction from t to $t + \tau$, where $\tau \sim Exp(\lambda)$, $\lambda = 1$. You may compute the random turning angle from the von Mises distribution and calculate the new position according to*

$$x_{t+\tau} \;=\; x_t + s\tau(\cos(\theta_t + \delta_\theta), \sin(\theta_t + \delta_\theta)). \tag{5}$$

It is enough to simulate the first 10^4 jumps. Assume $\kappa = 0.1, d_\tau = 0$ and check whether the walk has a preferable direction?

Problem 2. *Simulate another two dimensional random walk using a velocity-jump process, this time assume $\kappa = 0.5, d_\tau = 2$. And now, does the random walk have a preferable direction?*

Reflective boundary condition at $X(t) = 0$

This condition can be used when there is no chemical interaction between the boundary and diffusing molecules.

Consider solving a stochastic differential equation with the Euler-Maruyama method for the unidimensional case. We compute the next position $X(t + \Delta t)$ at time $t + \Delta t$ by

$$X(t + \Delta t) \;=\; X(t) + f(X(t), t)\Delta t + g(X(t), t)(\sqrt{\Delta t})\eta, \quad \eta \sim \mathcal{N}(0, 1). \tag{6}$$

1. generate the normally distributed random number η.
2. compute possible position $X(t + \Delta t)$ according to Eq. (6).
3. if $X(t + \Delta t)$ is less than 0, then set instead

$$X(t + \Delta t) \;=\; -X(t) - f(X(t), t)\Delta t - g(X(t), t)(\sqrt{\Delta t})\eta.$$

References

[1] N. Hill and D.-P. Häder, "A biased random walk model for the trajectories of swimming micro-organisms," *Journal of Theoretical Biology*, vol. 186, no. 4, pp. 503–526, 1997.