



Motivation

- Explore forces on a colloidal particle from interactions with smaller particles as a function of the dynamics of the smaller particles.
- Analyze thermodynamic properties of the interactions.
- Analyze drag and Reynold's number on colloidal particle when an external force is applied.



Assumptions

- A particle's instantaneous velocity is a superposition of its characteristic velocity and the velocity generated from any external forces.
- The motion of a ballistic particle is driven by energy consumed from the external environment and is not in thermodynamic equilibrium. An example of this would be a E. Coli or chemically propelled particles.
- Particle motion is over-damped, i.e. returns to characteristic speed quickly after interactions.



Implementation

- Interactions between particles are facilitated via ballistic collision interactions.
- Boundary conditions are periodic.
- Particle motion is over-damped, i.e. returns to characteristic speed quickly after interactions.
- Interactions are memory-less, i.e. only depend on position and energy of particles.
- Two sets of nano-particle behavior are explored: Brownian and Ballistic



Characterization of Colloidal Particle Dynamics

Calculate the Mean Square Displacement in the absence of drift

$$MSD = \langle (x - x_0)^2 \rangle = \frac{1}{N} \sum_{n=1}^{N} (x_n(t) - x_n(0))^2$$

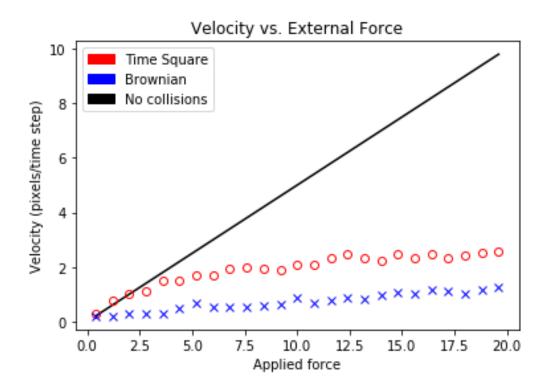
- Over 300 time steps the MSD for a particle with radius 120 pixel in a sea of 300 small Ballistic particles is 22 pixels.
- Over 300 time steps the MSD for a particle with radius 120 pixel in a sea of 300 small Brownian particles is 15 pixels.

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Times Square system with a small external force Brownian system with a small external force Times Square system with a large driving force Brownian system with a large external force





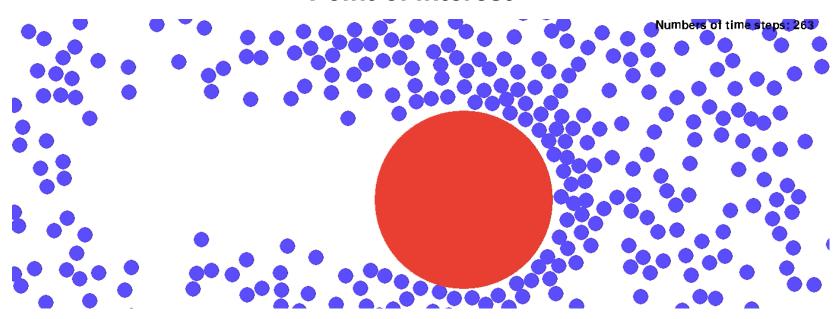
$$v_d = \frac{1}{2}a\tau = \frac{1}{2}\frac{\vec{F}}{m}\tau$$

$$\vec{F} = \vec{F}_{external} + \vec{F}_{interaction}$$

Plot for a large particle of radius 120 pixels in a sea of 300 small particles.



Point of interest



High density region forms in front of red particle and a wake forms behind red particle. This seems to mark a transition between low and high Reynold's number flow and will be explored further in the final project.



Next Steps

- Characterize the force on the large particle as a function of density of small particles, relative size, speed and mass of the particles.
- Simulate a sea of elliptical, E. Coli like molecules.
- Introduce more complex interaction terms between particles







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References

- Frenkel, D. & Smit, B. *Understanding molecular simulation: from algorithms to applications*. (Academic Press, 2012).
- Berg, H. C. Random walks in biology. (Princeton Univ. Press, 1983).
- Maggi, C., Paoluzzi, M., Angelani, L. & Leonardo, R. D. Memory-less response and violation of the fluctuation-dissipation theorem in colloids suspended in an active bath. *Scientific* Reports 7,(2017).