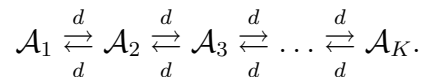


Classroom problem

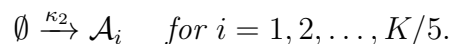
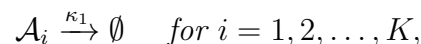
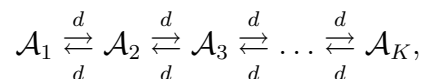
Problem 1. (*Compartment-based approach to Diffusion*) Consider a chemical species \mathcal{A} . Allow the molecules of \mathcal{A} to diffuse along the domain $[0, L] \times [0, h] \times [0, h]$, where $L = 1$ mm and $h = 25\mu\text{m}$. Divide the computational domain $[0, L] \times [0, h] \times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



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

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

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

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