Simulation Exercise 2024 Final Report Problems

Nagoya University Graduate School of Science
Takeshi Kawasaki, Instructor

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[**Instructions**] Solve the following problems (Question 1 and Question 2) by the deadline, and submit your answers along with the code used for numerical calculations via the designated section in the TACT system. The answers should be in a PDF file, and the code should be in a text file (with extensions like .cpp or .py) or a Python notebook (with the extension .ipynb). **Be sure to include the figures of the numerical results in the PDF.**

Question 1 (Single-Particle Brownian Motion in a Langevin Heat Bath)

Consider the motion of a particle of mass m driven by thermal fluctuations in a $\boxed{\text{2D}}$ solvent with temperature T and friction coefficient ζ. It is well-known that the motion of this particle can be modeled by the Langevin equation:

$$m\dot{\mathbf{v}}(t) = -\zeta \mathbf{v}(t) + \mathbf{F}_{\mathrm{B}}(t)$$

where the thermal fluctuation force $\mathbf{F}_{\mathrm{B}}(t)$ satisfies the fluctuation-dissipation theorem:

$$\left\langle \mathbf{F}_{\mathrm{B}}(t) \cdot \mathbf{F}_{\mathrm{B}}(t') \right\rangle = 4k_{\mathrm{B}}T\zeta\delta(t-t')$$

Let the unit of length be a and the unit of time be t_0. Consider how the motion of the particle driven by this model changes as its mass systematically varies.
[**Questions**]

(1) We discussed in the lecture that the thermal fluctuation force can be expressed as $\mathbf{F}_{\mathrm{B}}(t) = \sqrt{\frac{2k_{\mathrm{B}}T\zeta}{\Delta t}}\mathbf{R}_{\mathrm{G}}$ using a normal random number $\mathbf{R}_{\mathrm{G}}$ with variance 1. For nondimensionalization, let $\mathbf{v} = (a/t_0)\tilde{\mathbf{v}}$, and $\mathbf{F}_{\mathrm{B}}(t) = \sqrt{\frac{2k_{\mathrm{B}}T\zeta}{t_0\Delta\tilde{t}}}\mathbf{R}_{\mathrm{G}}$. Show that introducing the characteristic time scales $t_{\mathrm{D}} = \frac{m}{\zeta}$ and $t_{\mathrm{B}} = \frac{a^2\zeta}{k_{\mathrm{B}}T}$ allows the Langevin equation to be written as:

$$\frac{t_{\mathrm{D}}}{t_0}\dot{\tilde{\mathbf{v}}} = -\tilde{\mathbf{v}} + \sqrt{\frac{2t_0}{t_{\mathrm{B}}\Delta\tilde{t}}}\mathbf{R}_{\mathrm{G}}$$

(2) By setting the time unit t_0 in the nondimensionalized Langevin equation obtained in (1) to t_{B}, show that the equation can be expressed as:

$$m^*\dot{\tilde{\mathbf{v}}} = -\tilde{\mathbf{v}} + \sqrt{\frac{2}{\Delta\tilde{t}}}\mathbf{R}_{\mathrm{G}}$$

Here, show that m^* is a quantity proportional to the inertial mass: $mk_{\mathrm{B}}T/\zeta^2a^2$. ($m^*$ becomes a parameter of the equation, allowing the discussion of the inertial mass dependence of the particle's motion.)

(3) The mean square displacement of the particle driven by this model is theoretically given as:

$$\left\langle \Delta\mathbf{r}(t)^2 \right\rangle = \frac{4k_{\mathrm{B}}T}{\zeta}\left[t + \frac{m}{\zeta}e^{-\zeta t/m} - \frac{m}{\zeta}\right]$$

Show that nondimensionalizing this equation using the units of length a and time $t_0 = t_{\mathrm{B}}$ results in the nondimensionalized mean square displacement:

$$\left\langle \Delta\tilde{\mathbf{r}}^2 \right\rangle = 4m^* \left\{ \frac{\tilde{t}}{m^*} + e^{-\frac{\tilde{t}}{m^*}} - 1 \right\}$$

Under the initial conditions $\mathbf{r} = (0, 0)$ and $\mathbf{v} = (0, 0)$, solve the Langevin equation (2) numerically using the semi-implicit Euler method with a time step of $\Delta t = 0.01t_{\mathrm{B}}$, and answer the following questions.

[**Questions**]

(4) Plot the particle trajectory over the time interval $[0, 100t_{\mathrm{B}}]$ when the inertial mass m^* is systematically varied as $m^* = 0.1, 1.0, 10$. Output the particle position every $10\Delta t$ and connect these points with lines. Also, consider how the trajectory of Brownian motion changes as the inertial mass increases.

(5) Plot the mean square displacement $\left\langle \Delta\mathbf{r}(t)^2 \right\rangle$ over the time interval $[0.01t_{\mathrm{B}}, 100t_{\mathrm{B}})$ for $m^* = 0.1, 1.0, 10$, and compare the results with the theory obtained in (3). Note that $\langle \cdots \rangle$ represents a quantity averaged over time or ensemble. Furthermore, the upper limit of the time interval is semi-open, meaning it does not necessarily have to reach $100t_{\mathrm{B}}$. Additionally, relate the change in the mean square displacement to the change in the trajectory as the inertial mass increases. [Hint: ballistic region and diffusive region]

Question 2 (Classical Molecular Dynamics Method: Smoothing of Potential Cutoff)

In molecular dynamics calculations, it is common to introduce a cutoff length r_{cut} in the intermolecular potential to truncate the force calculation between particles that satisfy $r > r_{\mathrm{cut}}$. However, at the cutoff point $r = r_{\mathrm{cut}}$, the force often becomes discontinuous, requiring the cutoff point r_{cut} to be taken longer to reduce this discontinuity. On the other hand, taking a longer r_{cut} increases computational cost, so to solve this problem, the following smoothing potential, which ensures that the potential and its derivative are continuously connected at the cutoff point, is introduced:

$$U(r) = U_0(r) - U_0(r_{\mathrm{cut}}) - U_0'(r_{\mathrm{cut}})(r - r_{\mathrm{cut}})$$

where $U_0'(r) = \frac{\mathrm{d}U_0(r)}{\mathrm{d}r}$. Answer the following questions regarding this smoothing potential.

[**Questions**]

(1) Show that $U(r_{\mathrm{cut}}) = 0$ and $U'(r_{\mathrm{cut}}) = 0$. (In other words, the potential and force smoothly connect to zero at the cutoff point $r = r_{\mathrm{cut}}$, eliminating the discontinuity in force.)

Next, consider a system of 1000 2D disk particles with mass m and diameter a, interacting via the smoothing potential $U(r_{ij})$ given by the Lennard-Jones potential:

$$U_0(r_{ij}) = 4\epsilon \left\{ \left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{a}{r_{ij}}\right)^{6} \right\}$$

These particles are confined within a 2D periodic boundary condition of side length $L = 50a$. The cutoff length is set to $r_{\mathrm{cut}} = 2.0a$, which is slightly shorter than what was covered in the lecture. Answer the following questions related to the classical molecular dynamics simulation of these particles. In the simulation, let the unit of length be a, the unit of time be $t_0 = \sqrt{\frac{ma^2}{\epsilon}}$, and the dimensionless temperature (parameter) be $T^* = \frac{k_\mathrm{B}T}{\epsilon}$.

[**Questions**]

(2) Using a crystal configuration as the initial condition, simulate the particles' motion for $10t_0$ at a temperature of $T^* = 5.0$ under a Langevin heat bath, and plot the particle configuration afterwards. The time step for numerical calculation should be $\Delta t = 0.01t_0$.

(3) After (2), lower the temperature to $T^* = 0.2$ under a Langevin heat bath, simulate the particles' motion for $1500t_0$, and plot the particle configuration afterwards. The time step for numerical calculation should be $\Delta t = 0.01t_0$.

(4) After (3), remove the Langevin heat bath and switch to Newton's equations of motion. Simulate the particles' motion for $100t_0$, and plot the potential energy, kinetic energy, and their sum (mechanical energy) per particle as a function of time. Confirm that the mechanical energy is conserved (or shows a tendency towards conservation). Newton's equations of motion should be solved using the velocity Verlet method with a time step of $\Delta t = 0.001t_0$. Additionally, when plotting, ensure that the potential energy and kinetic energy fluctuations are visible, and that the mechanical energy appears constant by comparison.

The following problems are not mandatory, but you can attempt them if you have extra time. Appropriate credit will be given for extra effort.

(5) The distribution function of the velocity components, such as the x-component, of particles in thermal equilibrium at temperature T is known to satisfy the Maxwell-Boltzmann distribution:

$$f(v_x) = \sqrt{\frac{m}{2\pi k_\mathrm{B}T}}e^{-\frac{mv_x^2}{2k_\mathrm{B}T}}$$

Given that $f(v_x)$ has the dimension of the inverse of velocity, nondimensionalize $f(v_x)$ in the same manner as before, and show that:

$$\tilde{f}(\tilde{v}_x) = \sqrt{\frac{1}{2\pi T^*}}e^{-\frac{\tilde{v}^2}{2T^*}}$$

(6) Verify that the velocity distribution function $f(v_x)$ (as a normalized histogram) obtained from the actual simulation is consistent with the theoretical result in (5). When calculating the histogram, make sure to take sufficient time averages (e.g., averaging the data every t_0).