Internship report M1 – 2022

Brownian Motion near a Soft Surface
Supporting Information

Yilin YE

SUPERVISOR: Yacine AMAROUCHENE, David DEAN, Thomas SALEZ - *Université de Bordeaux, CNRS, Laboratoire Ondes et Matière d'Aquitaine, UMR 5798, F-33405, Talence, France*

Theoretical Analyses

Situation of the problem

The equations of motion are shown below [1]

$$\ddot{X}_G + \frac{2\varepsilon\xi}{3}\frac{\dot{X}_G}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_G}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta}-\ddot{X}_G}{\Delta^{5/2}}\right] - \sqrt{\frac{\varepsilon}{2}}\sin\alpha = 0$$

$$\ddot{\Delta} + \xi\frac{\dot{\Delta}}{\Delta^{3/2}} + \frac{\kappa\xi}{4}\left[21\frac{\dot{\Delta}^2}{\Delta^{9/2}} - \frac{(\dot{\Theta}-\dot{X}_G)^2}{\Delta^{7/2}} - \frac{15}{2}\frac{\ddot{\Delta}}{\Delta^{7/2}}\right] + \cos\alpha = 0$$

$$\ddot{\Theta} + \frac{4\varepsilon\xi}{3}\frac{\dot{\Theta}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{3}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{X}_G}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{X}_G-\ddot{\Theta}}{\Delta^{5/2}}\right] = 0$$

with $\alpha = 0$ for a plan case.

For the convenience, we simplify all coefficients as:

$$\ddot{\Delta} + a_1\frac{\dot{\Delta}}{\Delta^{3/2}} + a_2\frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3\frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3\frac{\dot{X}^2}{\Delta^{7/2}} + a_4\frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_5\frac{\ddot{\Delta}}{\Delta^{7/2}} + a_6 = 0$$

$$\ddot{X}_G + b_1\frac{\dot{X}}{\sqrt{\Delta}} + b_2\frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_4\frac{\ddot{\Theta}}{\Delta^{5/2}} + b_5\frac{\ddot{X}_G}{\Delta^{5/2}} + b_6 = 0$$

$$\ddot{\Theta} + c_1\frac{\dot{\Theta}}{\sqrt{\Delta}} + c_2\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3\frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + c_4\frac{\ddot{X}_G}{\Delta^{5/2}} + c_5\frac{\ddot{\Theta}}{\Delta^{5/2}} + c_6 = 0$$

with coefficients: $a_1 = \xi$, $a_2 = \frac{21\kappa\xi}{4}$, $a_3 = -\frac{\kappa\xi}{4}$, $a_4 = \frac{\kappa\xi}{2}$, $a_5 = -\frac{15\kappa\xi}{8}$, $a_6 = \cos(\alpha = 0) = 1$; $b_1 = \frac{2\varepsilon\xi}{3}$, $b_2 = \frac{19\kappa\xi\varepsilon}{24}$, $b_3 = -\frac{\kappa\xi\varepsilon}{6}$, $b_4 = \frac{\kappa\xi\varepsilon}{12}$, $b_5 = -\frac{\kappa\xi\varepsilon}{12}$, $b_6 = \sin(\alpha = 0) = 0$; and $c_1 = \frac{4\varepsilon\xi}{3}$, $c_2 = \frac{19\kappa\xi\varepsilon}{12}$, $c_3 = -\frac{\kappa\xi\varepsilon}{3}$, $c_4 = \frac{\kappa\xi\varepsilon}{6}$, $c_5 = -\frac{\kappa\xi\varepsilon}{6}$, $c_6 = 0$. In addition, we write $\ddot{\Delta}, \ddot{X}_G, \ddot{\Theta}$ as $\dot{v}_z, \dot{v}_x, \dot{v}_\theta$, $\dot{\Delta}, \dot{X}_G, \dot{\Theta}$ as v_z, v_x, v_θ, Δ, X_G, Θ as r_z, r_x, r_θ.

Effective friction matrix

Mass matrix

Consider the deterministic equation with mass according to the equations of motion mentioned above:

$$m_\alpha \cdot \dot{v}_\alpha = \left[F_{1\alpha}(\mathbf{x}) + F_{2\alpha\beta}(\mathbf{x})\dot{v}_\beta\right] - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta$$

we have

$$F_{1z} = -m_z a_6 = -m_z \qquad F_{1x} = -m_x b_6 = 0 \qquad F_{1\theta} = -m_\theta c_6 = 0$$

$$F_{2hzz} = -\frac{m_z a_5}{\Delta^{7/2}} \qquad F_{2hzx} = 0 \qquad F_{2hz\theta} = 0$$

$$F_{2hxz} = 0 \qquad F_{2hxx} = -\frac{m_x b_5}{\Delta^{5/2}} \qquad F_{2hx\theta} = -\frac{m_x b_4}{\Delta^{5/2}}$$

$$F_{2h\theta z} = 0 \qquad F_{2h\theta x} = -\frac{m_\theta c_4}{\Delta^{5/2}} \qquad F_{2h\theta\theta} = -\frac{m_\theta c_5}{\Delta^{5/2}}$$

Introduce the mass matrix as $M_{\alpha\beta} = \delta_{\alpha\beta} \cdot m_\alpha - F_{2h\alpha\beta}(\mathbf{x})$:

$$M = \begin{pmatrix} m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}} & 0 & 0 \\ 0 & m_x - \frac{\kappa\xi\varepsilon m_x}{12\Delta^{5/2}} & \frac{\kappa\xi\varepsilon m_x}{12\Delta^{5/2}} \\ 0 & \frac{\kappa\xi\varepsilon m_\theta}{6\Delta^{5/2}} & m_\theta - \frac{\kappa\xi\varepsilon m_\theta}{6\Delta^{5/2}} \end{pmatrix}$$

with its inverse matrix

$$M^{-1} = \begin{pmatrix} \frac{1}{m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}}} & 0 & 0 \\ 0 & \frac{12\Delta^{5/2} - 2\kappa\xi\varepsilon}{12\Delta^{5/2} m_x - 3\kappa\xi\varepsilon m_x} & \frac{\kappa\xi\varepsilon}{3m_\theta\left(\kappa\xi\varepsilon - 4\Delta^{5/2}\right)} \\ 0 & \frac{2\kappa\xi\varepsilon}{3m_x\left(\kappa\xi\varepsilon - 4\Delta^{5/2}\right)} & \frac{12\Delta^{5/2} - \kappa\xi\varepsilon}{12\Delta^{5/2} m_\theta - 3\kappa\xi\varepsilon m_\theta} \end{pmatrix}$$

The inverse matrix at first-order approximation of κ shows

$$M^{-1} \approx \begin{pmatrix} \frac{1}{m_z} + \frac{15\kappa\xi}{8\Delta^{5/2} m_z} & 0 & 0 \\ 0 & \frac{1}{m_x} + \frac{\kappa\xi\varepsilon}{12\Delta^{5/2} m_x} & -\frac{\kappa\xi\varepsilon}{12\Delta^{5/2} m_\theta} \\ 0 & -\frac{\kappa\xi\varepsilon}{6\Delta^{5/2} m_x} & \frac{1}{m_\theta} + \frac{\kappa\xi\varepsilon}{6\Delta^{5/2} m_\theta} \end{pmatrix}$$

Fokker-Planck equation for friction matrix

Let $\mathbb{P}(q,t)$ be the probability density function to find a particle in $[q, q+dq]$, as the general coordinate q satisfies

$$\dot{q}(t) = -W'(q) + \xi(t)$$

where $\xi(t)$ refers to the Wiener process. We have the Fokker-Planck equation as

$$\frac{\partial \mathbb{P}(q,t)}{\partial t} = \frac{\partial}{\partial q}\left[\frac{dW(q)}{dq} + T\frac{\partial}{\partial q}\right]\mathbb{P}(q,t)$$

Suppose that $\mathbf{x}, \mathbf{v}$ refer to the position and velocity, respectively. We consider the following deterministic equation

$$d\mathbf{x} = \mathbf{v}dt$$

$$d\mathbf{v} = -\mathbf{U}dt - \nabla\phi(\mathbf{x})dt$$

where $\phi(\mathbf{x})$ is the external potential only including gravity. We assume that $\mathbf{U}$ are generated by hydrodynamic interactions, which do not however affect the equilibrium Gibbs-Boltzmann distribution shown as

$$P_{eq}(\mathbf{x},\mathbf{v}) = \frac{1}{Z}\exp\left(-\frac{\beta\mathbf{v}^2}{2} - \beta\phi(\mathbf{x})\right)$$

Note, $\frac{\partial P}{\partial x_\alpha} = P\left(-\beta\frac{\partial\phi}{\partial x_\alpha}\right)$, $\frac{\partial P}{\partial v_\alpha} = P(-\beta v_\alpha)$, and $\beta^{-1} = k_B T \xrightarrow{k_B=1} T$.

Exploit the Fokker-Planck equation on the distribution probability P above as a function of time t.

$$\begin{aligned}\frac{\partial P}{\partial t} &= \frac{\partial}{\partial v_\alpha}\left[(U_\alpha + \nabla_\alpha\phi)P + T\frac{\partial P}{\partial v_\alpha}\right] + \frac{\partial}{\partial x_\alpha}\left(T\frac{\partial P}{\partial v_\alpha}\right) \\ &= \frac{\partial}{\partial v_\alpha}\left[(U_\alpha + \nabla_\alpha\phi)P + T\frac{\partial P}{\partial v_\beta}\frac{\partial v_\beta}{\partial v_\alpha}\right] + \frac{\partial}{\partial x_\alpha}\left[T \cdot P(-\beta v_\alpha)\right] \\ &= \frac{\partial}{\partial v_\alpha}\left[T\gamma_{\alpha\beta}\frac{\partial P}{\partial v_\beta} + U_\alpha P + \frac{\partial\phi}{\partial x_\alpha}P\right] - \frac{\partial}{\partial x_\alpha}(v_\alpha P)\end{aligned}$$

The last two terms would vanish since

$$\frac{\partial}{\partial v_\alpha}\left(\frac{\partial \phi}{\partial x_\alpha}P\right)=\left(\cancel{\frac{\partial}{\partial v_\alpha}\frac{\partial \phi}{\partial x_\alpha}}\right)\cdot P+\frac{\partial \phi}{\partial x_\alpha}\cdot\frac{\partial P}{\partial v_\alpha}=\frac{\partial \phi}{\partial x_\alpha}\cdot P(-\beta v_\alpha)$$

$$\frac{\partial}{\partial x_\alpha}(v_\alpha P)=\left(\cancel{\frac{\partial v_\alpha}{\partial x_\alpha}}\right)P+v_\alpha\left(\frac{\partial P}{\partial x_\alpha}\right)=v_\alpha\cdot P\cdot\left(-\beta\frac{\partial \phi}{\partial x_\alpha}\right)$$

So we have

$$\frac{\partial P}{\partial t}=\frac{\partial}{\partial v_\alpha}\left(T\gamma_{\alpha\beta}\frac{\partial P}{\partial v_\beta}+U_\alpha P\right)=\frac{\partial}{\partial v_\alpha}\left(-\gamma_{\alpha\beta}v_\beta P+U_\alpha P\right)$$

Therefore, at equilibrium $\frac{\partial P}{\partial t}=0$, we obtain the GB distribution for the steady state if

$$U_\alpha=\gamma_{\alpha\beta}v_\beta$$

We have for small velocities that

$$U_\alpha=\gamma_{\alpha\beta}v_\beta=\lambda_{\alpha\beta}(\mathbf{x})v_\beta+\Lambda_{\alpha\beta\gamma}(\mathbf{x})v_\beta v_\gamma$$

where the term $\lambda_{\alpha\beta}(\mathbf{x})$ is just the friction tensor without any elastic effects. Additional efforts should be taken on the second term by symmetry. We would like to have

$$\gamma_{\alpha\beta}=\lambda_{\alpha\beta}+\gamma_{2\alpha\beta}\qquad \gamma_{2\alpha\beta}=\Gamma_{\alpha\beta\gamma}v_\gamma$$

Consequently, we have

$$\Gamma_{\alpha\beta\gamma}(\mathbf{x})v_\beta v_\gamma=\Lambda_{\alpha\beta\gamma}(\mathbf{x})v_\beta v_\gamma$$

Without loss of generality, we take

$$\Lambda_{\alpha\beta\gamma}=\Lambda_{\alpha\gamma\beta}$$

which then gives

$$\Gamma_{\alpha\beta\gamma}+\Gamma_{\alpha\gamma\beta}=2\Lambda_{\alpha\beta\gamma}$$

In fact, velocity terms on different directions contribute equally for products, so

$$\Lambda_{\alpha\beta\gamma}=\Lambda_{\alpha\gamma\beta}$$

Also, mutual interactions means that terms with v_α contribute equally toward $\gamma_{\alpha\beta}v_\beta$, hence we obtain another constraint

$$\Gamma_{\alpha\beta\gamma}=\Gamma_{\beta\alpha\gamma}$$

Following the format of Langevin equation, $\gamma_{\alpha\beta}$ matrix above only contains terms about first derivatives

$$U_z=\gamma_{z\beta}v_\beta=a_1\frac{\dot\Delta}{\Delta^{3/2}}+a_2\frac{\dot\Delta^2}{\Delta^{9/2}}+a_3\frac{\dot\Theta^2+\dot X^2}{\Delta^{7/2}}+a_4\frac{\dot\Theta\dot X}{\Delta^{7/2}}$$
$$U_x=\gamma_{x\beta}v_\beta=b_1\frac{\dot X}{\sqrt{\Delta}}+b_2\frac{\dot\Delta\dot X}{\Delta^{7/2}}+b_3\frac{\dot\Delta\dot\Theta}{\Delta^{7/2}}$$
$$U_\theta=\gamma_{\theta\beta}v_\beta=c_1\frac{\dot\Theta}{\sqrt{\Delta}}+c_2\frac{\dot\Delta\dot\Theta}{\Delta^{7/2}}+c_3\frac{\dot\Delta\dot X}{\Delta^{7/2}}$$

From this we take the first equation for instance, finding

$$\sum_\alpha\lambda_{z\alpha}v_\alpha=\xi\frac{v_z}{\Delta^{3/2}}\qquad\Rightarrow\qquad\lambda_{zz}=\frac{\xi}{\Delta^{3/2}}\quad\lambda_{zx}=0\quad\lambda_{z\theta}=0$$

Similarly, we have

$$\sum_\alpha\lambda_{x\alpha}v_\alpha=\frac{2\varepsilon\xi v_x}{3\Delta^{1/2}}\qquad\Rightarrow\qquad\lambda_{xz}=0\quad\lambda_{xx}=\frac{2\varepsilon\xi}{3\Delta^{1/2}}\quad\lambda_{x\theta}=0$$

$$\sum_\alpha\lambda_{\theta\alpha}v_\alpha=\frac{4\varepsilon\xi v_\theta}{3\Delta^{1/2}}\qquad\Rightarrow\qquad\lambda_{\theta z}=0\quad\lambda_{\theta x}=0\quad\lambda_{\theta\theta}=\frac{4\varepsilon\xi}{3\Delta^{1/2}}$$

Consider

$$\sum_{\alpha\beta}\Lambda_{z\alpha\beta}v_\alpha v_\beta = \frac{21\kappa\xi v_z^2}{4\Delta^{9/2}} - \frac{\kappa\xi\left(v_x^2+v_\theta^2\right)}{4\Delta^{7/2}} + \frac{\kappa\xi v_x v_\theta}{2\Delta^{7/2}}$$

which furnishes

$$\Gamma_{zzz} = \frac{21\kappa\xi}{4\Delta^{9/2}} \qquad \Gamma_{zxx} = -\frac{\kappa\xi}{4\Delta^{7/2}} \qquad \Gamma_{z\theta\theta} = -\frac{\kappa\xi}{4\Delta^{7/2}}$$

Again

$$\sum_{\alpha\beta}\Lambda_{x\alpha\beta}v_\alpha v_\beta = \frac{19\kappa\xi\varepsilon v_z v_x}{24\Delta^{7/2}} - \frac{\kappa\xi\varepsilon v_x v_\theta}{6\Delta^{7/2}}$$

we get

$$\Gamma_{xxz} + \Gamma_{xzx} = \frac{19\kappa\xi\varepsilon}{24\Delta^{7/2}}$$

The symmetry $\Gamma_{\alpha\beta\gamma} = \Gamma_{\beta\alpha\gamma}$ now gives

$$\Gamma_{xxz} = \frac{19\kappa\xi\varepsilon}{24\Delta^{7/2}} - \Gamma_{xzx} = \frac{19\kappa\xi\varepsilon}{24\Delta^{7/2}} - \Gamma_{zxx} = \frac{\kappa\xi}{\Delta^{7/2}}\left(\frac{19\varepsilon}{24}+\frac{1}{4}\right)$$

Therefore, we could resolve all coefficients $\lambda_{\alpha\beta}$ and $\Gamma_{\alpha\beta\gamma}$ by this way:

$$\lambda_{\alpha\beta} = \begin{pmatrix} \frac{a_1}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{b_1}{\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{c_1}{\sqrt{\Delta}} \end{pmatrix}$$

$$\Gamma_{z\alpha\beta} = \begin{pmatrix} \frac{a_2}{\Delta^{9/2}} & 0 & 0 \\ 0 & \frac{a_3}{\Delta^{7/2}} & \frac{a_4+b_3-c_3}{2\Delta^{7/2}} \\ 0 & \frac{a_4-b_3+c_3}{2\Delta^{7/2}} & \frac{a_3}{\Delta^{7/2}} \end{pmatrix} \quad \Gamma_{x\alpha\beta} = \begin{pmatrix} 0 & \frac{a_3}{\Delta^{7/2}} & \frac{a_4+b_3-c_3}{2\Delta^{7/2}} \\ \frac{b_2-a_3}{\Delta^{7/2}} & 0 & 0 \\ \frac{-a_4+b_3+c_3}{2\Delta^{7/2}} & 0 & 0 \end{pmatrix} \quad \Gamma_{\theta\alpha\beta} = \begin{pmatrix} 0 & \frac{a_4-b_3+c_3}{2\Delta^{7/2}} & \frac{a_3}{\Delta^{7/2}} \\ \frac{-a_4+b_3+c_3}{2\Delta^{7/2}} & 0 & 0 \\ \frac{c_2-a_3}{\Delta^{7/2}} & 0 & 0 \end{pmatrix}$$

Combine those coefficients together by $\gamma_{\alpha\beta} = \lambda_{\alpha\beta} + \Gamma_{\alpha\beta\gamma}v_\gamma$, we obtain

$$\gamma_{\alpha\beta} = \begin{pmatrix} \frac{a_1}{\Delta^{3/2}} + \frac{a_2 v_z}{\Delta^{9/2}} & \frac{v_\theta(a_4+b_3-c_3)}{2\Delta^{7/2}} + \frac{a_3 v_x}{\Delta^{7/2}} & \frac{v_x(a_4-b_3+c_3)}{2\Delta^{7/2}} + \frac{a_3 v_\theta}{\Delta^{7/2}} \\ \frac{v_\theta(a_4+b_3-c_3)}{2\Delta^{7/2}} + \frac{a_3 v_x}{\Delta^{7/2}} & \frac{(b_2-a_3)v_z}{\Delta^{7/2}} + \frac{b_1}{\sqrt{\Delta}} & \frac{v_z(-a_4+b_3+c_3)}{2\Delta^{7/2}} \\ \frac{v_x(a_4-b_3+c_3)}{2\Delta^{7/2}} + \frac{a_3 v_\theta}{\Delta^{7/2}} & \frac{v_z(-a_4+b_3+c_3)}{2\Delta^{7/2}} & \frac{(c_2-a_3)v_z}{\Delta^{7/2}} + \frac{c_1}{\sqrt{\Delta}} \end{pmatrix}$$

and its 1-order approximation of κ:

$$\gamma_{\alpha\beta} \approx \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} + \frac{21\kappa\xi v_z}{4\Delta^{9/2}} & \frac{\kappa\xi((\varepsilon+3)v_\theta-3v_x)}{12\Delta^{7/2}} & -\frac{\kappa(\xi(3v_\theta+(\varepsilon-3)v_x))}{12\Delta^{7/2}} \\ \frac{\kappa\xi((\varepsilon+3)v_\theta-3v_x)}{12\Delta^{7/2}} & \frac{2\xi\varepsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi(19\varepsilon+6)v_z}{24\Delta^{7/2}} & -\frac{\kappa(\xi(\varepsilon+1)v_z)}{4\Delta^{7/2}} \\ -\frac{\kappa(\xi(3v_\theta+(\varepsilon-3)v_x))}{12\Delta^{7/2}} & -\frac{\kappa(\xi(\varepsilon+1)v_z)}{4\Delta^{7/2}} & \frac{4\xi\varepsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi(19\varepsilon+3)v_z}{12\Delta^{7/2}} \end{pmatrix}$$

Effective friction matrix

Therefore, the deterministic equation turns to

$$m_\alpha \cdot \dot{v}_\alpha - F_{2\alpha\beta}(\mathbf{x})\dot{v}_\beta = M_{\alpha\beta}\dot{v}_\beta = F_{1\alpha}(\mathbf{x}) - m_\alpha \cdot \gamma_{\alpha\beta}v_\beta$$

and then we could finally find the effective friction matrix as $\gamma_{\text{eff}} = M_{\alpha\beta}^{-1} m_\alpha \cdot \gamma_{\alpha\beta}v_\beta$

$$\dot{v}_\beta = M_{\alpha\beta}^{-1}\left(F_{1\alpha}(\mathbf{x}) - m_\alpha \cdot \gamma_{\alpha\beta}v_\beta\right)$$

$$\gamma_{\text{eff}} = M_{\alpha\beta}^{-1} \cdot \begin{pmatrix} m_Z & 0 & 0 \\ 0 & m_X & 0 \\ 0 & 0 & m_\Theta \end{pmatrix} \cdot \gamma_{\alpha\beta}$$

with elements below:

$$\gamma_{\text{eff},zz} \approx \frac{\xi}{\Delta^{3/2}} + \kappa\left(\frac{15\xi^2}{8\Delta^4} + \frac{21\xi v_z}{4\Delta^{9/2}}\right)$$

$$\gamma_{\text{eff},xx} \approx \frac{2\xi\varepsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(4\sqrt{\Delta}\xi\varepsilon^2 + 18v_z + 57\varepsilon v_z\right)}{72\Delta^{7/2}}$$

$$\gamma_{\text{eff},\theta\theta} \approx \frac{4\xi\varepsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(8\sqrt{\Delta}\xi\varepsilon^2 + 57\varepsilon v_z + 9v_z\right)}{36\Delta^{7/2}}$$

$$\gamma_{\text{eff},xz} = \gamma_{\text{eff},zx} \approx \frac{\kappa\xi\left((\varepsilon+3)v_\theta - 3v_x\right)}{12\Delta^{7/2}}$$

$$\gamma_{\text{eff},\theta z} = \gamma_{\text{eff},z\theta} \approx \frac{\kappa\xi\left((3-\varepsilon)v_x - 3v_\theta\right)}{12\Delta^{7/2}}$$

$$\gamma_{\text{eff},\theta x} = \gamma_{\text{eff},x\theta} \approx -\frac{\kappa\xi\left(16\Delta^3\xi\varepsilon^2 + 36\Delta^{5/2}(\varepsilon+1)v_z\right)}{144\Delta^6}$$

Modified noise correlator amplitude

After the effective friction matrix γ_{eff}, we consider the random forces and their correlator amplitudes. For the 1D case in the bulk, we only need the square root of friction coefficient. Similarly, we could suppose that $\gamma_{\text{eff}} \approx \Psi + \kappa\Phi$, as well as $\gamma_{\text{eff}}^{1/2} \approx \psi + \kappa\chi$, then we have

$$\gamma_{\text{eff}} = \gamma_{\text{eff}}^{1/2}\gamma_{\text{eff}}^{1/2} = (\psi+\kappa\chi)(\psi+\kappa\chi) \approx \psi\psi + \kappa(\psi\chi + \chi\psi)$$

so we resolve $\psi_{ij} = \sqrt{\Psi_{ij}}$, and $\chi_{ij} = \frac{\Phi_{ij}}{\sqrt{\Psi_{ii}}+\sqrt{\Psi_{jj}}}$.

The results seem plausible and enough with the first-order correction of κ. However, as for γ_{eff}, several velocities have been included. In 1D case, we make Laplace and the its inverse transform for solutions, while here we have to consider that as a matrix equation

$$\tilde{\dot{\mathbf{v}}} = -\widetilde{\gamma_{\text{eff}}\cdot\mathbf{v}} + \widetilde{M^{-1}\cdot\delta\mathbf{F}}$$

Note, γ_{eff} is not a constant matrix, which should be included inside the Laplace transform.

Dissect γ_{eff} as $\gamma_{\text{eff}} = \gamma_0 + \gamma_1(\kappa) + \gamma_{1v}(\kappa, v_i)$,

$$\gamma_0 = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{2\xi\varepsilon}{3\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{4\xi\varepsilon}{3\sqrt{\Delta}} \end{pmatrix} \qquad \gamma_1 = \begin{pmatrix} \frac{15\kappa\xi^2}{8\Delta^4} & 0 & 0 \\ 0 & \frac{\kappa\xi^2\varepsilon^2}{18\Delta^3} & -\frac{\kappa\xi^2\varepsilon^2}{9\Delta^3} \\ 0 & -\frac{\kappa\xi^2\varepsilon^2}{9\Delta^3} & \frac{2\kappa\xi^2\varepsilon^2}{9\Delta^3} \end{pmatrix}$$

$$\gamma_{1v} = \begin{pmatrix} \frac{21\kappa\xi v_z}{4\Delta^{9/2}} & \frac{\kappa\xi((\varepsilon+3)v_\theta-3v_x)}{12\Delta^{7/2}} & \frac{\kappa\xi((3-\varepsilon)v_x-3v_\theta)}{12\Delta^{7/2}} \\ \frac{\kappa\xi((\varepsilon+3)v_\theta-3v_x)}{12\Delta^{7/2}} & \frac{\kappa\xi(6+19\varepsilon)v_z}{24\Delta^{7/2}} & -\frac{\kappa\xi(\varepsilon+1)v_z}{4\sqrt{\Delta}} \\ \frac{\kappa\xi((3-\varepsilon)v_x-3v_\theta)}{12\Delta^{7/2}} & -\frac{\kappa\xi(\varepsilon+1)v_z}{4\sqrt{\Delta}} & \frac{\kappa\xi(19\varepsilon+3)v_z}{12\Delta^{7/2}} \end{pmatrix}$$

where γ_0 is constant matrix, independent on κ; γ_1 depends on κ; and γ_{1v} depends on κ and velocities v_i. Hence we could separate the transform as $\widetilde{\gamma_{\text{eff}}\cdot\mathbf{v}} = \gamma_0\cdot\tilde{\mathbf{v}} + \gamma_1\cdot\tilde{\mathbf{v}} + \widetilde{\gamma_{1v}\cdot\mathbf{v}}$. Since γ_0 is a diagonal matrix, we write $\gamma_{i0} = \gamma_{i0}$ for the convenience. Also, we suppose that $\gamma_{1v,ij} = g_{ij\alpha}v_\alpha$, where $g_{ij\alpha}$ refers to the coefficient of v_α in $\gamma_{1v,ij}$, such as $g_{12x} = -\frac{\kappa\xi v_x}{4\Delta^{7/2}}$. A symmetric γ_{eff} results in symmetric γ_0 and γ_1, so is $g_{ij\alpha}$.

It would be raisonnable to consider the perturbation on κ, for this elastic compliance parameter $\kappa \ll 1$ (about $10^{-4} \sim 10^{-3}$). We write $\mathbf{v} = \mathbf{v}_0 + \mathbf{v}_1$, where the former is on 0 order while the latter 1 order. Similarly, the mass matrix and random forces would be treated in the same way.

$$\dot{\mathbf{v}} = \dot{\mathbf{v}}_0 + \dot{\mathbf{v}}_1 = -\gamma_{\text{eff}}\cdot\mathbf{v} + M^{-1}\cdot\delta\mathbf{F} = -(\gamma_0+\gamma_1+\gamma_{1v})\cdot(\mathbf{v}_0+\mathbf{v}_1) + (M_0^{-1}+M_1^{-1})\cdot(\delta\mathbf{F}_0+\delta\mathbf{F}_1)$$

We only keep terms of 0 and 1 order of κ:

$$\dot{\mathbf{v}}_0 = -\gamma_0\cdot\mathbf{v}_0 + M_0^{-1}\cdot\delta\mathbf{F}_0$$

$$\dot{\mathbf{v}}_1 = -\gamma_0\cdot\mathbf{v}_1 - \gamma_1\cdot\mathbf{v}_0 - \gamma_{1v}\cdot\mathbf{v}_0 + M_0^{-1}\cdot\delta\mathbf{F}_1 + M_1^{-1}\cdot\delta\mathbf{F}_0$$

After Laplace transform, we have

$$s\widetilde{\mathbf{v}}_0 - \mathbf{v}(0) = -\gamma_0 \cdot \widetilde{\mathbf{v}}_0 + M_0^{-1} \cdot \widetilde{\delta \mathbf{F}_0}$$

$$s\widetilde{\mathbf{v}}_1 = -\gamma_0 \cdot \widetilde{\mathbf{v}}_1 - \gamma_1 \cdot \widetilde{\mathbf{v}}_0 - \widetilde{\gamma_{1v} \cdot \mathbf{v}_0} + M_0^{-1} \cdot \widetilde{\delta \mathbf{F}_1} + M_1^{-1} \cdot \widetilde{\delta \mathbf{F}_0}$$

Note $\mathscr{L}_t \left[\int_0^t f(\tau) g(t-\tau)\, d\tau\right](s) = (\mathscr{L}_t[f(t)](s))\,(\mathscr{L}_t[g(t)](s))$. 0-order solutions are rather simple:

$$v_{i0}(t) = v_{i0}(0) e^{-\gamma_{i0} t} + \int_0^t \mathrm{d}\tau \frac{\delta F_{i0}(\tau)}{m_i} \exp\left[-\gamma_{i0}(t-\tau)\right]$$

Follow the same process we have done previously, we get the amplitude of noise correlator:

$$\left\langle \delta F_{i0}(\tau_1) \delta F_{j0}(\tau_2) \right\rangle = 2 k_B T m_i \gamma_{i0} \delta_{ij} \delta(\tau_1 - \tau_2)$$

As for the 1-order correction v_{i1}, we have

$$(s+\gamma_{i0})\widetilde{v_{i1}} = -\sum_j \gamma_{1,ij} \widetilde{v_{i0}} - \sum_j \sum_k g_{ijk} (\widetilde{v_{j0} \cdot v_{k0}}) + M_{0i}^{-1} \widetilde{\delta F_{i1}} + \sum_j M_{1,ij}^{-1} \widetilde{\delta F_{j0}}$$

Laplace and its inverse transform have been calculated. To be clear, we decompose $\mathbf{v}_1$ as

$$\mathbf{v}_1 = \mathbf{v}_{gv} + \left(\mathbf{v}_{vv} + \mathbf{v}_{vf} + \mathbf{v}_{fv} + \mathbf{v}_{ff}\right) + \mathbf{v}_{fm} + \mathbf{v}_{mf}$$

with the following expressions along the direction i:

$$v_{i,gv} = \frac{\gamma_{1,ij}}{\gamma_{i0} - \gamma_{j0}} \left[\left(e^{-\gamma_{i0} t} - e^{-\gamma_{j0} t}\right) v_j(0) + \int_0^t \mathrm{d}\tau \frac{\delta F_{j0}(\tau)}{m_j} \left[e^{-\gamma_{i0}(t-\tau)} - e^{-\gamma_{j0}(t-\tau)} \right] \right]$$

$$v_{i,vv} = -g_{ijk} v_j(0) v_k(0) \cdot \frac{e^{-(\gamma_{j0}+\gamma_{k0})t} - e^{-\gamma_{i0} t}}{\gamma_{i0} - \gamma_{j0} - \gamma_{k0}}$$

$$v_{i,fv} = -g_{ijk} v_k(0) \int_0^t \mathrm{d}\tau \delta F_{j0}(\tau) \frac{e^{-(\gamma_{j0}+\gamma_{k0})(t-\tau)} - e^{-\gamma_{i0}(t-\tau)}}{m_j \left(\gamma_{i0} - \gamma_{j0} - \gamma_{k0}\right)}$$

$$v_{i,vf} = -g_{ijk} v_j(0) \int_0^t \mathrm{d}\tau \delta F_{k0}(\tau) \frac{e^{-(\gamma_{j0}+\gamma_{k0})(t-\tau)} - e^{-\gamma_{i0}(t-\tau)}}{m_k \left(\gamma_{i0} - \gamma_{j0} - \gamma_{k0}\right)}$$

$$v_{i,ff} = -\frac{g_{ijk}}{m_j m_k} \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}x \delta F_{j0}(x) e^{-\gamma_{j0}(\tau - x)} \int_0^\tau \mathrm{d}y \delta F_{k0}(y) e^{-\gamma_{k0}(\tau-y)} e^{-\gamma_{i0}(t-\tau)}$$

$$v_{i,fm} = \int_0^t \mathrm{d}\tau \frac{\delta F_{i1}(\tau)}{m_i} e^{-\gamma_{i0}(t-\tau)} \qquad v_{i,mf} = M_{1,ij}^{-1} \int_0^t \mathrm{d}\tau \delta F_{j0}(\tau) e^{-\gamma_{i0}(t-\tau)}$$

However, higher order correlation functions would be introduced due to $v_{vv}, v_{fv}, v_{vf}, v_{ff}$ while calculating noise correlator amplitudes and diffusion coefficients, such as $\langle v_i v_j v_k \rangle$, $\langle v_i v_j \delta F_{k0} \rangle$, $\langle v_i \delta F_{j0} \delta F_{k0} \rangle$, $\langle \delta F_{i0} \delta F_{j0} \delta F_{k0} \rangle$. In fact, we pose that there is no correlation between velocities and random forces $\langle v_i \delta F_j \rangle = 0$, as well as $\langle \delta F_{i0} \rangle = 0$. Therefore, we are inclined to neglect these odd-power terms below.

Note, as for $\mathbf{v}_{gv}$, $\lim_{\gamma_{i0}\to\gamma_{j0}} \frac{e^{-\gamma_{i0}t} - e^{-\gamma_{j0}t}}{\gamma_{i0} - \gamma_{j0}} = -t e^{-\gamma_{i0} t}$. With all coefficients known, we could resolve $\mathbf{v}_1$. Then we take $v_{z1}(t)$ for instance for the following calculation.

$$v_{z1}(t) = -v_z(0)\gamma_{1,zz} t e^{-\gamma_{z0} t} + \int_0^t \mathrm{d}\tau e^{-\gamma_{z0}(t-\tau)} \left\{ \left[\frac{\delta F_{z1}(\tau)}{m_z} + M_{zz1}^{-1} \delta F_{z0}(\tau) \right] - \gamma_{1,zz}(t-\tau) \frac{\delta F_{z0}(\tau)}{m_z} \right\}$$

Still, we consider the velocity square average up to 1-order κ:

$$\left\langle v_z^2(t) \right\rangle = \left\langle \left[v_{z0}(t) + v_{z1}(t)\right]^2 \right\rangle \approx \left\langle v_{z0}^2(t) \right\rangle + 2 \left\langle v_{z0}(t) v_{z1}(t) \right\rangle$$

Suppose there exists the correlation between 0-order and 1-order random force, $\langle \delta F_{z0}(\tau_1) \delta F_{z1}(\tau_2) \rangle = K_z \cdot \delta(\tau_1 - \tau_2)$. So at long time limit $t \to \infty$, $\left\langle v_z^2(t) \right\rangle$ would converge to

$$\left\langle v_z^2(t) \right\rangle = k_B T \left[\frac{1}{m_z} + 2\left(M_{1,zz}^{-1} - \frac{\gamma_{1,zz}}{2 m_z \gamma_{z0}} \right) \right] + \frac{K}{m_z^2 \gamma_{z0}}$$

Since $\langle v_z^2(t)\rangle = \frac{k_B T}{m_z}$, we obtain the amplitude K_z

$$K_z = k_B T m_z \left(\gamma_{1,zz} - 2\gamma_{z0} m_z M^{-1}_{1,zz}\right)$$

Hence the modified noise amplitude of z up to 1-order correction turns to

$$\begin{aligned}
&\langle \delta F_z(\tau_1)\delta F_z(\tau_2)\rangle \approx \langle \delta F_{z0}(\tau_1)\delta F_{z0}(\tau_2)\rangle + 2\langle \delta F_{z0}(\tau_1)\delta F_{z1}(\tau_2)\rangle \\
&= 2k_B T m_z \gamma_{z0}\delta(\tau_1-\tau_2) + 2k_B T m_z \left(\gamma_{1,zz} - 2\gamma_{z0} m_z M^{-1}_{1,zz}\right)\delta(\tau_1-\tau_2) \\
&= 2k_B T m_z \delta(\tau_1-\tau_2)\cdot\left(\gamma_{z0} + \gamma_{1,zz} - 2\gamma_{z0} m_z M^{-1}_{1,zz}\right)
\end{aligned}$$

Note $M^{-1}_{1,zz} = \frac{15\kappa\xi}{8\Delta^{5/2} m_z}$, $\gamma_{z0} + \gamma_{1,zz} = \frac{\xi}{\Delta^{3/2}} + \frac{15\kappa\xi^2}{8\Delta^4}$, we calculate

$$\gamma_{z0} + \gamma_{1,zz} - 2\gamma_{z0} m_z M^{-1}_{1,zz} = \frac{\xi}{\Delta^{3/2}} - \frac{15\kappa\xi^2}{8\Delta^4}$$

and then an amazingly concise result:

$$\langle \delta F_z(\tau_1)\delta F_z(\tau_2)\rangle = 2k_B T m_z \delta(\tau_1-\tau_2)\cdot(\gamma_{z0} - \gamma_{1,zz})$$

which is always valid at 1-order correction. Since $\gamma_{z0} = \frac{a_1}{\Delta^{3/2}}$, $\gamma_{1,zz} = -\frac{a_1 a_5}{\Delta^4}$, $M^{-1}_{1,zz} = -\frac{a_5}{\Delta^{5/2} m_z}$, we verify

$$\gamma_{z0} + \gamma_{1,zz} - 2\gamma_{z0} m_z M^{-1}_{1,zz} = \frac{a_1}{\Delta^{3/2}} + \frac{a_5 a_1}{\Delta^4} = \gamma_{z0} - \gamma_{1,zz}$$

Furthermore, we could repeat the same procedure for v_{1x} and $v_{1\theta}$, deriving the modified noise correlator amplitudes K_x and K_θ. There are non-zero non-diagonal elements in γ_1, so we get additional terms shown below:

$$\begin{aligned}
v_{x1}(t) = &-v_x(0)\gamma_{1,xx} t e^{-\gamma_{x0}t} + \frac{v_\theta(0)\gamma_{1,x\theta}}{\gamma_{x0}-\gamma_{\theta0}}\left(e^{-\gamma_{x0}t} - e^{-\gamma_{\theta0}t}\right) \\
&- \gamma_{1,xx}\int_0^t \mathrm{d}\tau (t-\tau) e^{-\gamma_{x0}(t-\tau)} \frac{\delta F_{x0}(\tau)}{m_x} \\
&+ \frac{\gamma_{1,x\theta}}{\gamma_{\theta0}-\gamma_{x0}}\int_0^t \mathrm{d}\tau \left(e^{-\gamma_{\theta0}(t-\tau)} - e^{-\gamma_{x0}(t-\tau)}\right)\frac{\delta F_{\theta0}(\tau)}{m_\theta} \\
&+ \int_0^t \mathrm{d}\tau e^{-\gamma_{x0}(t-\tau)}\left[M^{-1}_{1,xx}\delta F_{x0}(\tau) + M^{-1}_{1,x\theta}\delta F_{\theta0}(\tau) + \frac{\delta F_{x1}(\tau)}{m_x}\right]
\end{aligned}$$

$$\begin{aligned}
v_{\theta1}(t) = &-v_\theta(0)\gamma_{1,\theta\theta} t e^{-\gamma_{\theta0}t} + \frac{v_x(0)\gamma_{1,\theta x}}{\gamma_{x0}-\gamma_{\theta0}}\left(e^{-\gamma_{x0}t} - e^{-\gamma_{\theta0}t}\right) \\
&+ \frac{\gamma_{1,\theta x}}{\gamma_{\theta0}-\gamma_{x0}}\int_0^t \mathrm{d}\tau \left(e^{-\gamma_{\theta0}(t-\tau)} - e^{-\gamma_{x0}(t-\tau)}\right)\frac{\delta F_{x0}(\tau)}{m_x} \\
&- \gamma_{1,\theta\theta}\int_0^t \mathrm{d}\tau (t-\tau) e^{-\gamma_{\theta0}(t-\tau)} \frac{\delta F_{\theta0}(\tau)}{m_\theta} \\
&+ \int_0^t \mathrm{d}\tau e^{-\gamma_{\theta0}(t-\tau)}\left[M^{-1}_{1,\theta x}\delta F_{x0}(\tau) + M^{-1}_{1,\theta\theta}\delta F_{\theta0}(\tau) + \frac{\delta F_{\theta1}(\tau)}{m_\theta}\right]
\end{aligned}$$

Again, we suppose $\langle \delta F_{x0}(\tau_1)\delta F_{x1}(\tau_2)\rangle = K_x\cdot\delta(\tau_1-\tau_2)$, and $\langle \delta F_{\theta0}(\tau_1)\delta F_{\theta1}(\tau_2)\rangle = K_\theta\cdot\delta(\tau_1-\tau_2)$ for $\langle v_x^2\rangle$ and $\langle v_\theta^2\rangle$. At long time limit $t\to\infty$, they converge to:

$$\begin{aligned}
\langle v_x^2(t)\rangle &= k_B T\left[\frac{1}{m_x} + 2\left(M^{-1}_{1,xx} - \frac{\gamma_{1,xx}}{2m_x\gamma_{x0}}\right)\right] + \frac{K}{m_x^2\gamma_{x0}} \\
\langle v_\theta^2(t)\rangle &= k_B T\left[\frac{1}{m_\theta} + 2\left(M^{-1}_{1,\theta\theta} - \frac{\gamma_{1,\theta\theta}}{2m_\theta\gamma_{x0}}\right)\right] + \frac{K}{m_\theta^2\gamma_{\theta0}}
\end{aligned}$$

Since they should be equal to $\frac{k_BT}{m_x}$, $\frac{k_BT}{m_\theta}$, respectively, we get:

$$K_x = k_BTm_x\left(\gamma_{1,xx} - 2m_xM^{-1}_{1,xx}\gamma_{x0}\right)$$
$$K_\theta = k_BTm_\theta\left(\gamma_{1,\theta\theta} - 2m_\theta M^{-1}_{1,\theta\theta}\gamma_{\theta 0}\right)$$

Similar to the modified noise correlator on z, we obtain again concise results:

$$\langle\delta F_x(\tau_1)\delta F_x(\tau_2)\rangle = 2k_BTm_x\delta(\tau_1-\tau_2)\cdot(\gamma_{x0}-\gamma_{1,xx})$$
$$\langle\delta F_\theta(\tau_1)\delta F_\theta(\tau_2)\rangle = 2k_BTm_\theta\delta(\tau_1-\tau_2)\cdot(\gamma_{\theta 0}-\gamma_{1,\theta\theta})$$

Mean square displacement

We have already obtained noise correlator amplitudes by $\left\langle v^2(t)\right\rangle$. At the same time, we could also derive the mean square displacement (MSD) by $\langle v(0)v(t)\rangle$. Reminder, there is no correlation between $v_i(t)$ and $\delta F_j(t)$, $\left\langle v_i(t_1)\delta F_j(t_2)\right\rangle = 0$. But we assume that $\langle v_x(0)v_\theta(0)\rangle = \langle v_\theta(0)v_x(0)\rangle = k_BT/m_{x\theta}$. And note $m_x\left\langle v_x^2(0)\right\rangle/2 = k_BT/2$, $m_\theta\left\langle v_\theta^2(0)\right\rangle/2 = k_BT/2$.

$$\begin{aligned}
&\langle v_x(0)v_x(t)\rangle = \langle v_x(0)\left[v_{x0}(t)+v_{x1}(t)\right]\rangle = \langle v_x(0)v_{x0}(t)\rangle + \langle v_x(0)v_{x1}(t)\rangle\\
&= \frac{k_BT}{m_x}e^{-\gamma_{x0}t}\left(1-\gamma_{1,xx}t\right) + \frac{k_BT}{m_{x\theta}}\frac{\gamma_{1,x\theta}}{\gamma_{x0}-\gamma_{\theta 0}}\left(e^{-\gamma_{x0}t}-e^{-\gamma_{\theta 0}t}\right)\\
&\langle v_\theta(0)v_\theta(t)\rangle = \langle v_\theta(0)\left[v_{\theta 0}(t)+v_{\theta 1}(t)\right]\rangle = \langle v_\theta(0)v_{\theta 0}(t)\rangle + \langle v_\theta(0)v_{\theta 1}(t)\rangle\\
&= \frac{k_BT}{m_\theta}e^{-\gamma_{\theta 0}t}\left(1-\gamma_{1,\theta\theta}t\right) + \frac{k_BT}{m_{x\theta}}\frac{\gamma_{1,\theta x}}{\gamma_{x0}-\gamma_{\theta 0}}\left(e^{-\gamma_{x0}t}-e^{-\gamma_{\theta 0}t}\right)
\end{aligned}$$

Define MSD as $\left\langle\Delta r_i^2(t)\right\rangle = \left\langle\int_0^t \mathrm{d}\tau_1\int_0^t \mathrm{d}\tau_2 v_i(\tau_1)v_i(\tau_2)\right\rangle$. We compute this value by its derivative as a function of $\langle v_i(0)v_i(t)\rangle$, since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\Delta r_i^2(t)\right\rangle = 2\int_0^t \mathrm{d}\tau\,\langle v_i(0)v_i(\tau)\rangle$$

After two integrations, we have $\left\langle\Delta r_i^2(t)\right\rangle$

$$\begin{aligned}
\left\langle\Delta r_x^2(t)\right\rangle &= \left\langle\Delta r_x^2(0)\right\rangle + k_BT\times\left(\frac{\frac{e^{-t\gamma_{x0}}-1}{\gamma_{x0}}+t}{m_x\gamma_{x0}} + \frac{\gamma_{1,x\theta}\left(\frac{e^{-t\gamma_{x0}}-1}{\gamma_{x0}}+t\right)}{\gamma_{x0}m_{x\theta}\left(\gamma_{x0}-\gamma_{\theta 0}\right)} - \frac{\gamma_{1,x\theta}\left(\frac{e^{-t\gamma_{\theta 0}}-1}{\gamma_{\theta 0}}+t\right)}{\gamma_{\theta 0}m_{x\theta}\left(\gamma_{x0}-\gamma_{\theta 0}\right)} - \frac{\gamma_{1,xx}\left(t-\frac{2-e^{-t\gamma_{x0}}(t\gamma_{x0}+2)}{\gamma_{x0}}\right)}{m_x\gamma_{x0}^2}\right)\\
&\overset{t\to 0}{\approx}\left\langle\Delta r_x^2(0)\right\rangle + \frac{k_BT}{m_x}t^2 - \frac{\left(k_BT\left(m_x\gamma_{1,x\theta}+m_{\mathrm{x}\theta}\left(\gamma_{x0}+\gamma_{1,xx}\right)\right)\right)}{3\left(m_xm_{\mathrm{x}\theta}\right)}t^3
\end{aligned}$$

$$\begin{aligned}
\left\langle\Delta r_\theta^2(t)\right\rangle &= \left\langle\Delta r_\theta^2(0)\right\rangle + k_BT\times\left(\frac{\frac{e^{-t\gamma_{\theta 0}}-1}{\gamma_{\theta 0}}+t}{m_\theta\gamma_{\theta 0}} + \frac{\gamma_{1,\theta x}\left(\frac{e^{-t\gamma_{x0}}-1}{\gamma_{x0}}+t\right)}{\gamma_{x0}m_{x\theta}\left(\gamma_{x0}-\gamma_{\theta 0}\right)} - \frac{\gamma_{1,\theta x}\left(\frac{e^{-t\gamma_{\theta 0}}-1}{\gamma_{\theta 0}}+t\right)}{\gamma_{\theta 0}m_{x\theta}\left(\gamma_{x0}-\gamma_{\theta 0}\right)} - \frac{\gamma_{1,\theta\theta}\left(t-\frac{2-e^{-t\gamma_{\theta 0}}(t\gamma_{\theta 0}+2)}{\gamma_{\theta 0}}\right)}{m_\theta\gamma_{\theta 0}^2}\right)\\
&\overset{t\to 0}{\approx}\left\langle\Delta r_\theta^2(0)\right\rangle + \frac{k_BT}{m_\theta}t^2 - \frac{\left(k_BT\left(m_\theta\gamma_{1,\theta x}+m_{\mathrm{x}\theta}\left(\gamma_{\theta 0}+\gamma_{1,\theta\theta}\right)\right)\right)}{3\left(m_\theta m_{\mathrm{x}\theta}\right)}t^3
\end{aligned}$$

Additionally, cross mean "square" displacement could also been derived between x and θ.

$$\langle\Delta r_x(t)\cdot\Delta r_\theta(t)\rangle = \int_0^t\left[\frac{\mathrm{d}}{\mathrm{d}t}\langle\Delta r_x(\tau)\cdot\Delta r_\theta(\tau)\rangle\right]\mathrm{d}\tau + \langle\Delta r_x(0)\cdot\Delta r_\theta(0)\rangle$$

Since $\Delta r_x(t) = \int_0^t v_x(\tau)\mathrm{d}\tau$, $\Delta r_\theta(t) = \int_0^t v_\theta(\tau)\mathrm{d}\tau$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Delta r_x(t)\cdot\Delta r_\theta(t)\rangle = \int_0^t\langle v_x(t)v_\theta(\tau)\rangle\,\mathrm{d}\tau + \int_0^t\langle v_x(\tau)v_\theta(t)\rangle\,\mathrm{d}\tau$$

Consider cross velocity product average up to 1-order of κ:

$$\begin{aligned}
&\langle v_x(\tau_1)v_\theta(\tau_2)\rangle\approx\\
&\quad\langle v_{x0}(\tau_1)v_{\theta 0}(\tau_2)\rangle + \langle v_{x0}(\tau_1)v_{\theta 1}(\tau_2)\rangle + \langle v_{x1}(\tau_1)v_{\theta 0}(\tau_2)\rangle
\end{aligned}$$

Only taking $\left\langle v_x^2(0)\right\rangle$, $\left\langle v_\theta^2(0)\right\rangle$, $\langle v_x(0)v_\theta(0)\rangle = \frac{k_BT}{m_{x\theta}}$ mentioned previously into account, we insist that $\langle \delta F_x(\tau_1)\delta F_\theta(\tau_2)\rangle = 0$, and $\left\langle v_i(\tau_1)\delta F_j(\tau_2)\right\rangle = 0$. Therefore, we could easily calculate each term:

$$\begin{aligned}
\langle v_{x0}(\tau_1)v_{\theta 0}(\tau_2)\rangle &= \langle v_x(0)v_\theta(0)\rangle e^{-\gamma_{0x}\tau_1}e^{-\gamma_{0\theta}\tau_2} \\
\langle v_{x0}(\tau_1)v_{\theta 1}(\tau_2)\rangle &= \left\langle v_x^2(0)\right\rangle \frac{e^{-\gamma_{0x}\tau_1}\gamma_{1,\theta x}}{\gamma_{0x}-\gamma_{0\theta}}\left(e^{-\gamma_{0x}\tau_2}-e^{-\gamma_{0\theta}\tau_2}\right) - \langle v_x(0)v_\theta(0)\rangle \gamma_{1,\theta\theta}\tau_2 e^{-\gamma_{0x}\tau_1}e^{-\gamma_{0\theta}\tau_2} \\
\langle v_{x1}(\tau_1)v_{\theta 0}(\tau_2)\rangle &= \left\langle v_\theta^2(0)\right\rangle \frac{e^{-\gamma_{0\theta}\tau_2}\gamma_{1,x\theta}}{\gamma_{0x}-\gamma_{0\theta}}\left(e^{-\gamma_{0x}\tau_1}-e^{-\gamma_{0\theta}\tau_1}\right) - \langle v_x(0)v_\theta(0)\rangle \gamma_{1,xx}\tau_1 e^{-\gamma_{0x}\tau_1}e^{-\gamma_{0\theta}\tau_2}
\end{aligned}$$

We jump the explicit calculation process, giving the final result directly:

$$\begin{aligned}
&\langle \Delta r_x(t)\cdot\Delta r_\theta(t)\rangle = \langle \Delta r_x(0)\cdot\Delta r_\theta(0)\rangle \\
&+ \frac{\gamma_{1,\theta x}\left(e^{t\gamma_{x0}}-1\right)e^{-t(\gamma_{\theta 0}+2\gamma_{x0})}\left(\gamma_{\theta 0}e^{t\gamma_{\theta 0}}\left(e^{t\gamma_{x0}}-1\right)-\gamma_{x0}\left(e^{t\gamma_{\theta 0}}-1\right)e^{t\gamma_{x0}}\right)}{\gamma_{\theta 0}\gamma_{x0}^2\left(\gamma_{x0}-\gamma_{\theta 0}\right)}\left\langle v_x^2(0)\right\rangle \\
&+ \frac{\gamma_{1,x\theta}\left(e^{t\gamma_{\theta 0}}-1\right)e^{-t(2\gamma_{\theta 0}+\gamma_{x0})}\left(\gamma_{\theta 0}e^{t\gamma_{\theta 0}}\left(e^{t\gamma_{x0}}-1\right)-\gamma_{x0}\left(e^{t\gamma_{\theta 0}}-1\right)e^{t\gamma_{x0}}\right)}{\gamma_{\theta 0}^2\gamma_{x0}\left(\gamma_{x0}-\gamma_{\theta 0}\right)}\left\langle v_\theta^2(0)\right\rangle \\
&+ \frac{e^{-t(\gamma_{\theta 0}+\gamma_{x0})}}{\gamma_{\theta 0}^2\gamma_{x0}^2}\langle v_x(0)v_\theta(0)\rangle \times \\
&\quad \left[\gamma_{x0}\left(\gamma_{\theta 0}\left(\left(e^{t\gamma_{x0}}-1\right)\left(e^{t\gamma_{\theta 0}}+t\gamma_{1,\theta\theta}-1\right)+t\gamma_{1,xx}\left(e^{t\gamma_{\theta 0}}-1\right)\right)\right.\right. \\
&\quad \left.\left.-\gamma_{1,\theta\theta}\left(e^{t\gamma_{\theta 0}}-1\right)\left(e^{t\gamma_{x0}}-1\right)\right)-\gamma_{\theta 0}\gamma_{1,xx}\left(e^{t\gamma_{\theta 0}}-1\right)\left(e^{t\gamma_{x0}}-1\right)\right]
\end{aligned}$$

Numerical Simulations

Discretisation algorithm

We set $N_{\max} = 60000$ for the following numerical simulations. Besides, we introduce another parameter, the time scaling ratio $t_r = 1/200$, which means that we would split the time unit into 200 intervals, for the sake of much smooth numerical results. Consider the real time unit less than the typical time of Brownian motion, for example 1ms; so we use $dt = \frac{1\text{ms}\cdot c}{r\sqrt{2\varepsilon}}\cdot t_r$ in the simulation codes.

Dimensionless variables

In order to non-dimensionalize the problem, we follow the variables used in [1]:

$$\delta = \Delta\cdot r\varepsilon \qquad x_G = X_G\cdot r\sqrt{2\varepsilon} \qquad \theta = \Theta\cdot\sqrt{2\varepsilon}$$

Introduce $t = T\cdot r\sqrt{2\varepsilon}/c$, where c is the maximum velocity for free fall particles. So the velocities in reality would be replaced by those shown in our equations of motion:

$$v_\Delta = \frac{v_z}{c}\cdot\sqrt{\frac{2}{\varepsilon}} \qquad v_X = \frac{v_x}{c} \qquad v_\Theta = \frac{v_\theta r}{c}$$

where c is a free fall velocity scale constant

$$c = \sqrt{2gr\rho^*/\rho}$$

and $\rho^* = \rho_{\text{sty}} - \rho_{\text{sol}}$, $\rho = \rho_{\text{sol}} = 1.00$ g/cm^3, $\rho_{\text{sty}} = 1.06$ g/cm^3. Similarly, related to velocities, accelerations and forces would be treated in the same way according to their direction.

$$\dot v_\Delta = \dot v_z\cdot\frac{2r}{c^2} \qquad \dot v_X = \dot v_x\cdot\frac{r\sqrt{2\varepsilon}}{c^2} \qquad \dot v_\Theta = \dot v_\theta\cdot\frac{r^2\sqrt{2\varepsilon}}{c^2}$$

$$\left\langle \widehat{\delta F_z}(\tau_1)\cdot\widehat{\delta F_z}(\tau_2)\right\rangle = \langle \delta F_z(\tau_1)\cdot\delta F_z(\tau_2)\rangle \times \frac{2}{c^2\varepsilon}$$

$$\left\langle \widehat{\delta F_x}(\tau_1)\cdot\widehat{\delta F_x}(\tau_2)\right\rangle = \langle \delta F_x(\tau_1)\cdot\delta F_x(\tau_2)\rangle \times \frac{1}{c^2}$$

$$\left\langle \widehat{\delta F_\theta}(\tau_1)\cdot\widehat{\delta F_\theta}(\tau_2)\right\rangle = \langle \delta F_\theta(\tau_1)\cdot\delta F_\theta(\tau_2)\rangle \times \frac{r^2}{c^2}$$

Euler-Maruyama method

In Itô calculus, the Euler–Maruyama method is used for the approximate numerical solution of a stochastic differential equation (SDE). Consider the equation

$$dX_t = a(X_t,t)dt + b(X_t,t)dW_t$$

with initial condition $X_0 = x_0$, where W_t stands for the Wiener process, and suppose that we wish to solve this SDE on some interval of time $[0,T]$. Then the Euler-Maruyama approximation to the true solution X is the Markov chain Y defined as follows:

- partition the interval $[0,T]$ into N equal subintervals of width $\Delta t = T/N > 0$: $0 = \tau_0 < \tau_1 < \cdots < \tau_N = T$
- set $Y_0 = x_0$
- recursively define Y_n for $0 \leqslant n \leqslant N-1$ by

$$Y_{n+1} = Y_n + a(Y_n,\tau_n)\Delta t + b(Y_n,\tau_n)\Delta W_n$$

  where the random variables ΔW_n are independent and identically distributed normal random variables with expected value zero and variance Δt.

Discrete-Time Langevin Integration

Consider a Langevin equation with the external force $f(t)$, namely the gravity and the spurious force for us:

$$dv = \frac{f(t)}{m}dt - \gamma v dt + \sqrt{\frac{2\gamma}{\beta m}}dW(t)$$

we exploit the discretisation algorithm based on [2] with the following splitting steps:

$$\begin{aligned}
\mathbf{v}\left(n+\frac{1}{4}\right) &= \sqrt{a}\cdot\mathbf{v}(n) + \left[\frac{1}{\beta}(\mathbf{1}-\mathbf{a})\cdot\mathbf{m}^{-1}\right]^{1/2}\cdot\mathbf{N}^{+}(n)\\
\mathbf{v}\left(n+\frac{1}{2}\right) &= \mathbf{v}\left(n+\frac{1}{4}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot\mathbf{m}^{-1}\cdot\mathbf{f}(n)\\
\mathbf{r}\left(n+\frac{1}{2}\right) &= \mathbf{r}(n) + \frac{\Delta t}{2}\mathbf{b}\cdot\mathbf{v}\left(n+\frac{1}{2}\right)\\
&\mathscr{H}(n) \to \mathscr{H}(n+1)\\
\mathbf{r}(n+1) &= \mathbf{r}\left(n+\frac{1}{2}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot\mathbf{v}\left(n+\frac{1}{2}\right)\\
\mathbf{v}\left(n+\frac{3}{4}\right) &= \mathbf{v}\left(n+\frac{1}{2}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot\mathbf{m}^{-1}\cdot\mathbf{f}(n+1)\\
\mathbf{v}(n+1) &= \sqrt{a}\cdot\mathbf{v}\left(n+\frac{3}{4}\right) + \left[\frac{1}{\beta}(\mathbf{1}-\mathbf{a})\cdot\mathbf{m}^{-1}\right]^{1/2}\cdot\mathbf{N}^{-}(n+1)
\end{aligned}$$

where $a_{ij} = \delta_{ij}\exp(-\gamma_i\Delta t)$, $\mathscr{N}^{\pm}$ are independent normally distributed random variables with zero mean and unit variance, $b_{ij} = \delta_{ij}\sqrt{\frac{2}{\gamma_i\Delta t}\tanh\frac{\gamma_i\Delta t}{2}}$

References

[1] T. Salez, L. Mahadevan, *J. Fluid Mech.* **2015**, *779*, 181-196, **Elastohydrodynamics of a sliding, spinning and sedimenting cylinder near a soft wall**.

[2] D. A. Sivak, J. D. Chodera, and G. E. Crooks, *J. Phys. Chem. B* **2014**, *188(24)*, 6466-6474, **Time step rescaling recovers continuous-time dynamical properties for discrete-time Langevin integration of nonequilibrium systems**.