Summary of Zhe's tasks and project

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1 Before Project

1.1

Write the Brownian Dynamics code without hydrodynamics interaction by matlab, which is similar to the work on https://github.com/stochasticHydroTools/HydroGrid/blob/master/example/brownian_walkers.py
The iteration can be described as following:

$$r^{n+1} = r^n + \sqrt{2D\Delta t} \cdot \mathcal{N}(0,1)$$

1.2

Write a error-bar plot code by matlab to evaluate the "$ln(P) \sim r^2$", using Monto-Carlo methods to estimate the error.
Use data from 1.1 to test this plot code.
Attention should be paid to that the input and output of these codes script should be in standard and suitable format.

1.3 No Wall situation

Considering a particle in Stokes fluid, the force equilibrium eq. should be:

$$m_f g = F = 6\pi a \eta v$$

where the right term comes from the stokes viscosity formula.
Hence, we got the sedimentary velocity :

$$v = \frac{1}{6\pi a \eta} F \triangleq \mu F$$

By law of Stokes-Einstein, the diffusion coefficient can be written as below,

$$D = k_B T \mu$$

1.4 With-Wall situation

The parallel and perpendicular motion can be separated.

$$v_{//} = \mu_{//} F_{//}$$

$$D_{//} = k_B T \mu_{//}$$

where $\frac{\mu_{//}(h)}{\mu_0} = 1 - \frac{9a}{16h} + \frac{2a^3}{16h^3} - \frac{a^5}{16h^5}$,which is approximation of low order.

1.5 Parameter choice

$$P(h) \sim e^{-k(h-H)^2/2k_B T}$$

Firstly, choose k and H
s.t.
1.$H \geq 5 \ or \ 4\sigma$
2.The particle should not be too closed to the wall. It is better to set H=5a or 4a
Moreover, it's very import to choose time step Δt s.t. $\sigma \in [0.9, 1.1]\sigma_{true}$
It's recommended that $\Delta t \in [0.1, 0.25]\tau$, where τ is the relaxation time.
Notation: random seed should be reset at every repeat.
Finally, it's also important to set the initial gaussian distribution (i.e. the σ_0).
$\sigma_0 >> \sigma_z$, where $\sigma_0 \geq 5 - 10\sigma$ is recommended.
Define the packing fraction $\phi = \pi a^2 n_0 \sim 1$,where $n_0 = \frac{N}{\int_0^\infty e^{-r^2/2\sigma_0^2} 2\pi r dr}$

2 Project

Using periodic boundary, $n = \frac{N}{L^2}$. The initial distribution is 2D uniform distribution and there's no particle-particle potential.
Define:

$$F(k;t) = \Sigma e^{i\vec{k}\cdot\vec{r}}$$

Grid the domain and doing 2D FFT on the number of particles in each cells and we can get the $k = (\kappa_x \frac{2\pi}{L_x}, \kappa_y \frac{2\pi}{L_y})$
Define the dynamic structure factor:

$$\mathcal{S}(k,\tau) =< F(k;t+\tau) F^*(k;t) >$$

,which is the auto correlation function of F(f;t).
By regression like 'ln($\mathcal{S}(k,\tau) \sim \tau$)', we can get the diffusion coefficient $D_c(k)$ of any wavenumber k since

$$\mathcal{S}(k;t) = n e^{-k^2 D_c(k) \tau}$$