3D Particle Diffusions

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Brownian Motion

Fluid (η)

Newton's Second Law:

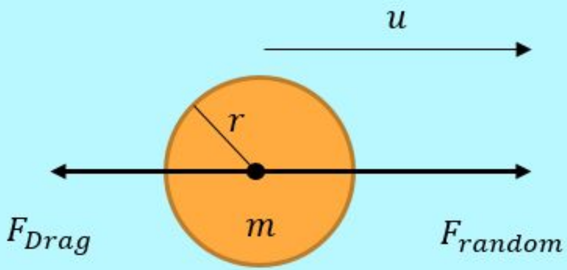
$$F_{net} = ma$$

For the Sphere:

$$m\frac{du}{dt} = -\gamma u + F_{random}$$

In Low Reynolds Number Flow:

$$\gamma = 6\pi\eta r$$

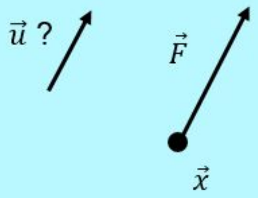


Stoke Flows

- How to simulate the process of Brownian motion computationally

$$\mu \Delta \vec{u} = \nabla p - \vec{F}$$
$$\nabla \cdot \vec{u} = 0$$
$$\Rightarrow \Delta p = \nabla \cdot \vec{F}$$

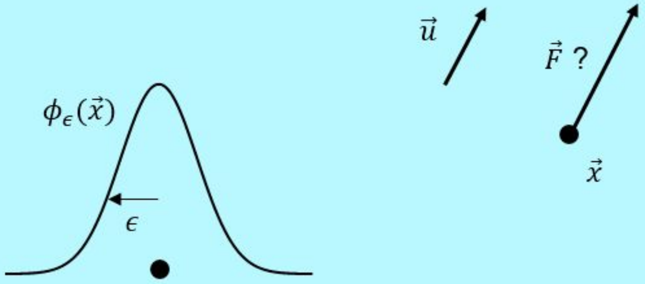
μ is the viscosity of the fluid, $\vec{u}(\vec{x})$ is the velocity of the fluid, $p(\vec{x})$ is the pressure, $\vec{F}(\vec{x})$ is an external force, and $(\vec{x})$ is a point in the fluid. $\Delta \equiv \nabla \cdot \nabla$ is the Laplacian.



Method of Regularized Stokeslets (MRS)

$$\vec{F}(\vec{x}) = \vec{f}_0 \phi_\epsilon(\vec{x} - \vec{x}_0)$$

$$\int \phi_\epsilon(\vec{x} - \vec{x}_0) d\vec{x} = 1$$



Cortez, R., Fauci, L., & Medovikov, A.S. (2005). *The method of regularized Stokeslets in three dimensions: Analysis, validation, and application to helical swimming.* Physics of Fluids, 17(3) 031504

MRS

Blob function $\phi_\epsilon(x - x_0) = \dfrac{15\epsilon^4}{8\pi(r^2+\epsilon^2)^{7/2}},$

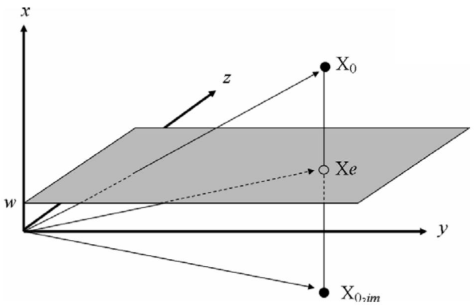
$$\mathbf{u}(\mathbf{x}) = \sum_{k=1}^{N} \frac{-\mathbf{f}_k}{4\pi\mu}\left[\ln\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right) - \frac{\epsilon\left(\sqrt{r_k^2+\epsilon^2}+2\epsilon\right)}{\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right)\sqrt{r_k^2+\epsilon^2}}\right]$$
$$+ \frac{1}{4\pi\mu}[\mathbf{f}_k\cdot(\mathbf{x}-\mathbf{x}_k)](\mathbf{x}-\mathbf{x}_k)\left[\frac{\sqrt{r_k^2+\epsilon^2}+2\epsilon}{\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right)^2\sqrt{r_k^2+\epsilon^2}}\right],$$

Due to the linear relationship between force and velocity, this formula can be written as

U = MF

Method of Images for Regularized Stokeslets (MIRS)

$$
\begin{aligned}
\mathbf{U}(\mathbf{x}_e) = \sum_{k=1}^{M} & \left[\mathbf{f}_k H_1(|\mathbf{x}_k^*|) + (\mathbf{f}_k \cdot \mathbf{x}_k^*)\mathbf{x}_k^* H_2(|\mathbf{x}_k^*|)\right] - \left[\mathbf{f}_k H_1(|\mathbf{x}_k|) + (\mathbf{f}_k \cdot \mathbf{x}_k)\mathbf{x}_k H_2(|\mathbf{x}_k|)\right] - h_k^2 [\mathbf{g}_k D_1(|\mathbf{x}_k|) \\
& + (\mathbf{g}_k \cdot \mathbf{x}_k)\mathbf{x}_k D_2(|\mathbf{x}_k|)] - 2h_k \left[\frac{H_1'(|\mathbf{x}_k|)}{|\mathbf{x}_k|} + H_2(|\mathbf{x}_k|)\right](\mathbf{L}_k \times \mathbf{x}_k) + 2h_k \Big[(\mathbf{g}_k \cdot \mathbf{e}_1)\mathbf{x}_k H_2(|\mathbf{x}_k|) \\
& + (\mathbf{x}_k \cdot \mathbf{e}_1)\mathbf{g}_k H_2(|\mathbf{x}_k|) + (\mathbf{g}_k \cdot \mathbf{x}_k)\mathbf{e}_1 \frac{H_1'(|\mathbf{x}_k|)}{|\mathbf{x}_k|} + (\mathbf{x}_k \cdot \mathbf{e}_1)(\mathbf{g}_k \cdot \mathbf{x}_k)\mathbf{x}_k \frac{H_2'(|\mathbf{x}_k|)}{|\mathbf{x}_k|}\Big],
\end{aligned}
$$



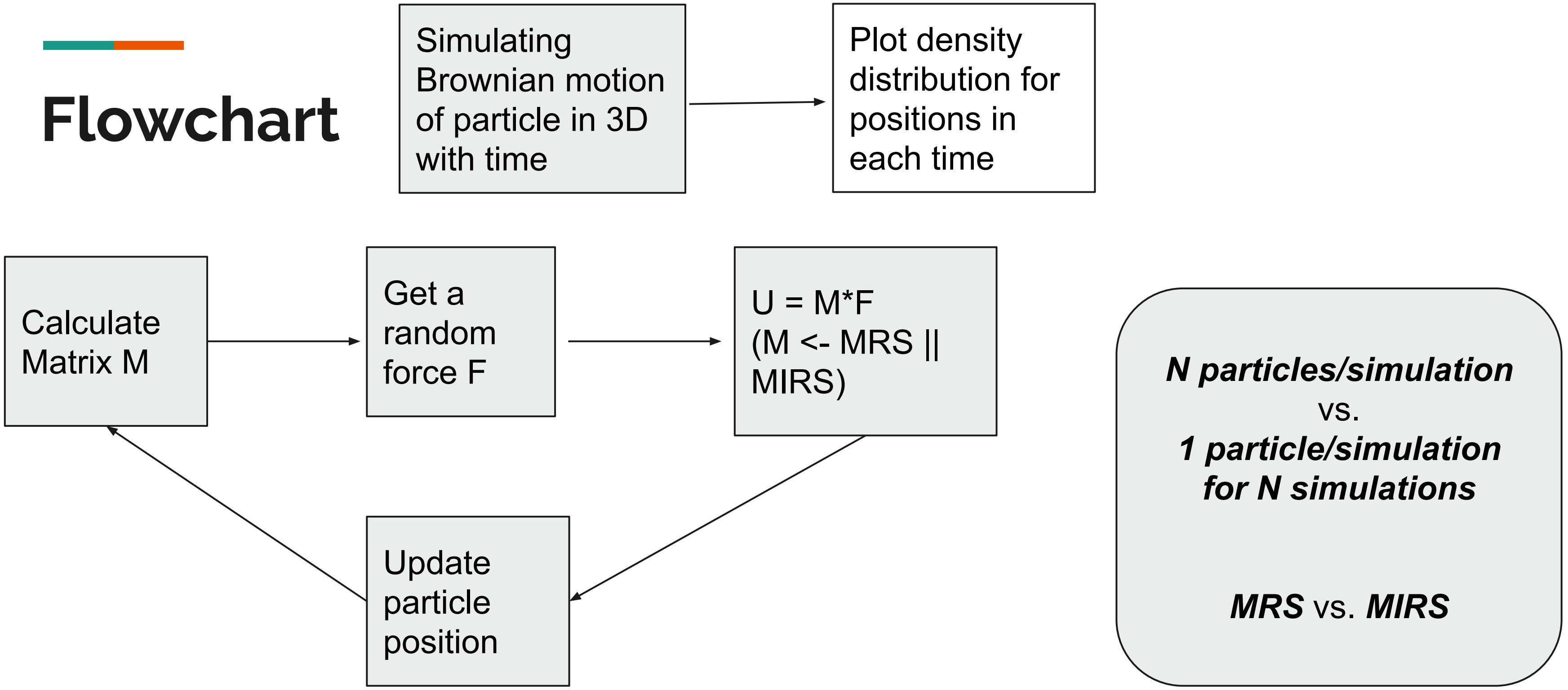
Schematic of the fluid domain with the wall at $x = w$, the location of the Stokeslet at $\mathbf{x}_0$ and the image point.

Due to the linear relationship between force and velocity, this formula can be written as

U = MF

Ainley, J., Durkin, S., Embid, R., Boindala, P., & Cortez, R. (2008). *The method of images for regularized Stokeslets.* Journal of Computational Physics, 227(9), 4600–4616.

Flowchart



Simulating Brownian motion of particle in 3D with time
Plot density distribution for positions in each time
Calculate Matrix M
Get a random force F
U = M*F (M <- MRS || MIRS)
Update particle position
N particles/simulation
vs.
1 particle/simulation for N simulations
MRS vs. **_MIRS_**

3-D Task 1: Find Drag Radius as a Function of ϵ

- Impose a constant velocity $\vec{u}$ to a blob of size ϵ, find the drag force $\vec{F}$, and use the Stokes Drag Formula $F = (6\pi\eta r)u$ ...

$$F_D = 6\pi\eta r U$$

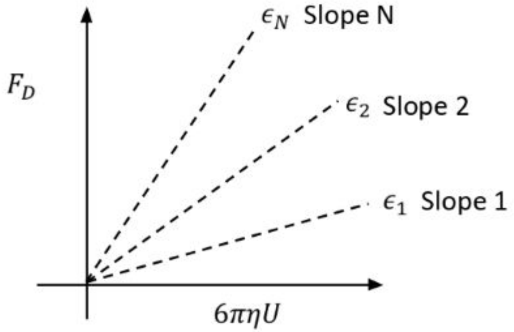


Figure 1. F_D versus $6\pi\eta U$ for various values of ϵ.

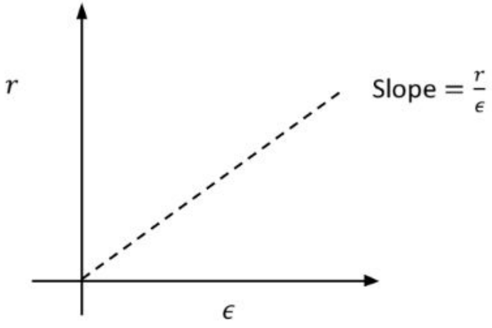
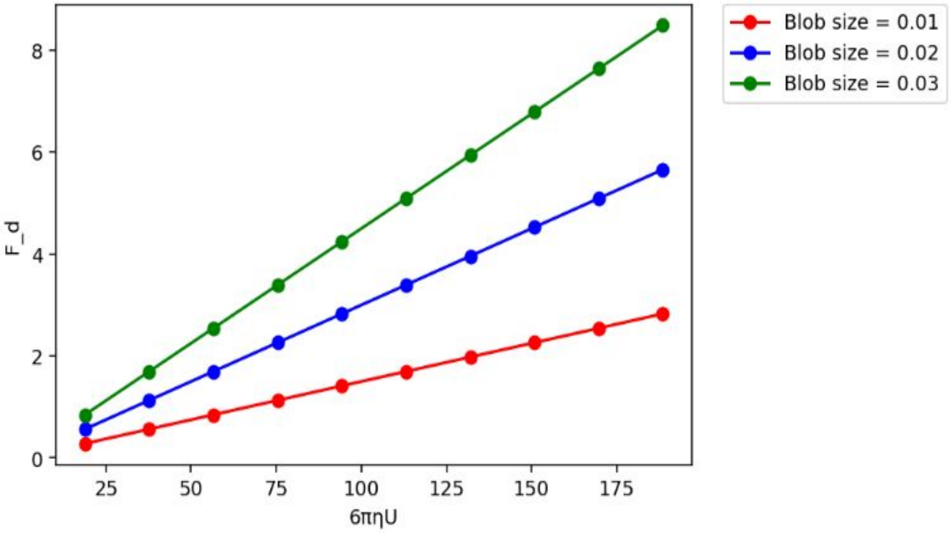
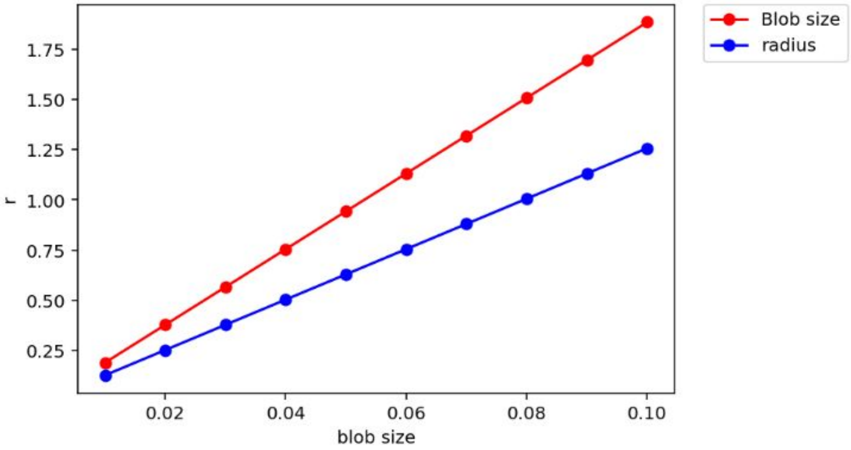


Figure 2. $\frac{F_D}{6\pi\eta U} = r$ versus ϵ. The slope gives a scaling from ϵ to r.

Result

Blob size $\mathcal{E}$ = 1.5*r* where *r* is the radius of a particle.

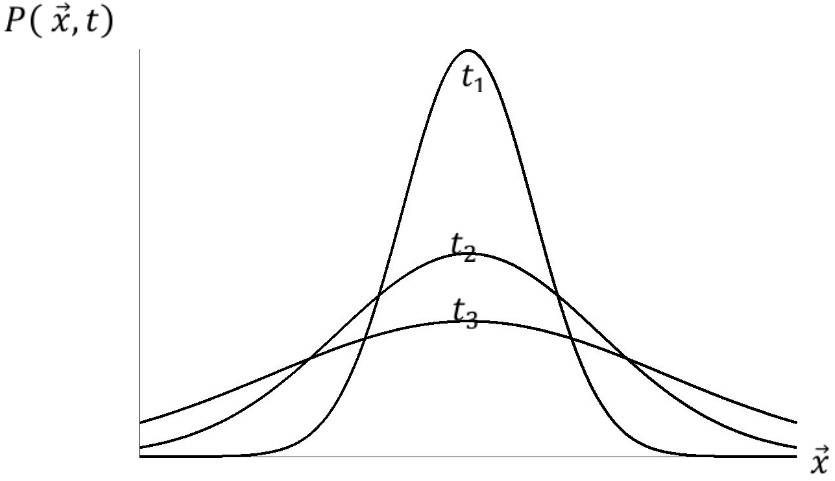




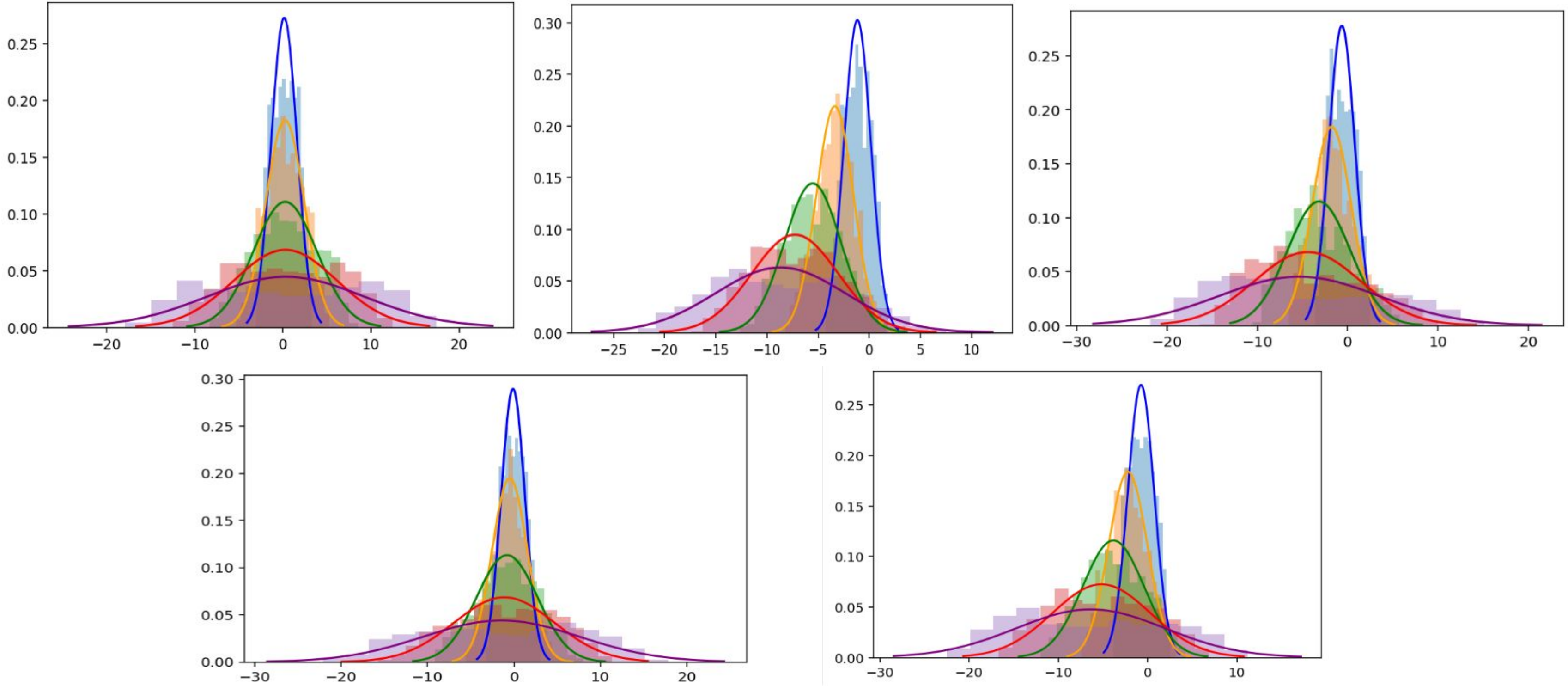
2. Simulate Brownian Motion

- Add in a random force at each time step, calculate the probability density of the particle being found at position $\vec{x}$ at time t.

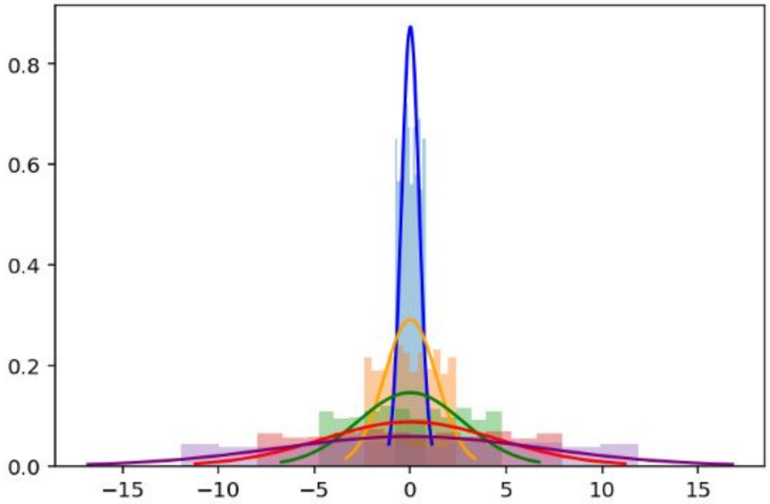
$$P(\vec{x},t) = \frac{1}{\sqrt{(4\pi D t)^3}} e^{-\frac{\vec{x}^2}{4Dt}}$$



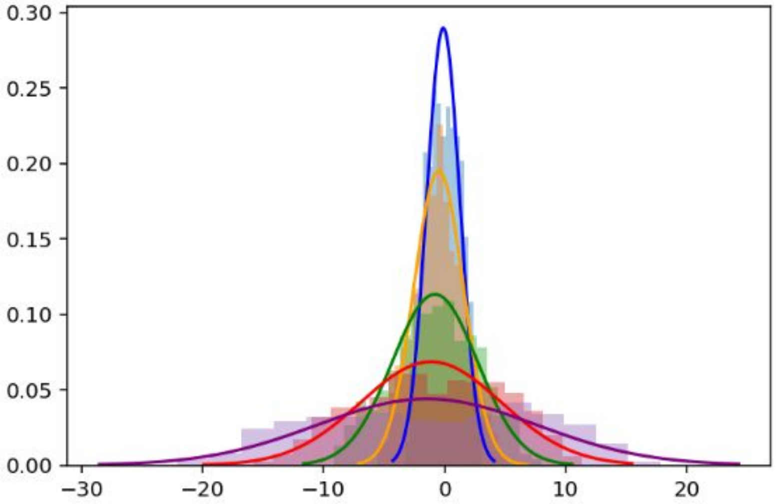
Results for N particles/simulation using MRS (no surface)



Results for 1 particle/simulation with N simulations using MRS (no surface)

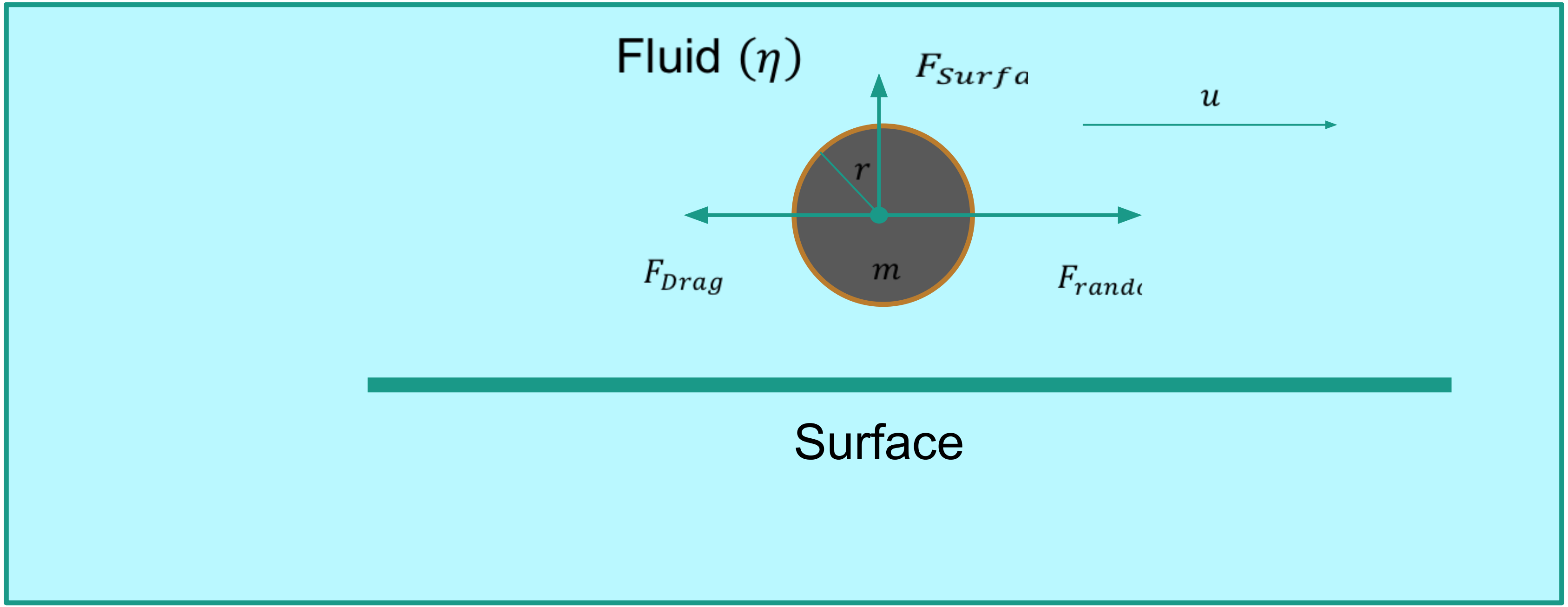


1 particle N simulations



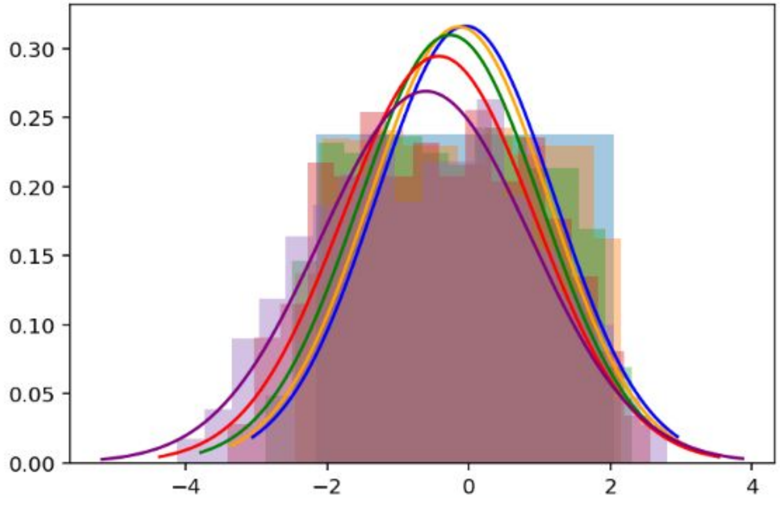
N particles

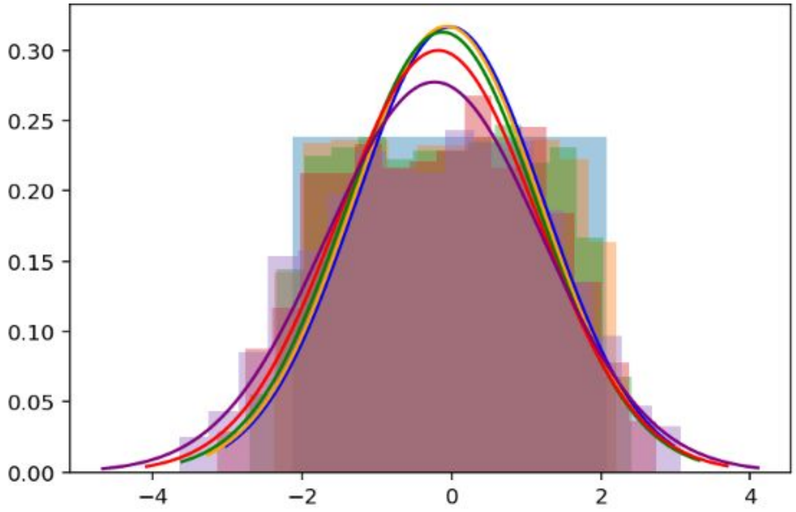
3-D Task 3: Impose Surface Hydrodynamic Interactions



Results for N particles/simulation using MIRS

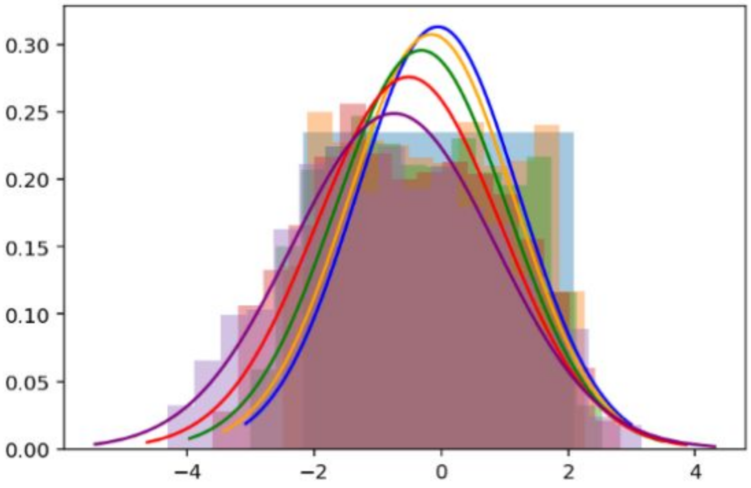
(density distribution in the y; surface at -2.5 x)

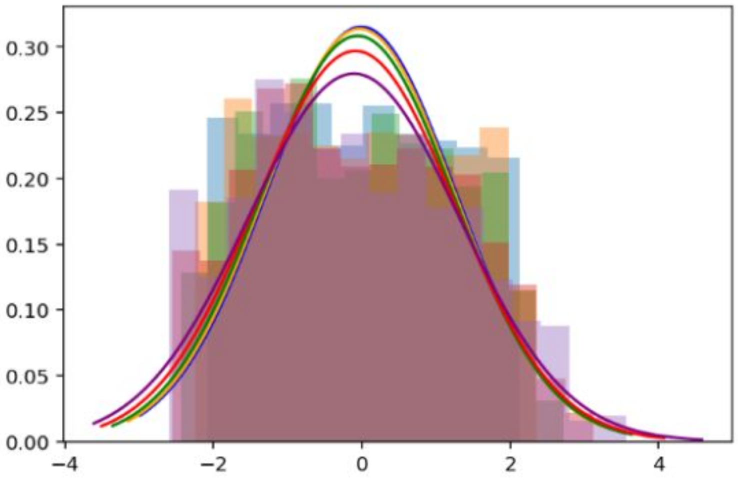




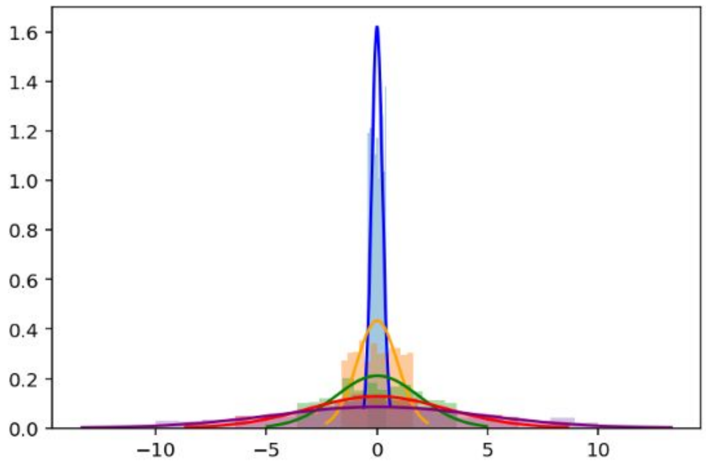
Results for N particles/simulation using MIRS

(density distribution in the x direction; surface at x = -2.5)

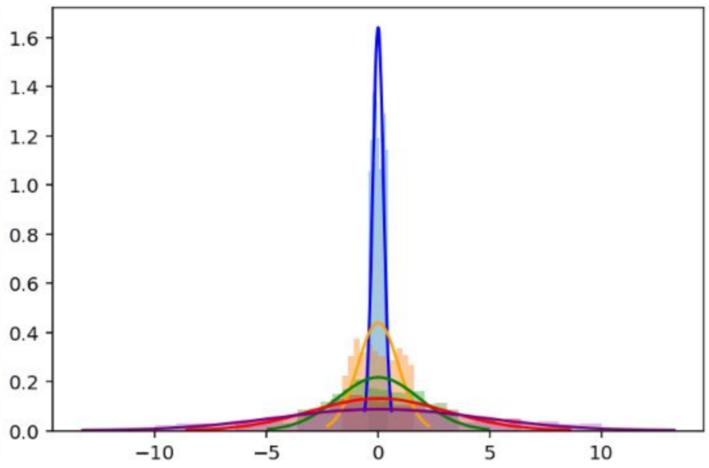




Results for 1 particle/simulation with N simulations using MIRS (density distribution in the y or z direction; surface at x = -1)

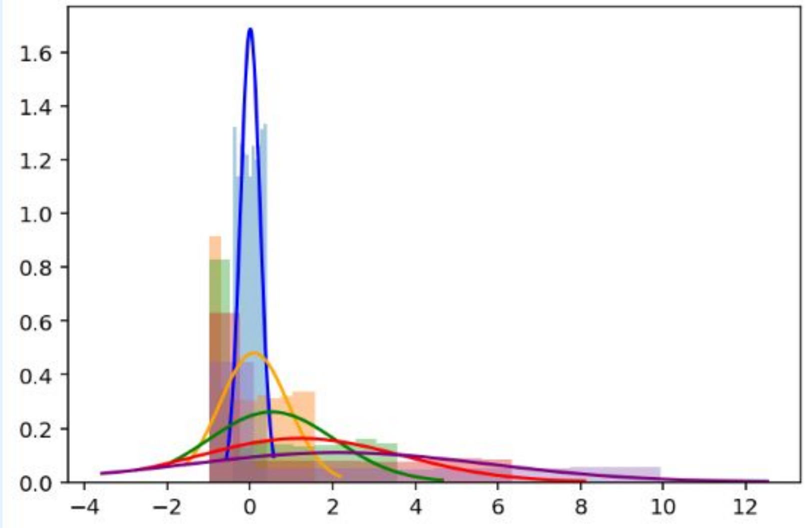


Y axis



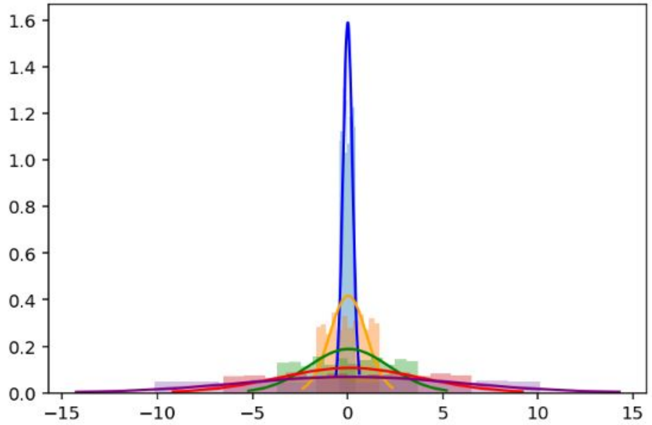
Z axis

Results for 1 particle/simulation with N simulations using MIRS (density distribution in the x direction; surface at x = -1)

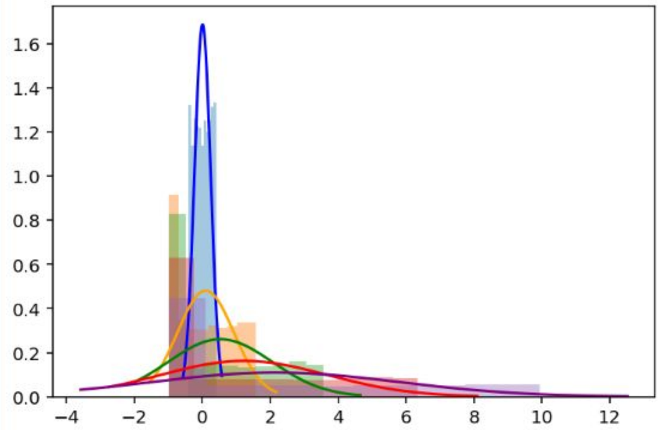


Conclusion 1: Surface Effect (No Particle-Particle Interactions)

1 particle/simulation for N simulations **(density distribution in the x direction)**



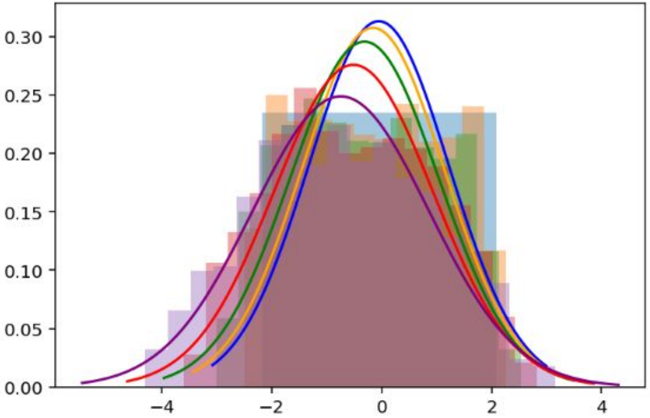
MRS (infinite 3D space)



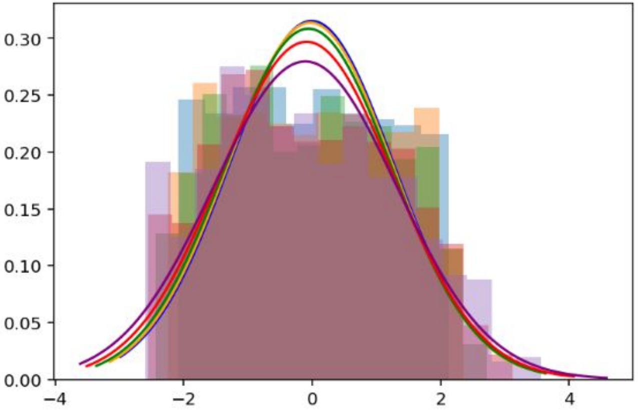
MIRS (surface at x = -1)

Conclusion 2: Surface Effect *and* Particle-Particle Interactions

N particles/simulation **(density distribution in the x direction)**



MRS (infinite 3D space)



MIRS (surface at x = -2.5)

Lessons & Future directions

- Time management
- Communication with advisors regularly
- Similarity to machine learning

Future directions

- Realistic random force
- Further applications

Acknowledgement

- Nicholas Coltharp
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- Dr. Nguyen
- Dr. Lewis for coming today!