Problem Sheet 4

1. This is a warm-up problem. You are asked to verify a few results from the Lecture Notes. You do not need to write long derivations (a few lines for each point (a)–(g) will be enough).

(a) Derive the equations (13.10)–(13.11) for the evolution of the mean vector $\mathbf{M}(t)$ of the diffusion-advection compartment-based model.

(b) Derive the PDE (13.19) for the density of bacteria.

(c) Derive formula (13.27) by solving the ODE (13.24) in the interval $[t, t+\Delta t]$ with initial conditions $X(t)$, $V(t)$ and $Y_2(t)$.

(d) Derive formula (13.38) for the stationary distribution $p_s(u)$.

(e) Show that the one-particle solvent model (14.4)–(14.7) can be equivalently written as equations (14.9)–(14.12) for four variables $X(t)$, $V(t)$, $U(t)$ and $Z(t)$.

(f) Solve equations (15.3)–(15.4) and derive formula (15.5) for positions of heat bath particles of the solvent modelled as a system of harmonic oscillators.

(g) Use conservation of energy to derive equation (16.9).

2. Consider N animals following a velocity jump process on the unit circle $\{\,(\cos(\theta), \sin(\theta)) \mid \theta = [0, 2\pi)\,\}$. Each animal moves either clockwise or anticlockwise with unit angular speed. Let $\omega_i(t) = \pm 1$, $i = 1, 2, \ldots, N$, be the angular velocity of the i-th animal, where $+1$ is for the anticlockwise rotation and -1 is for the clockwise rotation. Let us define the average angular velocity of the whole group by

$$u(t) = \frac{1}{N} \sum_{i=1}^{N} \omega_i(t),$$

i.e. $u(t) \in [-1, 1]$. We will assume that the i-th animal changes its direction according to the Poisson process with the turning frequency

$$\lambda \equiv \lambda(\omega_i(t), u(t)) = 1 + 10\Big(1 - \omega_i(t)\, u(t)\Big)^2.$$

(a) Let $N = 1$, i.e. we only consider one animal in part (a). Let $p^-(\theta, t)$ (resp. $p^+(\theta, t)$) be the probability that this animal moves clockwise (resp. anticlockwise). Write a system of partial differential equations which describe the time evolution of p^+ and p^-. Write a partial differential equation satisfied by $p = p^+ + p^-$.

(b) Let $N \geq 1$. Let $A(t)$ be the number of animals which move anticlockwise. Let $P(a, t)$ be the probability that $A(t) = a$. Write the master equation for $P(a, t)$.

(c) Let $N \gg 1$. Show that the system has two favourable states: either the group (most of the animals) moves clockwise or the group moves anticlockwise. What is the average time taken for the group to change its direction of movement?

3. Simulate the diffusion-advection example from Section 13.1 using the velocity jump SSA (a8)–(c8) where the turning frequency λ is given by (13.16). Plot the density of particles at time $t = 2$ minutes. You should obtain the same result as shown in Figure 13.1(b).

4. Consider the model (13.33)–(13.34) from Section 13.3. Write a computer code which can simulate this model and investigate how the average time taken for the group to change its direction depends on the interaction radius $R \in (0, 2)$. Use $N = 20$ locusts. Plot the stationary distribution of the (total) average velocity given by (13.35) for $R = 0.5$ and $R = 1$. Compare with Figure 13.3(c) which was computed for $R = 2$. Plot the average switching time as a function of R.

5. Consider the full one-particle solvent model expressed in terms of four variables as (14.9)–(14.12).

(a) Show that the corresponding friction kernel $\kappa(\tau)$ can be written in the form (14.29). Prove the generalized fluctuation-dissipation theorem (14.28) for this $\kappa(\tau)$.

(b) Consider limit $\alpha_4 \to \infty$ in (14.29). Show that $\kappa(\tau)$ in (14.29) converges to $\kappa(\tau)$ which we obtained for the three variable model, namely to equation (14.24), in the limit $\alpha_4 \to \infty$.

6. Assume that the noise term $R(t)$ is given as a linear combination of normally distributed random numbers in equation (14.44). Find coefficients $c_0, c_1, c_2, \ldots, c_{k_m}$ so that $R(t)$ satisfies the generalized fluctuation-dissipation theorem given in equation (14.43). That is,

(a) derive system of linear equations (14.46) for coefficients $c_1, c_2, \ldots, c_{\min\{k_m, k\}}$,

(b) derive equation (14.48) for computation of coefficient c_0.

7. Consider the solvent model introduced in Section 15.2.

(a) Use the conservation of momentum and energy to derive formulas for post-collision velocities of the colliding diffusing (heavy) and solvent (light) particles, given in equations (15.17)–(15.18).

(b) Derive formula (15.33) for the effective noise term β_i.

8. Consider a three-dimensional domain, a ball of radius $\overline{R}$, which contains a particle, a ball of radius $R < \overline{R}$, at its centre. Let r denote the distance from the common centre of both balls and assume that we have other particles uniformly distributed in spherical shell $R \le r \le \overline{R}$, which all exert force (16.3) on the particle at the origin. Use the potential $\Phi(r) = r^{-a}$, where $a > 0$ is a constant, and denote the density of particles by ϱ. Calculate the total energy of their interactions, i.e. evaluate

$$\int_R^{\overline{R}} \Phi(r)\, \varrho\, 4\pi r^2 \, \mathrm{d}r$$

and show that it can be considered independent of $\overline{R}$, provided that $\overline{R}$ is sufficiently large and $a > 3$. What happens for $a < 3$?

9. Consider the molecular dynamics modelling introduced in Lecture 16.

(a) Differentiate the Hamiltonian (16.12) with respect of time and use ODEs (16.10)–(16.11) to show that the Hamiltonian (16.12) is constant for all solutions of ODEs (16.10)–(16.11).

(b) Consider the solvent described as a system of harmonic oscillators studied in Section 15.1 and described by system of ODEs (15.1)–(15.4). Define the potential energy function $U(\mathbf{q})$ and state variable $[\mathbf{q}(t), \mathbf{p}(t)]$ so that equations (15.1)–(15.4) can be equivalently rewritten in the Hamiltonian form (16.10)–(16.11).

(c) Use the Protein Data Bank at `http://www.rcsb.org/` Search for "actin" and "cyclin" proteins. How many atoms do these proteins consists of? Look at their 3D structures. Experiment with presentation styles (spacefill, surface). Do you see any differences between these proteins?

A couple of additional questions (OPTIONAL)

10. Since some of you took Part A optional course Integral Transforms, I have included the following optional question. However, even if you did not take Part A Integral Transforms, you could attempt it. All you need is some basic properties of the Laplace transform, defined by (14.52).

(a) Derive equation (14.51) relating velocity autocorrelation function $\chi(\tau)$ and friction kernel $\kappa(\tau)$.

(b) Consider the three-equation model (14.14)–(14.16). Show that its velocity autocorrelation function $\chi(\tau)$ can be obtained as

$$\chi(\tau) = \frac{\sigma^2}{\kappa(0)}\,\mathscr{L}^{-1}\left(\frac{s+\alpha_2}{s^2+\alpha_2 s+\alpha_1}\right)$$

This formula can also be obtained by passing to the limit $\alpha_4 \to \infty$ in (14.53).

(c) By inverting the Laplace transform in part (b), derive equation (14.55) for the velocity autocorrelation function $\chi(\tau)$ of the three-equation model (14.14)–(14.16).

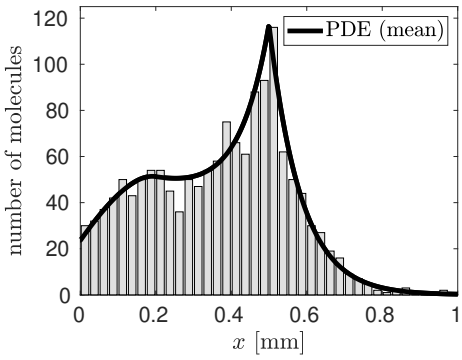
11. In Section 13.1 we presented methods for adding an additional advection (drift, taxis) term to the individual-based and compartment-based models of diffusion. The same approach can be used to design the corresponding reaction-diffusion-advection SSAs. In this question, you are asked to add an additional drift term to the example presented in Section 11.1. As in Section 11.1, the molecules of chemical species A diffuse in the elongated domain $[0,L]\times[0,h]\times[0,h]$ (see Figure 11.1(a)) with the diffusion constant $D = 10^{-4}\ \mathrm{mm}^2\,\mathrm{sec}^{-1}$. They are also transported to the middle of the domain by the additional advective term (13.15). Initially, there are no molecules in the system. Molecules are produced in the part of the domain $[0,L/5]\times[0,h]\times[0,h]$ at a rate $k_2 = 2\times 10^{-5}\ \mu\mathrm{m}^{-3}\,\mathrm{sec}^{-1}$ and are degraded at a rate $k_1 = 10^{-3}\,\mathrm{sec}^{-1}$ in the whole domain.

(a) Design the compartment-based model, i.e. as in Sections 8.2 and 11.1, divide the computational domain $[0,L]\times[0,h]\times[0,h]$ into $K = L/h = 40$ compartments of volume h^3 and denote the number of molecules of chemical species A in the i-th compartment $[(i-1)h, ih)\times[0,h]\times[0,h]$ by A_i. Then this reaction-diffusion-advection process is described by the system of chemical reactions generalizing the reaction-diffusion system (11.1)–(11.3): the chain of reactions (11.1) is modified to the diffusion-advection model (13.9). Calculate the numbers of molecules in each compartment at time $t = 15$ min using the Gillespie SSA (a4)–(d4).

(b) Solve the PDE describing the time evolution of the concentration, $a(x,t)$, of molecules of A at point x and time t, which is given by

$$\frac{\partial a}{\partial t} = D\,\frac{\partial^2 a}{\partial x^2} - \frac{\partial}{\partial x}\big(\tilde{f}a\big) + k_2\,\chi_{[0,L/5]} - k_1 a,$$

where $\chi_{[0,L/5]}$ is the characteristic function of the interval $[0,L/5]$. Plot the solution of this PDE in the same figure as the result of your compartment-based reaction-diffusion-advection SSA. You should obtain results comparable to the figure on the right.



(c) Design an individual-based (molecular-based) SSA of the same process by modifying the SSA (a12)–(c12), which is a molecular-based algorithm for simulating the reaction-diffusion example from Section 11.1. That is, the trajectories of individual molecules will be modelled by (13.7). Use this model to compute the same result as in parts (a)–(b), i.e. you should aim to get the same figure as it is shown on the right.