R lab simulation seminar

Chapter 2: Brownian dynamics simulations under shear flow

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Agenda

Section 1

Browninan dynamics simulations under shear flow

1.1 Deformation of the system

In this chapter, we deal with overdamped Brownian dynamics simulation under shear flow. First we define the shear strain for $\alpha\beta$ direction $\gamma_{\alpha\beta}$, which is represented as

$$\gamma_{\alpha\beta} = \frac{\partial R_\beta(x_\alpha)}{\partial x_\alpha}, \tag{1}$$

where $x_\alpha \in x, y, z$ and $R_\beta(x_\alpha)$ is the deformation from the original position for $\beta(\in x, y, z)$ direction at x_α.
Now, let us focus on the flow behavior in the shear flow in the xy direction. Therefore, the shear strain γ_{xy} is the main player. We display γ_{xy} simply as γ.
Here we aim to calculate the shear rate $\dot{\gamma}(= \frac{\mathrm{d}\gamma}{\mathrm{d}t})$ dependences of the stress σ and the viscosity η (flow curve), which are called "flow curves" and then the flow behaviors of systems are widely examined.

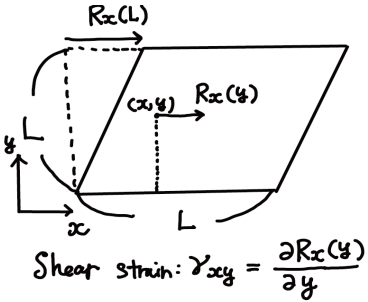


FIG 1: Definition on the strain.

1.2 Browninan dynamics simulations under shear flow

In this subsection we deal with the motions of the brownian particles under shear flow. First, let us consider the equation of motion of underdamped particles which give steady shear flow in the xy direction represented as

$$m\frac{\mathrm{d}\mathbf{v}_j(t)}{\mathrm{d}t} = -\zeta(\mathbf{v}_j(t) - \dot{\gamma}y_j\mathbf{e}_x) + \mathbf{F}^{\mathrm{I}}_j(t) + \mathbf{F}^{\mathrm{B}}_j(t). \tag{2}$$

Here, $\mathbf{F}^{\mathrm{I}}_j(t)$ is the interaction force applied to the particle j, and $\mathbf{F}^{\mathrm{B}}_j(t)$ is the thermal fluctuation force acting on the particle j which satisfies the following fluctuation dissipation theorem:

$$\langle \mathbf{F}^{\mathrm{B}}_j(t)\mathbf{F}^{\mathrm{B}}_k(t')\rangle = 2k_BT\zeta\delta(t-t')\delta_{jk}\mathbf{1}. \tag{3}$$

The equation of motion when the viscosity of the solvent is large and the motion of colloidal particles can be regarded as the overdamped is represented as follows:

$$\zeta(\mathbf{v}_j(t) - \dot{\gamma}y_j\mathbf{e}_x) = \mathbf{F}^{\mathrm{I}}_j(t) + \mathbf{F}^{\mathrm{B}}_j(t), \tag{4}$$

where the shear strain γ (dimensionless number) is given by

$$\gamma(t) = \int_{t'}^{t'+t} \dot{\gamma}(s)\mathrm{d}s. \tag{5}$$

1.2 Browninan dynamics simulations under shear flow II

For the steady shear flow the shear rate $\dot{\gamma}(t)$ is constant, whereas for the oscillatory shear flow $\dot{\gamma}(t)$ is given by

$$\dot{\gamma}(t) = \gamma_0 \omega \sin \omega t \tag{6}$$

where γ_0 is the amplitude of the oscillation strain.

1.3 Lees-Edwards periodic boundary condition

As the way of computing shear flow in the particle simulations, here I am going to introduce a trick of a periodic boundary condition. For generating the Couette flow, as represented in Fig. **2**, the simulation cell should be deformed. Such periodic boundary condition is called Lees Edwards periodic boundary condition (i.e., deforming brick mnodel) [A. W. Lees and S. F. Edwards, J. Phys. C: Solid State Phys. 5, 1921 (1972)]. The periodic boundary determination is performed as shown in Fig. **3**.

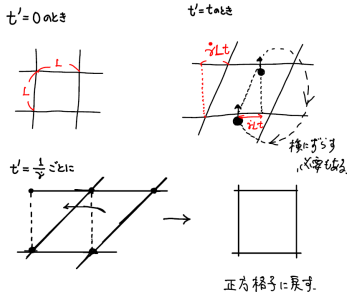
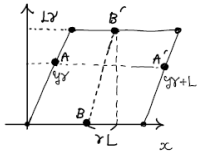


FIG 2: The Lees Edwards boundary condition (deformation brick model).

1.3 Lees-Edwards periodic boundary condition II

・座標の更新



x方向 (A ⇔ A')

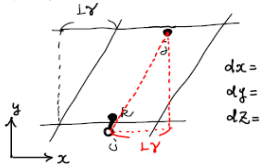
```
if(x[j] < y[j]×gamma)
    x[j] += L;
else if (x[j] < y[j]gamma - tL)
    x[j] -= L;
```

y方向 (B ⇔ B')

```
if (y[j] < 0){
    y[j] += L;
    x[j] += y[j]×gamma; }

else if (y[j] > L){
    y[j] -= L;
    x[j] -= y[j]×gamma; }
```

・相互作用:



dx = x[j] - x[k]
dy = y[j] - y[k]
dz = z[j] - z[k]

この場合 x方向は、通常の周期境界条件と同様。
y方向は、x方向にもずらす必要がある。まずy方向から判定する。

```
{ if (dy > 0.5L){
    dy -= L;
    dx -= LY ; }
  if (dy < -0.5L){
    dy += L;
    dx += LY ; }
```

.... y方向

```
{ if (dx > 0.5L)
    dx -= L;
  else if (dx < -0.5L)
    dx += L;
```

... x方向
.... 逆方向も

シミュレーションの際には γ(t) を用意する方が良い

```
{ γ += γ̇ × dt
  if (γ > 1.0) γ = 0 ;
```

γが 1.0 に達する度に γ=0 に更新する.

1.4 Cell list method under shear flow

Here let us discuss how to construct cell list under shear flow. First, the system should be divided into several parallelogram regions similar to the Lees-Edwards boundary (Figure **4**). Here, the bottom length of the cell R_{CL} must satisfy $R_{\mathrm{CL}} > \sqrt{2} r_{\mathrm{c}}$ for the potential cutoff r_{c}. Other than this, the way of computation is the same as the case without shear flow.

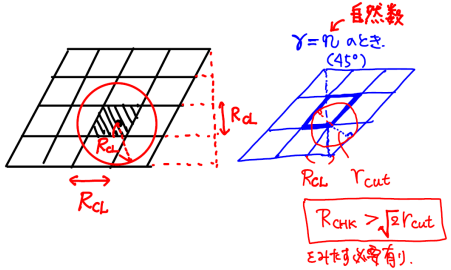


FIG 4: A cell list of the Lees Edwards boundary condition. Here,the bottom length of the cell R_{CL} must satisfy $R_{\mathrm{CL}} > \sqrt{2} r_{\mathrm{c}}$ for the potential cutoff r_{c}.

Section 2

Calculation method for stress and viscosity

2.1 Virial theorem for pressure

Here, I introduce a method for calculating physical quantities which are often estimated in simulations under shear flow. First, the pressure in **the three dimensional system** is calculated from Virial's theorem as

$$P = \frac{Nk_{\mathrm{B}}T}{V} + \frac{1}{3V}\left\langle \sum_j \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{I}} \right\rangle. \tag{7}$$

Here, the $\langle \cdots \rangle$ represents the time average such as

$$\langle \mathcal{A} \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}t \mathcal{A}(t). \tag{8}$$

In Eq. (7), the first term on the right side is called the dynamical term, and the second term is the interaction term. In ideal gases, the second term disappears, and in condensed systems, the second term often becomes important. In the overdamped limit, the first term is negligible.

2.2 Virial theorem in pressure calculations in confined by walls

First, the total virial is divided into the contribution of the internal force due to the interparticle interaction force and the contribution of the external force, which is the force applied to the wall such as

$$\underbrace{\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j \right\rangle}_{[1]} = \underbrace{\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{I}} \right\rangle}_{[2]} + \underbrace{\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{E}} \right\rangle}_{[3]} \tag{9}$$

First, the term [1] is transformed into

$$\begin{aligned} \underbrace{\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j \right\rangle}_{[1]} &= \left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot m\ddot{\mathbf{r}}_j \right\rangle \\ &= -\left\langle \sum_{j=1}^{N} m\dot{\mathbf{r}}_j \cdot \dot{\mathbf{r}}_j \right\rangle \\ &= -Nk_{\mathrm{B}}T. \end{aligned} \tag{10}$$

2.2 Virial theorem in pressure calculations in confined by walls II

The term [2] remains unchanged, and the term [3] can be transformed by the continuum limit and the Gaussian theorem such that

$$\begin{aligned}\underbrace{\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{E}} \right\rangle}_{[3]} &= -\iint \mathbf{r} \cdot (P \mathrm{d}\mathbf{S}) \\ &= -P \iiint \nabla \cdot \mathbf{r} (\mathrm{d}V) \\ &= -3PV\end{aligned}$$

Therefore we obtain

$$P = \frac{N k_{\mathrm{B}} T}{V} + \frac{1}{3V} \left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{I}}. \right\rangle \tag{11}$$

However, there is a problem with rounding error, and it should not be calculated in the computer simulations in this form. If it is used as it is, the larger the absolute value of the coordinate is, the more the rounding

2.2 Virial theorem in pressure calculations in confined by walls III

error is accumulated. In order to reduce rounding errors, the interaction term of Eq. (11) is modified as follows:

$$\begin{aligned}
\frac{1}{3V}\left\langle \sum_{j=1}^{N} \mathbf{r}_j \cdot \mathbf{F}_j^{\mathrm{I}} \right\rangle &= \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_j \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle + \frac{1}{3V}\left\langle \sum_{j<k} \mathbf{r}_j \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle \\
&= \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_j \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle + \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_k \cdot \mathbf{F}_{kj}^{\mathrm{I}} \right\rangle \\
&= \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_j \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle - \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_k \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle \\
&= \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_{jk} \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle . \qquad (12)
\end{aligned}$$

Hence we obtain

$$P = \frac{N k_{\mathrm{B}} T}{V} + \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_{jk} \cdot \mathbf{F}_{jk}^{\mathrm{I}} \right\rangle \qquad (13)$$

2.2 Virial theorem in pressure calculations in confined by walls IV

Since this equation takes the inner product of not $\mathbf{r}_j$ but $\mathbf{r}_{jk}$ and the force, the rounding error is reduced because it does not depend on the absolute value of the coordinate. More interestingly, the same equation as Eq. (15) can be applied even under the periodic boundary condition without explicitly introducing walls.

2.3 Virial theorem in pressure calculations under periodic boundary condition

This subsection refers [J. J. Erpenbeck and W. W. Wood, Statistical Mechanics, Part B (1977)]. In the case of the periodic boundary condition, the force is only the internal force because there is no wall. Therefore, the equation of Virial is as follows:

$$-\frac{Nk_{\mathrm{B}}T}{V} = \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}_{jk} \cdot \mathbf{F}^{\mathrm{I}}_{jk} \right\rangle \tag{14}$$

where $\mathbf{r}_{jk}$ is the inter-particle distance in the cell, and **the periodic boundary condition is not considered**. Here, the particle j is located at the lower boundary, and the interparticle distance considering the periodic boundary condition is $\mathbf{r}'_{jk} = \mathbf{r}_{jk} - L\mathbf{e}_{\mathbf{r}}$. Thus, the Virial equation is:

$$\begin{aligned} -\frac{Nk_{\mathrm{B}}T}{V} &= \left\langle \sum_{j>k} \mathbf{r}'_{jk} \cdot \mathbf{F}^{\mathrm{I}}_{jk} \right\rangle + L\left\langle \sum_{j>k,\ j\in\mathrm{boundary}} \mathbf{e}_{\mathbf{r}} \cdot P\Delta\mathbf{S}_{jk} \right\rangle \\ &= \left\langle \sum_{j>k} \mathbf{r}'_{jk} \cdot \mathbf{F}^{\mathrm{I}}_{jk} \right\rangle - 3PV \end{aligned}$$

2.3 Virial theorem in pressure calculations under periodic boundary condition II

Therefore the pressure under periodic boundary condition is represented as

$$P = \frac{Nk_{\mathrm{B}}T}{V} + \frac{1}{3V}\left\langle \sum_{j>k} \mathbf{r}'_{jk} \cdot \mathbf{F}^{\mathrm{I}}_{jk} \right\rangle. \tag{15}$$

The formula looks exactly the same as the one obtained with walls!

Section 3

Stress tensor

3.1 Stress tensor

Here we introduce the stress tensor such as

$$\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}, \tag{16}$$

where each component of the stress ($\alpha, \beta \in x, y, z$) is given by

$$\sigma_{\alpha\beta} = -\sum_{j=1}^{N} \frac{m v_j^\alpha v_j^\beta}{V} - \frac{1}{V} \left\langle \sum_{j>k} {x^\alpha}_{jk} F_{jk}^\beta \right\rangle. \tag{17}$$

By changing a bit the second term in the right hand side of the equation we obtain

$$\sigma_{\alpha\beta} = -\sum_{j=1}^{N} \frac{m v_j^\alpha v_j^\beta}{V} - \frac{1}{V} \left\langle \sum_{j>k} \frac{{x^\alpha}_{jk} {x^\beta}_{jk} F_{jk}}{r_{jk}} \right\rangle$$

Here the pressure is represented as

$$P = -\frac{1}{3} \mathrm{Tr} \overleftrightarrow{\sigma}$$

3.2 Derivation of the stress tensor

Consider the case of a wall. Here, we derive σ_{xy}. Decomposing Partial Virial into internal and external forces such that

$$\begin{aligned}\left\langle \sum_{j=1}^{N} x_j F_j^y \right\rangle &= \left\langle \sum_{j=1}^{N} x_j F_j^{I,y} \right\rangle + \left\langle \sum_{j=1}^{N} x_j F_j^{E,y} \right\rangle \\ &= \left\langle \sum_{j=1}^{N} x_j F_j^{I,y} \right\rangle + \sigma_{xy} V\end{aligned}$$

Here the left-hand side is transformed by the integration by part such as

$$\left\langle \sum_{j=1}^{N} x_j F_j^y \right\rangle = - \left\langle \sum_{j=1}^{N} m v_j^x v_j^y \right\rangle \tag{18}$$

Therefore xy component of the stress is given by

$$\sigma_{xy} = - \sum_{j=1}^{N} \langle \frac{m v_j^x v_j^y}{V} \rangle - \frac{1}{V} \left\langle \sum_{j>k} \frac{x_{jk} y_{jk} F_{jk}}{r_{jk}} \right\rangle .$$

3.2 Derivation of the stress tensor II

As in the case of pressure, the representation of the formula is identical in the case of wall and periodic boundary. If this is used, the shear viscosity when shear is applied in the xydirection is represented as

$$\eta = \sigma_{xy}/\dot{\gamma}. \tag{19}$$

Homework 7

Consider two-dimensional bi-disperse disk particles of $N_1 = N_2 = 500$ and $\sigma_2 = 1.4\sigma_1$ are filled in the cell of Lees Edwards boundary condition whose system size is L, and is driven by overdamped equation of motion of temperature at $T = 0$ such that

$$\zeta(\mathbf{v}_j(t) - \dot{\gamma} y_j \mathbf{e}_x) - \mathbf{F}_j^{\mathrm{I}}(t) = \mathbf{0}.$$

Here we adopt a shear stran γ for the $x$direction. Now introduce the interaction force $\mathbf{F}_j^{\mathrm{I}} = -\nabla_j U$with the harmonic potential

$$U(r_{jk}) = \frac{\epsilon}{2}\left(1 - \frac{r_{jk}}{\sigma_{jk}}\right)^2$$

The packing fraction of the particles is defined to be

$$\varphi = \frac{\pi}{4L^2}\sum_{j=1}^{N}\sigma_j^2.$$

Here, compute flow curves (σ_{xy} vs $\dot{\gamma}$ or η vs $\dot{\gamma}$) at $\varphi = 0.7, 0.75, 0.8, 0.82, 0.84, 0.86$. Note that when $\varphi = 0.84$ Newtonian behavior is not observed anymore and instead the system becomes solid: that transition is called **the jamming transition.**

(Refs.)[1]A. Ikeda, L. Berthier, and P. Sollich, Phys. Rev. Lett. 109, 018301 (2012), [2] T. Kawasaki, A. Ikeda, and L. Berthier, EPL 107, 28009 (2014), [3] T. Kawasaki, D. Coslovich, A. Ikeda, and L. Berthier, Phys. Rev. E 91, 012203 (2015), [4] T. Kawasaki and L. Berthier, Phys. Rev. E 94, 022615 (2016), [5] T. Kawasaki and L. Berthier, Phys. Rev. E 98, 012609 (2018).