Data Science Course Group (Sci.Grad): Simulation Tutorials
Lecture 4 Lecture Materials

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1. Lecture Schedule

- This practical course will be conducted in the first half of the spring semester.
- Lecture materials will be uploaded by **11:00 AM on the scheduled lecture day**.
- Schedule
  1. 4/15: Lecture 1
  2. 4/22: Lecture 2
  3. 4/30 (Tue): Lecture 3
  4. **5/13: Lecture 4 (Midterm Report Assignment Released)**
  5. 5/20: Lecture 5
  6. 5/27: Lecture 6 (**Midterm Report Assignment Submission Deadline**)
  7. **6/03: No Lecture**
  8. 6/10: Lecture 7 (**Final Report Assignment Released**)
  9. 6/17: Lecture 8
  10. 6/24: Lecture 9 (Makeup Class)

1.1. Syllabus

This practical course will cover the following topics (subject to change depending on progress):

1. Introduction
   - Usage of C (C++) for numerical calculations
   - Usage of Python for data analysis and visualization
   - Principles of numerical calculations
   - Round-off errors
   - Dimensional analysis in scientific computing
2. Numerical solutions of ordinary differential equations: Examples with damped oscillations and harmonic oscillators
   - Numerical integration of differential equations
   - Stability and conservation laws of orbits
3. Brownian motion of a single particle
   - Langevin equation (stochastic differential equations)
   - Generation of normal random numbers
   - Euler-Maruyama method
   - Time averaging and ensemble averaging
4. Brownian motion of multiple particles
   - Calculation methods for interaction forces
   - Non-equilibrium systems simulation: Example of phase separation phenomena
5. Molecular dynamics simulation of multiple particles
   - Position Verlet method and velocity Verlet method
   - Conservation laws in systems with multiple particles
6. Monte Carlo method
   - Review of statistical mechanics
   - Markov chain Monte Carlo method
   - Metropolis algorithm

Contents

2. Explanation of the 3rd Assignment

3rd Assignment

A small ball of mass m, considered as a point mass, is attached to a spring with spring constant k, with one end fixed. The ball moves in one dimension on a smooth horizontal surface, subjected to a viscous resistance force with a viscous resistance coefficient ζ. The equation of motion of the ball at time t, with position $x(t)$ and velocity $v(t)$, can be expressed as:

$$m\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -\zeta v(t) - kx(t) \tag{1}$$

Now, consider how the motion of the mass point changes significantly based on different values of the positive parameters (m, ζ, k).
[**Questions**]

(1) Express analytically the conditions under which the motion of the ball exhibits **damped oscillation (under-damping)**, over-damping, and critical damping, using m, ζ, and k.

(2) Let $\tilde{x}$ and $\tilde{t}$ be dimensionless variables representing length and time, respectively, where their relationship with the actual physical quantities given in the problem is $x = a\tilde{x}$, $t = t_0\tilde{t}$, and $\dot{x} = v = (a/t_0)\tilde{v}$. Here, a [m] and t_0 [s] are appropriately defined length and time scales. On the other hand, we can extract several physically meaningful time scales from the combination of physical quantities given in the equation of motion. These include the time scale of damped motion $t_d = \frac{m}{\zeta}$ and the time scale characterizing spring oscillation $t_s = \sqrt{m/k}$. Use these to non-dimensionalize the equation of motion, and then discretize it using the semi-implicit Euler method with a time step $\Delta\tilde{t}$ to derive a recurrence relation for $\tilde{v}(\tilde{t} + \Delta\tilde{t})$ and $\tilde{x}(\tilde{t} + \Delta\tilde{t})$.

(3) Now, by setting the time unit to $t_0 = t_s$ (Note: This is different from $t_0 = t_d$ as used in Lecture 3, now changed to t_s), one of the coefficients in the recurrence relation derived in problem (2) drops out, and it is found that t_s/t_d becomes the only parameter controlling the characteristics of the motion. Using the conditions estimated in problem (1), substitute appropriate values into t_s/t_d and numerically solve the recurrence relations discussed in problem (2) to reproduce damped oscillation (under-damping), over-damping, and critical damping, and plot the graph of $x(t)$. Set the initial conditions as $x(0) = a$, $\dot{x}(0) = 0$. Choose the computation time for $t > 0$ appropriately so that the characteristics of the motion can be observed, and set the time step $\Delta\tilde{t}$ appropriately within a range where the numerical solution converges.

2. Explanation of the 3rd Assignment (2)

[Explanation]

(1) Substituting $x(t) = Ae^{\lambda t}$ as the solution, λ must satisfy the following characteristic equation:

$$m\lambda^2 + \zeta\lambda + k = 0 \tag{2}$$

The discriminant of this quadratic equation is $D = \zeta^2 - 4mk$.
These relationships can be described using the time scales defined in the problem statement:

$$D = \zeta^2 - 4mk = m^2\left(\frac{1}{t_d^2} - 4\frac{1}{t_s^2}\right) \tag{3}$$

Therefore, the motion can be classified according to the discriminant, and the conditions that the parameter $\zeta^* = \frac{t_s}{t_d}$ must satisfy can be obtained:

- Over-damping: $D > 0$: $\frac{t_s}{t_d} > 2$
- Critical damping: $D = 0$: $\frac{t_s}{t_d} = 2$
- Under-damping: $D < 0$: $\frac{t_s}{t_d} < 2$

2. Explanation of the 3rd Assignment (3)

(2) Non-dimensionalizing the equation of motion:

$$m\frac{a}{t_0^2}\dot{\tilde{v}}(t) = -\zeta\frac{a}{t_0}\tilde{v}(t) - ka\tilde{x}(t) \tag{4}$$

Dividing both sides by $m\frac{a}{t_0^2}$ gives the dimensionless equation:

$$\dot{\tilde{v}}(t) = -\frac{\zeta t_0}{m}\tilde{v}(t) - \frac{kt_0^2}{m}\tilde{x}(t) \tag{5}$$

From this, the time scales $t_d = \frac{m}{\zeta}$ and $t_s = \sqrt{\frac{m}{k}}$ can be identified. Using these, the equation of motion can be expressed as:

$$\dot{\tilde{v}}(\tilde{t}) = -\frac{t_0}{t_d}\tilde{v}(\tilde{t}) - \frac{t_0^2}{t_s^2}\tilde{x}(\tilde{t}) \tag{6}$$

Discretizing this using the semi-implicit Euler method, the recurrence relations for $\tilde{v}(\tilde{t} + \Delta\tilde{t})$ and $\tilde{x}(\tilde{t} + \Delta\tilde{t})$ are:

$$\tilde{v}(\tilde{t} + \Delta\tilde{t}) = \tilde{v}(\tilde{t}) - \frac{t_0}{t_d}\tilde{v}(\tilde{t})\Delta\tilde{t} - \frac{t_0^2}{t_s^2}\tilde{x}(t)\Delta\tilde{t} \tag{7}$$

2. Explanation of the 3rd Assignment (4)

$$\tilde{x}(\tilde{t}+\Delta\tilde{t}) = \tilde{x}(\tilde{t}) + \boxed{\tilde{v}(\tilde{t}+\Delta\tilde{t})\Delta\tilde{t}} \tag{8}$$

Furthermore, by choosing the time scale as $t_0 = t_s$, the recurrence relation for $\tilde{v}(\tilde{t}+\Delta\tilde{t})$ becomes:

$$\tilde{v}(\tilde{t}+\Delta\tilde{t}) = \tilde{v}(\tilde{t}) - \frac{t_s}{t_d}\tilde{v}(\tilde{t})\Delta\tilde{t} - \tilde{x}(t)\Delta\tilde{t} \tag{9}$$

Thus, t_s/t_d becomes the parameter for this system.

(3) The simulation program and the plotting results (Fig. **1**) are shown below.

2. Explanation of the 3rd Assignment (5)

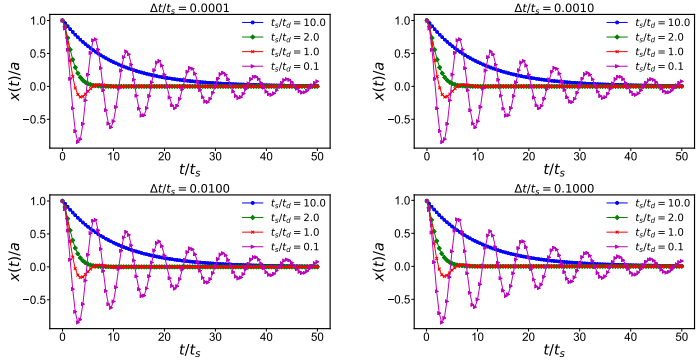

図 1: Numerical calculation results. The behavior when changing the parameter $\zeta^* = \frac{t_s}{t_d}$. $\zeta^* = 2$ represents critical damping, and the behavior changes significantly around this point. The convergence of the numerical calculation was confirmed for various Δt. It can be seen that even with $\Delta t = 0.1$, the calculation is reasonably accurate. However, errors occur on the order of $O(\Delta t)$.

2. Explanation of the 3rd Assignment (6)

Below is an example of the calculation program written in Python. Compare it with the C++ code from previous assignments.

リスト 1: Sample main calculation program “damp_osci.py” for the 3rd assignment. Available on the following GitHub repository: **[Link]**

```
1
2  import numpy as np
3  import sys
4
5  zeta=[10,2,1,0.1]
6  dt=[0.0001,0.001,0.01,0.1]
7
8  def damp_osci(dt,zeta):
9      v=0.
10     x=1.
11     t=0.
12     i=0
13     out=0.
14     f = open("./Lecture4/damp_osci_dt{:.4f}_zeta{:.1f}.dat".format(dt,zeta), 'w')
15     while i < (int)(50./dt):
16         v -= zeta*v*dt+x*dt
17         x+=v*dt
18         i+=1
```

2. Explanation of the 3rd Assignment (7)

```
        if(i*dt >=out):
            print("{:.4f} {:.20f} {:.20f}".format(i*dt,v,x))
            f.write("{:.4f} {:.20f} {:.20f}\n".format(i*dt,v,x))
            out+=0.5
    f.close()

for i in range(0,4):
    for j in range(0,4):
        print("dt={:.5f}".format(dt[i]))
        damp_osci(dt[i],zeta[j])
```

Below is a Python script used for plotting.

リスト 2: Sample plotting program “draw.py” for the 3rd assignment. Available on the following GitHub repository: **[Link]**

```


import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
%config InlineBackend.figure_format = 'retina'
import numpy as np
#plt.rcParams["text.usetex"] =True
```

2. Explanation of the 3rd Assignment (8)

```
9
10 plt.rcParams['font.family'] = 'Arial' 使用するフォント名#
11 plt.rcParams["font.size"] = 40
12
13 fig = plt.figure(figsize=(40,20))
14
15 dt=[0.0001,0.001,0.01,0.1]
16 zeta=[10,2,1,0.1]
17
18 for j in range(1,5):
19     ax = fig.add_subplot(2,2,j)
20     t, v0,x0  = np.loadtxt("./Lecture4/damp_osci_dt{:.4f}_zeta{:.1f}.dat".format(dt[j-1],zeta
           [0]), comments='#', unpack=True)
21     t, v1,x1  = np.loadtxt("./Lecture4/damp_osci_dt{:.4f}_zeta{:.1f}.dat".format(dt[j-1],zeta
           [1]), comments='#', unpack=True)
22     t, v2,x2  = np.loadtxt("./Lecture4/damp_osci_dt{:.4f}_zeta{:.1f}.dat".format(dt[j-1],zeta
           [2]), comments='#', unpack=True)
23     t, v3,x3  = np.loadtxt("./Lecture4/damp_osci_dt{:.4f}_zeta{:.1f}.dat".format(dt[j-1],zeta
           [3]), comments='#', unpack=True)
24     plt.title("$\Delta t/t_s ={:.4f}$".format(dt[j-1]),size=40)
25     plt.plot(t, x0, "o-",markersize=10,color="b",label=r"$t_s/t_d={:.1f}$".format(zeta[0]))
26     plt.plot(t, x1, "D-",markersize=10,color="g",label=r"$t_s/t_d={:.1f}$".format(zeta[1]))
27     plt.plot(t, x2, "x-",markersize=10,color="r",label=r"$t_s/t_d={:.1f}$".format(zeta[2]))
28     plt.plot(t, x3, ">-",markersize=10,color="m",label=r"$t_s/t_d={:.1f}$".format(zeta[3]))
```

2. Explanation of the 3rd Assignment (9)

```
29
30      #########
31      plt.tick_params(which='major',width = 1, length = 10)
32      plt.tick_params(which='minor',width = 1, length = 5)
33      ax.spines['top'].set_linewidth(4)
34      ax.spines['bottom'].set_linewidth(4)
35      ax.spines['left'].set_linewidth(4)
36      ax.spines['right'].set_linewidth(4)
37      plt.ylabel(r"$x(t)/a$",color='k', size=50)
38      plt.xlabel(r"$t/t_s$",color='k', size=50)
39
40      plt.legend(ncol=1, loc=1, borderaxespad=0, fontsize=35,frameon=False)
41      ##################################図のマージン設定
42      #
43      plt.subplots_adjust(wspace=0.3, hspace=0.35)
44
45  plt.savefig('./Lecture4/damp_osci.png')
46  plt.savefig('./Lecture4/damp_osci.pdf')
```

Contents

3.Langevin Heat Bath and Brownian Motion

Langevin Heat Bath and Brownian Motion

We consider the Langevin heat bath, which is often used as a thermal bath in molecular dynamics calculations, and the motion of particles driven by it. The particle motion here is Brownian motion, which is important not only in physics but also across fields such as chemistry and biology. The derivation of the theoretical solution is provided in the appendix, so please refer to it. The following reference was consulted in creating the appendix: [2] (R. Zwanzig, Nonequilibrium Statistical Mechanics (Oxford University Press, Oxford; New York, 2001)).

3.Langevin Heat Bath and Brownian Motion (2)

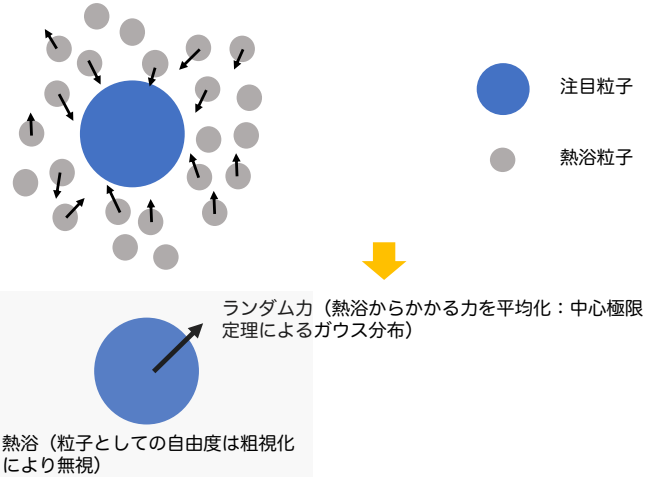

図 2: Concept of Langevin heat bath.

3.1. Langevin Equation and the Fluctuation-Dissipation Theorem

Langevin Equation

- The Brownian motion of a sphere with mass m moving in a d-dimensional solvent (heat bath) at temperature T with a friction coefficient ζ is described by the following Langevin equation:

$$\boxed{m\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} = -\zeta\mathbf{v}(t) + \mathbf{F}_{\mathrm{B}}(t)} \tag{10}$$

- Here, the thermal fluctuation force $\mathbf{F}_{\mathrm{B}}(t)$ is white noise (the two-time correlation function is a delta function of time = no correlation at different times) and is expressed as:

$$\boxed{\langle \mathbf{F}_{\mathrm{B}}(t) \cdot \mathbf{F}_{\mathrm{B}}(t') \rangle = 2d\zeta k_{\mathrm{B}} T \delta(t - t')} \tag{11}$$

  (This is the second type of fluctuation-dissipation theorem [Derivation can be found in the appendix]).
- In the next section, we will discretize this Langevin equation and solve it numerically.

3.2. Discretization of the Langevin Equation

- The Langevin equation maintains thermal equilibrium by being driven by random forces at each time step, with energy dissipated accordingly.
- Therefore, high precision is not required for the discretization of the Langevin equation; the (semi-implicit) Euler method is sufficient.
- The discretization method using the Euler method applied to such stochastic differential equations is called the Euler-Maruyama method [3].
- Next, we consider the treatment of the Dirac delta function that appears in the correlation function of the thermal fluctuation force.
- By integrating the time correlation function of the thermal fluctuation force (Eq. (49)) with the time step Δt, we obtain the relation:

$$2dk_{\mathrm{B}}T\zeta = \int_{-\infty}^{\infty} \mathrm{d}t' \left\langle \mathbf{F}(t'+t_0)\cdot\mathbf{F}(t_0)\right\rangle \sim \left\langle \mathbf{F}(t_0)^2\right\rangle \Delta t \tag{12}$$

- Therefore,

$$\left\langle \mathbf{F}(t_0)^2\right\rangle \sim \frac{2dk_{\mathrm{B}}T\zeta}{\Delta t} \tag{13}$$

indicating that the variance of each component of the thermal fluctuation force is $\frac{2k_{\mathrm{B}}T\zeta}{\Delta t}$.

3.2. Discretization of the Langevin Equation (2)

- Thus, the thermal fluctuation force is expressed as:

$$\mathbf{F}_{\mathrm{B}}(t) \sim \sqrt{\frac{2k_{\mathrm{B}}T\zeta}{\Delta t}}\mathbf{R}_{\mathrm{G}} \tag{14}$$

  where $\mathbf{R}_{\mathrm{G}}$ is a Gaussian random vector with a mean of $\mathbf{0}$ and a standard deviation of 1 for each component.
- Discretizing the Langevin equation (Eq. (48)) using the Euler-Maruyama method gives:

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) - \frac{\zeta}{m}\mathbf{v}(t)\Delta t + \sqrt{\frac{2k_{\mathrm{B}}T\zeta\Delta t}{m^2}}\mathbf{R}_{\mathrm{G}} \tag{15}$$

  In the following, we will nondimensionalize this discretized difference equation.

3.3. Nondimensionalization

In this section, we will nondimensionalize the discretized Langevin equation (Eq. (15)).

- Let the unit of length be the particle diameter a [m], and the unit of time be t_0 [s]. Setting $\mathbf{v} = \frac{a}{t_0}\tilde{\mathbf{v}}$, $t = t_0\tilde{t}$, and substituting into Eq. (15) gives:

$$\frac{a}{t_0}\tilde{\mathbf{v}}(\tilde{t}+\Delta\tilde{t}) = \frac{a}{t_0}(1-\frac{\zeta}{m}t_0\Delta\tilde{t})\tilde{\mathbf{v}}(\tilde{t}) + \sqrt{\frac{2k_{\mathrm{B}}T\zeta t_0\Delta\tilde{t}}{m^2}}\mathbf{R}_{\mathrm{G}} \tag{16}$$

  Dividing both sides of Eq. (16) by a/t_0 gives the equation in terms of nondimensional numbers:

$$\tilde{\mathbf{v}}(\tilde{t}+\Delta\tilde{t}) = (1-\frac{\zeta}{m}t_0\Delta\tilde{t})\tilde{\mathbf{v}}(\tilde{t}) + \sqrt{\frac{2k_{\mathrm{B}}T\zeta t_0^3\Delta\tilde{t}}{m^2a^2}}\mathbf{R}_{\mathrm{G}} \tag{17}$$

- Choosing the unit of time t_0 as $t_0 = \frac{m}{\zeta} = t_d$, which was used in the analysis of damped motion in the second lecture, simplifies the undetermined coefficient on the right-hand side of Eq. (17) to:

$$\tilde{\mathbf{v}}(\tilde{t}+\Delta\tilde{t}) = (1-\Delta\tilde{t})\tilde{\mathbf{v}}(\tilde{t}) + \sqrt{\frac{2mk_{\mathrm{B}}T}{a^2\zeta^2}\Delta\tilde{t}}\mathbf{R}_{\mathrm{G}} \tag{18}$$

- Here, since the coefficient attached to the thermal fluctuation force is a nondimensional number, we define it as: $T^* = \frac{mk_{\mathrm{B}}T}{a^2\zeta^2}$, which becomes the **parameter** in this calculation.[1]

3.3. Nondimensionalization (2)

- Generally, the parameters that appear in dynamic equations can often be expressed as the **ratio of time scales that characterize different physical phenomena**.
- In fact, taking the ratio of the time scale for damping motion relaxation $t_d = \frac{m}{\zeta}$ and the time scale characterizing diffusion $t_{\mathrm{B}} = \frac{a^2\zeta}{k_{\mathrm{B}}T} (= a^2/D)$ gives:

$$T^* = \frac{mk_{\mathrm{B}}T}{a^2\zeta^2} = \frac{t_d}{t_{\mathrm{B}}} \tag{19}$$

This indicates that as T^* increases, the diffusion time t_{B} becomes relatively shorter compared to the damping relaxation time.

- Thus, the nondimensionalized (velocity-related) Langevin equation becomes:

$$\tilde{\mathbf{v}}(\tilde{t} + \Delta\tilde{t}) = (1 - \Delta\tilde{t})\tilde{\mathbf{v}}(\tilde{t}) + \sqrt{2T^*\Delta\tilde{t}}\mathbf{R}_{\mathrm{G}} \tag{20}$$

Here, any nondimensional number can be assigned to T^*. Moreover, the results of the numerical calculations will systematically change depending on the value of T^*.

3.3. Nondimensionalization (3)

- Additionally, for position:

$$\tilde{\mathbf{r}}(\tilde{t}+\Delta\tilde{t}) = \tilde{\mathbf{r}}(\tilde{t}) + \tilde{\mathbf{v}}(\tilde{t}+\Delta\tilde{t})\Delta\tilde{t} \tag{21}$$

  This is the discretization used.

- Here, Eq. (21) is treated as an implicit method, and Eq. (20) as an explicit method. This is the **Semi-implicit Euler method**.
- Finally, after generating Gaussian random numbers $\mathbf{R}_{\mathrm{G}}$, numerical calculations can be performed. The method for generating Gaussian random numbers will be explained in the next section.

[1] An arbitrary number can be assigned, and the behavior of the solution qualitatively changes depending on its value.

3.4. Method for Generating Normal Random Numbers: Box-Muller Method [1]

In this section, we introduce the method for numerically generating normal random numbers.

- The Box-Muller method [1] is well-known for generating normal random numbers $\mathbf{R}_G$ with a variance of 1.

Box-Muller Method [1]

When U_1 and U_2 are uniformly distributed random numbers in the range $[0, 1]$, the following X_1 and X_2 are independent standard normal random numbers (with a variance of 1).

$$X_1 = \sqrt{-2\log U_1}\cos 2\pi U_2 \tag{22}$$

$$X_2 = \sqrt{-2\log U_1}\sin 2\pi U_2 \tag{23}$$

(Proof)

- By solving for U_1 and U_2 using Eqs. (22) and (23), we obtain:

$$\log U_1 = -\frac{X_1^2 + X_2^2}{2} \tag{24}$$

$$U_1 = e^{-\frac{X_1^2+X_2^2}{2}} \tag{25}$$

3.4. Method for Generating Normal Random Numbers: Box-Muller Method [1] (2)

- By dividing Eq. (22) by Eq. (23), we obtain:

$$\begin{aligned} \frac{X_2}{X_1} &= \tan 2\pi U_2 \\ U_2 &= \frac{1}{2\pi} \arctan \frac{X_2}{X_1} \end{aligned} \tag{26}$$

- Using these, it is shown that X_1 and X_2 are **independent Gaussian processes**.
- Now, introduce the probability density functions $P(X_1, X_2)$ and $\tilde{P}(U_1, U_2)$.
- The relationship between $P(X_1, X_2)$ and $\tilde{P}(U_1, U_2)$ is given by:

$$P(X_1, X_2)\mathrm{d}X_1\mathrm{d}X_2 = \tilde{P}(U_1, U_2)\mathrm{d}U_1\mathrm{d}U_2 \tag{27}$$

$$= \tilde{P}(U_1, U_2)\left|\frac{\partial(U_1, U_2)}{(X_1, X_2)}\right|\mathrm{d}X_1\mathrm{d}X_2 \tag{28}$$

3.4. Method for Generating Normal Random Numbers: Box-Muller Method [1] (3)

- Since U_1 and U_2 are independent uniform random numbers with a threshold of $[0, 1]$, we have:

$$\int_0^1 \mathrm{d}U_1 \int_0^1 \mathrm{d}U_2 \tilde{P}(U_1, U_2) = 1 \tag{29}$$

  leading to $\tilde{P}(U_1, U_2) = 1$. Therefore,

$$P(X_1, X_2) = \left| \frac{\partial(U_1, U_2)}{(X_1, X_2)} \right| \tag{30}$$

- Now, the Jacobian $|\frac{\partial(U_1, U_2)}{(X_1, X_2)}|$ is given by:

$$\left| \frac{\partial(U_1, U_2)}{(X_1, X_2)} \right| = \begin{vmatrix} \frac{\partial U_1}{\partial X_1} & \frac{\partial U_2}{\partial X_1} \\ \frac{\partial U_1}{\partial X_2} & \frac{\partial U_2}{\partial X_2} \end{vmatrix} \tag{31}$$

$$= \left| \frac{\partial U_1}{\partial X_1} \frac{\partial U_2}{\partial X_2} - \frac{\partial U_2}{\partial X_1} \frac{\partial U_1}{\partial X_2} \right| \tag{32}$$

3.4. Method for Generating Normal Random Numbers: Box-Muller Method [1] (4)

- Thus, by performing the appropriate differentiation, we obtain:

$$\left|\frac{\partial(U_1, U_2)}{(X_1, X_2)}\right| = \left| \frac{1}{2\pi} \frac{e^{-\frac{X_1^2+X_2^2}{2}}}{1+(\frac{X_2}{X_1})^2} - \frac{1}{2\pi} \frac{-X_2^2}{X_1^2} \frac{e^{-\frac{X_1^2+X_2^2}{2}}}{1+(\frac{X_2}{X_1})^2} \right| \tag{33}$$

$$= \frac{1}{2\pi} e^{-X_1^2+X_2^2/2} = \frac{1}{\sqrt{2\pi}} e^{-X_1^2/2} \frac{1}{\sqrt{2\pi}} e^{-X_2^2/2} \tag{34}$$

Thus,

$$P(X_1, X_2) = \frac{1}{\sqrt{2\pi}} e^{-X_1^2/2} \frac{1}{\sqrt{2\pi}} e^{-X_2^2/2} \tag{35}$$

Since $P(X_1, X_2) = p(X_1)p(X_2)$, it has been shown that X_1 and X_2 are **independent Gaussian processes**.

Differentiation of $y = \arctan x$

3.4. Method for Generating Normal Random Numbers: Box-Muller Method [1] (5)

For $y = \arctan x$, we have $x = \tan y$. Differentiating this with respect to y gives:

$$\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{1}{\cos^2 y} \tag{36}$$

Thus,

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \cos^2 y = \frac{1}{1 + \tan^2 y} = \frac{1}{1 + x^2} \tag{37}$$

3.5. Acceleration of the Box-Muller Method (Marsaglia Polar Method)

Improved Box-Muller Method (Marsaglia Polar Method) [4]

1. Using uniform random numbers u_1, u_2 within the range $[-1, 1]$, a two-dimensional vector

$$\mathbf{R} = (u_1, u_2) \tag{38}$$

is introduced. Here, $\mathbf{R}$ is randomly generated, and only pairs of random numbers that fall within a circle of radius 1 are selected (those outside are discarded).

2. The obtained $R^2 = u_1^2 + u_2^2$ is a uniform random number with a threshold of $[0, 1]$ (proof is provided below). Therefore, we can set $U_1 = R^2$ and obtain $\sqrt{-2\log U_1}$.

3. Next, the polar angle of $\mathbf{R}$ is uniformly distributed within the range $[0, 2\pi]$, which is equivalent to $2\pi U_2$. This implies that trigonometric functions with the argument $2\pi U_2$ can be indirectly obtained as:

$$\frac{u_1}{R} = \cos 2\pi U_2 \tag{39}$$

$$\frac{u_2}{R} = \sin 2\pi U_2 \tag{40}$$

- In the Box-Muller method, **trigonometric calculations are relatively heavy**, and generating a large number of random numbers incurs significant computational cost.
- Here, by adopting a clever computational method, we introduce the Marsaglia Polar Method [4], which **produces the same results as the Box-Muller method without directly calculating trigonometric functions**.

3.5. Acceleration of the Box-Muller Method (Marsaglia Polar Method) (2)

(Proof of 2)

If we set $X = R^2$, the relationship between the probability density function $f(X)$ and the probability density function $g(R)$ concerning R is:

$$f(X)\mathrm{d}X = g(R)\mathrm{d}R = g(R)\frac{\partial R}{\partial X}\mathrm{d}X \tag{41}$$

Here, since $g(R)$ is proportional to R^2, we have $g(R) = CR$. By performing the following integration:

$$\int_0^1 g(R)\mathrm{d}R = \left[\frac{C}{2}R^2\right]_0^1 = \frac{C}{2} = 1 \tag{42}$$

we find $C = 2$. Therefore, $\frac{\partial R}{\partial X} = \frac{1}{2R}$, leading to:

$$f(X)\mathrm{d}X = \frac{2R}{2R}\mathrm{d}X = 1\mathrm{d}X \tag{43}$$

Since $f(X) = 1$, it is shown that R^2 is a uniform random number with a threshold of $[0, 1]$.

3.5. Acceleration of the Box-Muller Method (Marsaglia Polar Method) (3)

リスト 3: Algorithm for generating normal random numbers (Box-Muller Method). The following program ”BM.h” is available from the GitHub repository **[Link]**. It can be included as a subroutine or as a header.

```
1
2
3  double unif_rand(double left, double right)
4  {
5    return left + (right - left)*rand()/RAND_MAX;
6  }
7  double gaussian_rand(void)
8  {
9    static double iset = 0;
10   static double gset;
11   double fac, rsq, v1, v2;
12
13   if (iset == 0) {
14     do {
15       v1 = unif_rand(-1, 1);
16       v2 = unif_rand(-1, 1);
17       rsq = v1*v1 + v2*v2;
18     } while (rsq >= 1.0 || rsq == 0.0);
19     fac = sqrt(-2.0*log(rsq)/rsq);
20
21     gset = v1*fac;
```

3.5. Acceleration of the Box-Muller Method (Marsaglia Polar Method) (4)

```
22      iset = 0.50;
23      return v2*fac;
24    } else {
25      iset = 0;
26      return gset;
27    }
28  }
```

[2] When dividing into annular segments, the area of the small section is proportional to R

Contents

4. Various Types of Averages

Numerical calculation results include statistical errors, so various averaging operations are performed during analysis to extract physically significant elements. Here, two commonly used averaging methods are introduced.

4.1. Time Averaging

Time Averaging

Time averaging is the process of averaging the values of physical quantities at each time in a steady state.

- This operation is performed on physical quantities $X(t)$ in a steady state and is actually calculated as

$$\langle X \rangle_{t_0} = \lim_{T \to \infty} \frac{1}{T} \int_0^T \mathrm{d}t_0 X(t_0) \tag{44}$$

- Similarly, when this operation is applied to a two-time correlation function $C(t, t_0) = X(t + t_0)X(t_0)$, it becomes

$$C(t) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \mathrm{d}t_0 C(t, t_0) \tag{45}$$

At this time, $C(t) = \langle X(t + t_0)X(t_0) \rangle_{t_0}$, or more simply $C(t) = \langle X(t)X(0) \rangle$.

4.2. Ensemble Averaging

Ensemble Averaging

Ensemble averaging refers to the averaging process carried out by summing up the results of multiple independent and identical trials (experiments).

- When the physical quantity of the α-th sample in thermal equilibrium is A_i, the ensemble average is

$$\langle A \rangle_{\text{ens}} = \frac{1}{N_{\text{ens}}} \sum_{\alpha=1}^{N_{\text{ens}}} A_\alpha \tag{46}$$

- (Reference) This is equivalent to the statistical mechanical average as follows:

$$\langle A \rangle_{\text{ens}} = \frac{\text{Tr} A(\mathbf{q}, \mathbf{p}) e^{-\beta \hat{H}(\mathbf{q},\mathbf{p})}}{Z} \tag{47}$$

Here, Z is the partition function: $Z = \text{Tr} e^{-\beta \hat{H}(\mathbf{q},\mathbf{p})}$.

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5. Assignment 4

Assignment 4 Implementation of Single Particle Brownian Motion

Consider the motion of a single particle driven by thermal fluctuation forces in a three-dimensional solvent with temperature T and friction coefficient ζ. The motion of this particle can be modeled by the Langevin equation $m\dot{\mathbf{v}}(t) = -\zeta\mathbf{v}(t) + \mathbf{F}_{\mathrm{B}}(t)$, as is widely known. When this Langevin equation is non-dimensionalized by taking the units of length and time as a and $\frac{m}{\zeta}$ respectively, the parameter $T^* = \frac{mk_{\mathrm{B}}T}{a^2\zeta^2}$ appears, as discussed in the lecture. Based on this, answer the following questions regarding the motion of this particle. Note that the following $\langle\cdots\rangle$ denotes quantities that have been sufficiently averaged over ensemble and time.

(1) Derive the analytical solution for the mean squared displacement $\left\langle \Delta\mathbf{r}(t)^2 \right\rangle = \frac{2dk_{\mathrm{B}}T}{\zeta}\left\{t - \frac{m}{\zeta}e^{-\zeta t/m} - \frac{m}{\zeta}\right\}$, and express it using the parameter T^* after non-dimensionalizing it.

(2) For any T^*, confirm that the theoretical solution derived in (1) matches the numerical solution. The numerical solution should be obtained using the semi-implicit Euler-Maruyama method.

(3) Calculate the velocity autocorrelation function of the particle $C(t) = \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$.

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6.1. Derivation of the Fluctuation-Dissipation Theorem

In this section, we will prove the (second kind) fluctuation-dissipation theorem from the Langevin equation. Although this principle may be omitted without affecting the course, understanding the basic principles is important for studying natural sciences, so an outline is provided below.

- The Brownian motion of a sphere of mass m moving in a solvent (heat bath) at temperature T with a drag coefficient ζ can be modeled by the following Langevin equation:

$$\boxed{m\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} = -\zeta\mathbf{v}(t) + \mathbf{F}_{\mathrm{B}}(t)} \tag{48}$$

- Here, the thermal fluctuation force $\mathbf{F}_{\mathrm{B}}(t)$ is white noise (the two-time correlation function is a delta function in time) and satisfies

$$\boxed{\langle \mathbf{F}_{\mathrm{B}}(t)\mathbf{F}_{\mathrm{B}}(t')\rangle = B\delta(t-t')\mathbf{1}} \tag{49}$$

  where $\mathbf{1}$ is the identity matrix, and $\mathbf{F}_{\mathrm{B}}(t)$ shows a Gaussian distribution with variance $\sqrt{B\delta(t-t')}$ due to the central limit theorem.

- Next, we determine the value of the correlation coefficient B based on the properties of particles moving in a heat bath at temperature T.

6.1. Derivation of the Fluctuation-Dissipation Theorem (2)

- According to classical equilibrium statistical mechanics, the equipartition theorem tells us that, for a spatial dimension d,

$$\boxed{\langle \mathbf{v}(t)^2 \rangle = \frac{dk_{\mathrm{B}}T}{m}} \tag{50}$$

  where k_{B} is the Boltzmann constant. The relationship between the Boltzmann constant and the gas constant R is given by $nR = Nk_B$, where n is the number of moles and N is the number of particles.

- By solving the Langevin equation (Eq. 48) using the method of variation of constants, the velocity vector is given by

$$\mathbf{v}(t) = \frac{1}{m}\int_{-\infty}^{t} \mathrm{d}t' \mathbf{F}_{\mathrm{B}}(t') e^{-\gamma(t-t')} \tag{51}$$

  Here, for simplicity, we set $\zeta = m\gamma$.

6.1. Derivation of the Fluctuation-Dissipation Theorem (3)

- The mean square of the velocity vector, expressed as a double integral, is given by

$$\begin{aligned}
\left\langle \mathbf{v}(t)^2 \right\rangle &= \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t} \mathrm{d}t_2 \left\langle \mathbf{F}_\mathrm{B}(t_1) \cdot \mathbf{F}_\mathrm{B}(t_2) \right\rangle e^{-\gamma(t-t_1)} e^{-\gamma(t-t_2)} \\
&= \frac{1}{m^2} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t} \mathrm{d}t_2 dB\delta(t_1 - t_2) e^{-2\gamma(t-t_1-t_2)} \\
&= \frac{1}{m^2} \int_{-\infty}^{t} \mathrm{d}t_1 dB e^{-2\gamma(t-t_1)} \\
&= \frac{1}{m^2} \int_{0}^{\infty} \mathrm{d}t' dB e^{-2\gamma t'} \\
&= \frac{Bd}{2m^2\gamma}
\end{aligned} \tag{52}$$

- Since $\left\langle \mathbf{v}(t)^2 \right\rangle = \frac{dk_\mathrm{B}T}{m}$ and noting that $m\gamma = \zeta$, the value of B is determined as

$$\boxed{B = 2\zeta k_\mathrm{B} T} \tag{53}$$

6.1. Derivation of the Fluctuation-Dissipation Theorem (4)

- Therefore, the correlation function of the thermal fluctuation force satisfies

$$\boxed{\langle \mathbf{F}_{\mathrm{B}}(t)\mathbf{F}_{\mathrm{B}}(t')\rangle = 2\zeta k_{\mathrm{B}}T\delta(t-t')\mathbf{1}} \tag{54}$$

This relationship, which expresses the balance between fluctuation forces (noise) and dissipation (impedance) in thermal equilibrium systems, is known as the
(second kind) fluctuation-dissipation theorem (FDT).

6.2. Velocity Autocorrelation Function

Next, we theoretically derive the velocity autocorrelation function of a particle moving in a Langevin heat bath. (This is important for understanding diffusion processes.)

- Taking the inner product of both sides of the Langevin equation with $\mathbf{v}(0)$ and averaging, we obtain

$$m\frac{\mathrm{d}\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle}{\mathrm{d}t} = -\zeta\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle + \langle \mathbf{F}_{\mathrm{B}}(t)\cdot\mathbf{v}(0)\rangle \tag{55}$$

Since the force at time t and the velocity at time 0 are uncorrelated, the second term on the right-hand side drops out. Letting the velocity autocorrelation function be $C(t) = \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle$, we have

$$\boxed{m\frac{\mathrm{d}C(t)}{\mathrm{d}t} = -\zeta C(t)} \tag{56}$$

Thus, $C(t)$ is described by a simple decaying differential equation. For $t > 0$, we obtain

$$C(t) = C(0)e^{-\gamma t} \tag{57}$$

Moreover, by the symmetry of correlation functions under time translation symmetry[3], we have

$$\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle = \langle \mathbf{v}(t-t)\cdot\mathbf{v}(-t)\rangle = \langle \mathbf{v}(0)\cdot\mathbf{v}(-t)\rangle \tag{58}$$

From this, setting $t' = -t$ (negative value), we get

$$C(t') = C(0)e^{\gamma t'} \tag{59}$$

6.2. Velocity Autocorrelation Function (2)

- Noting that $C(0) = \frac{dk_{\mathrm{B}}T}{m}$, and summarizing these results for general t, we obtain

$$\boxed{C(t) = \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle = \frac{dk_{\mathrm{B}}T}{m} e^{-\gamma|t|}} \tag{60}$$

Moreover, in the steady state, time translation symmetry holds for correlation functions, so

$$\boxed{C(t_1 - t_2) = \langle \mathbf{v}(t_1) \cdot \mathbf{v}(t_2) \rangle = \frac{dk_{\mathrm{B}}T}{m} e^{-\gamma|t_1 - t_2|}} \tag{61}$$

[3] The property that the value does not change even if the time of the two-time correlation function is shifted by an equal amount.

6.3. Mean Squared Displacement

Next, we theoretically examine the short-time and long-time behavior of a particle moving in a Langevin heat bath. In particular, diffusion behavior is observed in the long-time limit.

- The mean squared displacement is given by

$$\left\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \right\rangle \to 2dDt \quad (t \to \infty) \tag{62}$$

  where D is the **diffusion coefficient**.
- We now demonstrate that such behavior is reproduced by the solution of the Langevin equation, and also show the short-time behavior simultaneously.
- The displacement $\mathbf{r}(t) - \mathbf{r}(0)$ is obtained by integrating $\mathbf{v}(t)$:

$$\mathbf{r}(t) - \mathbf{r}(0) = \int_0^t \mathrm{d}t' \mathbf{v}(t') \tag{63}$$

  Thus, the mean squared displacement, written as a double integral, is

$$\begin{aligned} \left\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \right\rangle = \left\langle \Delta\mathbf{r}(t)^2 \right\rangle &= \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \left\langle \mathbf{v}(t_1) \cdot \mathbf{v}(t_2) \right\rangle \\ &= \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \frac{dk_\mathrm{B}T}{m} e^{-\gamma|t_1 - t_2|} \end{aligned} \tag{64}$$

6.3. Mean Squared Displacement (2)

We now divide the entire integration region into $t_1 > t_2$ and $t_1 < t_2$. Since the value of the integral is equal due to symmetry, we can restrict the calculation to $t_1 > t_2$ and multiply by 2 to account for the entire region (the integration region is shown in Figure **3**). Then,

$$\begin{aligned}
\left\langle \Delta \mathbf{r}(t)^2 \right\rangle &= \frac{2dk_{\mathrm{B}}T}{m} \int_0^t \mathrm{d}t_2 \int_{t_2}^t \mathrm{d}t_1 e^{-\gamma(t_1 - t_2)} \\
&= \frac{-2dk_{\mathrm{B}}T}{m\gamma} \int_0^t \mathrm{d}t_2 \left(e^{-\gamma(t-t_2)} - 1 \right) \\
&= \frac{2dk_{\mathrm{B}}T}{m\gamma} \left\{ t + \frac{1}{\gamma} e^{-\gamma t} - \frac{1}{\gamma} \right\} \qquad (65)
\end{aligned}$$

6.3. Mean Squared Displacement (3)

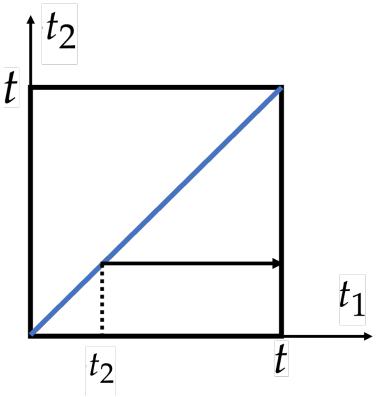

図 3: The integration region in equation (65) (first integrate with respect to t_1 over the region $t_2 \leq t_1 \leq t$, then integrate with respect to t_2 over the region $0 \leq t_2 \leq t$).

- We now consider the long-time and short-time behavior of the mean squared displacement.

6.3. Mean Squared Displacement (4)

- **Long-time behavior:** When $t \gg \gamma = 1/\gamma = m/\zeta$, the exponential and constant terms drop out in equation (65), leaving only the linear term in t:

$$\boxed{\left\langle \Delta \mathbf{r}(t)^2 \right\rangle \sim \frac{2dk_\mathrm{B}T}{m\gamma} t = \frac{2dk_\mathrm{B}T}{\zeta} t \equiv 2dDt} \tag{66}$$

  Thus, long-time behavior shows diffusion. Furthermore, the relation

$$\boxed{D = \frac{k_\mathrm{B}T}{\zeta}} \tag{67}$$

  is obtained, known as the Einstein relation.
- **Short-time behavior:** For $t \ll \gamma = 1/\gamma = m/\zeta$, expanding the exponential term in equation (65) using a Maclaurin series gives $e^{-\gamma t} \sim 1 - \gamma t + \frac{1}{2}\gamma^2$. Substituting this into equation (65), we obtain

$$\boxed{\left\langle \Delta \mathbf{r}(t)^2 \right\rangle \sim \frac{2dk_\mathrm{B}T}{m} t^2} \tag{68}$$

  Thus, short-time behavior shows t^2 behavior (ballistic motion). Additionally, since the average velocity in the equipartition theorem is $\left\langle \mathbf{v}(t)^2 \right\rangle = \frac{2dk_\mathrm{B}T}{m}$, we have $\left\langle \Delta \mathbf{r}(t)^2 \right\rangle \sim \left\langle (\mathbf{v}(t)t)^2 \right\rangle$, indicating uniform linear motion of velocity $\langle \mathbf{v}(t) \rangle$.

6.4. First Fluctuation-Dissipation Theorem and Green-Kubo Formula

So far, we have discussed the relationship between correlation functions and transport coefficients in thermal equilibrium systems and weakly non-equilibrium systems. Here, we consider the relationship between the velocity autocorrelation function and the diffusion coefficient.

- By integrating the velocity autocorrelation function $\langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle = \frac{k_B T}{m} e^{-\gamma |t|}$ over time, we obtain

$$\int_0^\infty \mathrm{d}t \, \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle = \frac{d k_B T}{\gamma m} = \frac{d k_B T}{\zeta} = dD \tag{69}$$

This shows that the diffusion coefficient is given by

$$D = \frac{1}{d} \int_0^\infty \mathrm{d}t \, \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle \tag{70}$$

This discussion can be extended to various systems such as thermal conduction and electrical conduction. In general, such a balance relationship between correlation functions and transport coefficients that ensures thermal equilibrium is known as the first fluctuation-dissipation theorem. It is also referred to as the Green-Kubo formula[4] [5, 6].

[4] A linear response theory discussing perturbations under weak external fields

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