CHEM-LV03 Analysis and Simulation of Stochastic Reaction-diffusion Systems
Department of Chemical and Metallurgical Engineering
Aalto University
Summer 2022 Exercise 6

Classroom problem

Problem 1. *(Compartment-based approach to Diffusion) Consider a chemical species $\mathcal{A}$. Allow the molecules of $\mathcal{A}$ to diffuse along the domain $[0, L] \times [0, h] \times [0, h]$, where $L = 1$ mm and $h = 25\mu m$. Divide the computational domain $[0, L] \times [0, h] \times [0, h]$ into $K = L/h = 40$ compartments each of volume h^3, and denote the number of molecules of $\mathcal{A}$ in the ith compartment $[(i-1)h, ih) \times [0, h] \times [0, h])]$ by $N_{\mathcal{A}_i}$, where i runs from 1 to K.*

$$\mathcal{A}_1 \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_2 \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_3 \underset{d}{\overset{d}{\rightleftarrows}} \dots \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_K.$$

Design a stochastic simulation algorithm for this reaction-diffusion system with initially 1000 molecules of $\mathcal{A}$ distributed uniformly at $[10h, 12h) \times [0, h] \times [0, h]$. Draw one realisation from your algorithm and plot the number of molecules at each compartment for different instants t. Consider the first 5×10^5 reactions and the following rate constants:

$$\kappa_1 = 1 \times 10^{-3}, \quad \kappa_2 = 2 \times 10^{-5}.$$

Problem 2. *(Compartment-based approach to Reaction-Diffusion) Consider a chemical species $\mathcal{A}$ being subjected to two reactions. Allow the molecules of $\mathcal{A}$ to diffuse along the domain $[0, L] \times [0, h] \times [0, h]$, where $L = 1$ mm and $h = 25\mu m$. Divide the computational domain $[0, L] \times [0, h] \times [0, h]$ into $K = L/h = 40$ compartments each of volume h^3, and denote the number of molecules of $\mathcal{A}$ in the ith compartment $[(i-1)h, ih) \times [0, h] \times [0, h])]$ by $N_{\mathcal{A}_i}$, where i runs from 1 to K.*

$$\mathcal{A}_1 \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_2 \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_3 \underset{d}{\overset{d}{\rightleftarrows}} \dots \underset{d}{\overset{d}{\rightleftarrows}} \mathcal{A}_K,$$

$$\mathcal{A}_i \xrightarrow{\kappa_1} \emptyset \quad \text{for } i = 1, 2, \dots, K,$$

$$\emptyset \xrightarrow{\kappa_2} \mathcal{A}_i \quad \text{for } i = 1, 2, \dots, K/5.$$

The domain is divided into two different regions $[0, L/5]$ and $[L/5, L]$ as a prepatterning, that is, it is expected that the chemical $\mathcal{A}$ is produced in only part of the domain.

Design a stochastic simulation algorithm for this reaction-diffusion system with initially zero molecules of $\mathcal{A}$. Draw one realisation from your algorithm and plot the number of molecules at each compartment for different instants t. Consider the first 2×10^5 reactions and the following rate constants:

$$\kappa_1 = 1 \times 10^{-3}, \quad \kappa_2 = 2 \times 10^{-5}.$$

Problem 3. *(Reaction-Diffusion PDE) The following PDE approximates the concentration of molecules along the domain $[0, L] \times [0, h] \times [0, h]$:*

$$\frac{\partial a}{\partial t} = D\frac{\partial^2 a}{\partial x^2} + \kappa_2 \chi_{[0,L/5]} - \kappa_1 a,$$

with zero-flux boundary conditions

$$\frac{\partial a}{\partial x}(0,t) = \frac{\partial a}{\partial x}(L,t) = 0.$$

Here, $a(x,t)$ is the concentration of molecules of $\mathcal{A}$ at point x and time t, and $\chi_{[0,L/5]}$ is the characteristic function of the interval $[0, L/5]$, so that $\chi_{[0,L/5]}(x) = 1$ if $x \in [0, L/5]$, and equals zero otherwise.

Solve the PDE above and compare the values of $a(x,t)h^3$ with the results from the compartment-based approach.

Problem 4. *(Velocity-jump process) Design another stochastic simulation algorithm for the reaction-diffusion system of Problem 2, this time with a velocity-jump process as the underlying diffusion model.*

(a) for each molecule, compute its x-coordinate at time $t + \Delta t$ according to the following steps:

- *generate a random number r uniformly distributed in (0,1).*
- *assume that a particle moves along the x-axis at a constant speed s. Compute the position of the molecule at time $t + \Delta t$ by*

  $$X(t + \Delta t) = X(t) + V(t)\Delta t,$$

  where the velocity can have only two values $V(t) = \pm s$. Here, assume $s = 1 \times 10^{-2}$ and $\Delta t = 0.01$.
- *apply reflective boundary conditions if $X(t + \Delta t)$ is less than 0 or greater than L.*
- *check if the particle turns in the time interval $[t, t+\Delta t)$, that is, check whether $r < \lambda \Delta t$. If so, then let $V(t + \Delta t) = -V(t)$. Otherwise, set $V(t + \Delta t) = V(t)$. The turning frequency λ is given by*

  $$\lambda = \frac{s^2}{2D}.$$

(b) for each molecule, generate a random number r_1 uniformly distributed in the interval (0,1). If $r_1 < \kappa_1 \Delta t$, then remove the molecule from the system.

(c) generate a random number r_1 uniformly distributed in the interval (0,1). If $r_2 < (\kappa_2 h^2 L/5)\Delta t$, then generate another random number r_3 uniformly distributed in the interval (0,1) and introduce a new molecule at the position with x-coordinate equal to $r_3 L/5$.

(d) repeat the steps above until you reach your stopping criteria.

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

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

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

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