# Nano-particle interactions with a micro-particle

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## 1 Introduction

The dynamics of small objects in fluids has been a subject of interest ever since Robert Brown observed the jiggling of pollen grain in a water bath through his microscope in 1827. In 1905 Albert Einstein fleshed out a theory for Brownian motion. Here the motion of a micro-particle is studied in four distinct environments. The micro-particle is immersed in a sea of much smaller particles. The particles interact according to distinct sets of rules and the effects of the kinetics on the micro-particles motion is explored.

## 2 Nano-Particle Environments

A variety of environments were prepared for the macro-particle. Each with the smaller particles motion governed by a simple set of rules. The four environments prepared in this experiment were Brownian particles, Times Square, run-and-tumble, and ballistic. Each of these environments is described in detail in the respective section. After preparing the environments a macro-particle was immersed in each. The smaller particles interacted with the large particles and the dynamics, i.e. RMS displacement and velocity, of the larger particle were studied. Next an external force was applied to the macro-particle and caused it to move through the sea of small particles. The interaction with the small particles produced a drag force on the macro-particle. The drag coefficient and viscosity are modeled for each environment. In some cases the motion of the macro-particle caused micro-particles to coalesce and form high density regions in front and in the wake of the macro-particles. Comparing the high-density region with the lower density region encourages one to think of a phase transition in the nano-particle bath. This is discussed further in Section 3.

### 2.1 Brownian

In the absence of an external force Brownian particles takes steps following a normal distribution centered at $\vec{r} = 0$ with variance determined by the temperature, or energy, of the surrounding environment. In Python the Brownian motion was implemented using the scipy.stats.norm.rvs(scale $= \sigma$) function to model a normal distribution with variance $\sigma$.

The RMS displacement of the Brownian particles is shown for a particular case in the figure below.

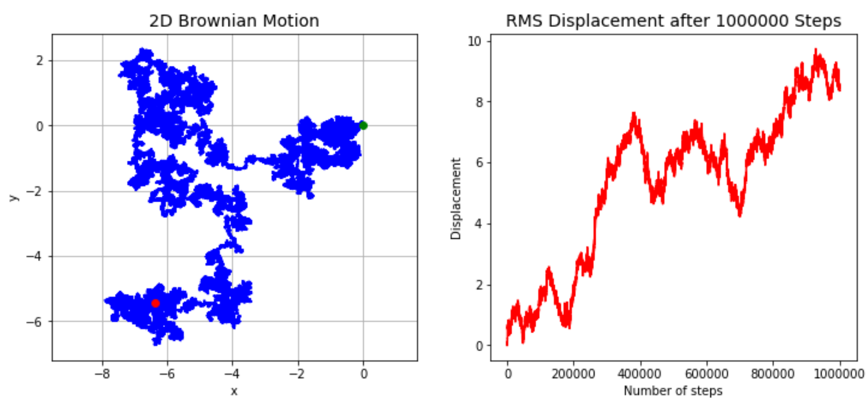


Fig. 1 - An example of the trajectory and RMS displacement of a Brownian Particle.

## 2.2 Run-and-Tumble

Run-and-tumble particles travel in a straight line (ballistic) path for a number of steps until a random variable stops the motion and changes the direction of the particle's trajectory. The straight line path corresponds to a "run" and the stopping and changing directions corresponds to a "tumble". The image below, produced by Elgeti and Gopner [4], shows the trajectory of a run-and-tumble particle over the course of five steps.

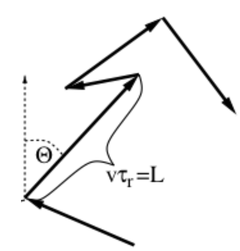


Fig. 3 - Schematic of a run-and-tumble trajectory. A "run" with velocity $v$ over a time $\tau$ is followed by a "tumble" or change in orientation $\theta$[4].

The dynamics of a run-and-tumble particle were implemented computationally by have the particle move forward a set distance each time step. A random variable was introduced to determine when the particle should change direction. The dynamics for a single particle run are shown above. The step size used matches the variance of the normal distribution used to generate the Brownian motion in Fig. 1.

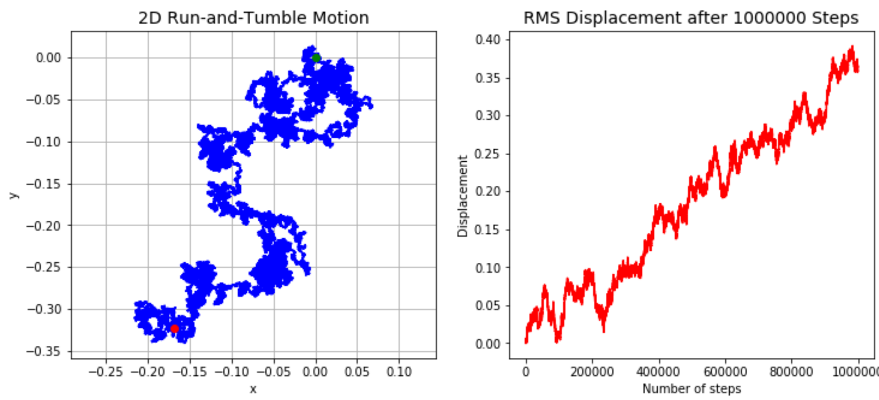


Fig. 3 - An example of the trajectory and RMS displacement of a Run-and-Tumble Particle.

The RMS displacement for the run-and-tumble particle was significantly less than that of the Brownian particle. This suggests that the steps size, or particle energies, may not be comparable in magnitude. Further investigation is needed regarding how to compare Brownian and run-and-tumble trajectories appropriately.

### 2.3 Ballistic

The dynamics of ballistic particles are governed by interactions among particles. Each particle moved in a straight line with constant speed until it collides with another particle. Particles collide elastically and the dynamics of each particle depends largely on the density of particles in the sea. The plot of a single particle's motion is excluded here as a single particle displacement would simply increases linearly with the number of steps the particle takes.

## 3 Interactions with Large Particle

After setting up the dynamics for a sea of particles a larger particle was introduced to the sea and the dynamics of the large particle were studied. To begin the displacement of the larger particle was tracked in the absence of external forces. The quantity of interest being the mean squared displacement (MSD)

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

After the dynamics without external forces were characterized and external force was applied the large particle and the interactions with the smaller particles were studied in the presence of an external force. This can be realized experimentally by introducing a para-magnetic bead to a sea of smaller particles, like E. Coli [3].

The forces on the colloidal particle were taken to be the sum of the external forces on the particle and the forces exerted via interactions with the smaller particles,

$$\vec{F} = \vec{F}_{external} + \vec{F}_{interaction}. \tag{2}$$

The drag force exerted by the smaller particles was then obtained by tracking the displacement and velocity of the large particle,

$$v_d = \frac{1}{2} a\tau = \frac{1}{2}\frac{\vec{F}}{m}\tau. \tag{3}$$

The forces exerted on the colloidal particle were found to depend on the relative size of the colloidal and nano-particles, the density of nano-particles, and the dynamics of the nano-particle bath, among other factors. The relation of the motion of the colloidal particle to the dynamics of the sea of nano-particles was of particular interest. Here the motion of the colloidal particle in the sea of Brownian particle is compared to motion in a sea of ballistic particles.

## 3.1 Interactions with Brownian Particles

When sufficent force was applied to the colloidal particle in a sea of Brownian particles a "wall" of condensed nano-particle formed in front of the colloidal particle, Fig. 4. Additionally, a wake formed behind the colloidal particle.

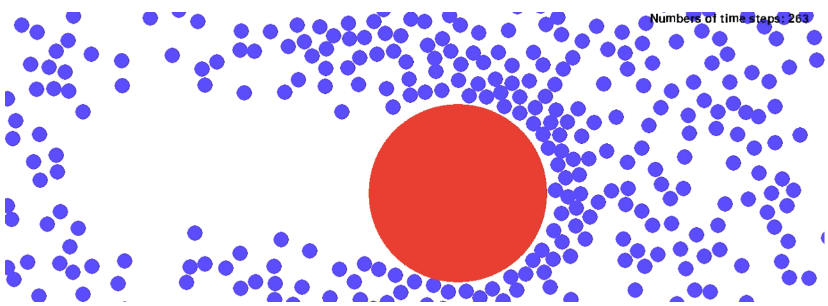


Fig. 4 - When a sufficiently large force is applied small particles (blue) build up in front of the large red particle. Additionally, a wake forms behind the red particle.

## 3.2 Time Square Interaction

Time Square model describes nano-particles that undergo ballistic motion, i.e. move was a fixed velocity and change direction only upon collisions with another particle. In this model the tourists (nano-particles) wander in straight lines, unaware of their surroundings until they make a head on collision with another particle. The large particle represents a hurried New Yorker trying desperately to make their morning commute. As the New Yorker moves faster it collides with more and more tourists and is inevitably slowed down by the collisions.

An example of the Times Square interaction at a particlular time is shown below.

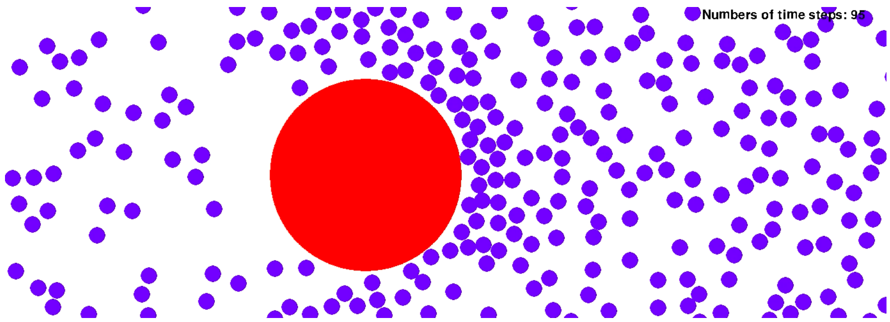


Fig. 5 - Interactions of a colloidal particle with a sea of ballistic nano-particles.

The Times Square interactions did not facilitated the build up of nano-particles in front of the sphere as strongly as the Brownian bath did. Additionally, the formatiion of a wake is less apparent in the Times Square case. This seems reasonable since the nano-particles follow ballistic trajectories and have no reason to change direction when entering the void left behind the larger particle.

### 3.3 Brownian and Time Square Comparison

The drag force on the colloidal particle seemed to depend strongly on the underlying dynamics of the nano-particles. A sample curve for the velocity on the colloidal particle as a function of the strengh of the applied force is shown below. The Brownian sea of particles appeared to be more viscous than the ballistic particle bath.

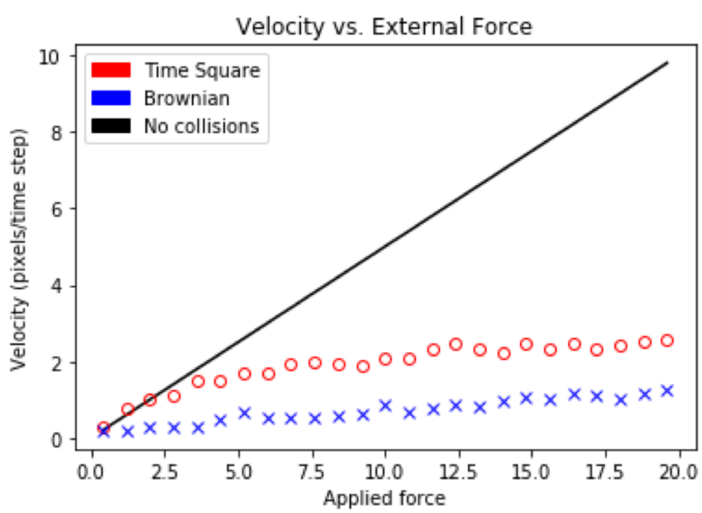


Fig. 6 - Velocity as a function of external force.

# 4 Numerical Scaling

The nano-particle environments described in Section 2 are all memory-less as such will scale linearly with the number of time steps $N$. The sclaling with the number of particle goes as $\mathcal{O}(N^2)$, as shown in the figure below.

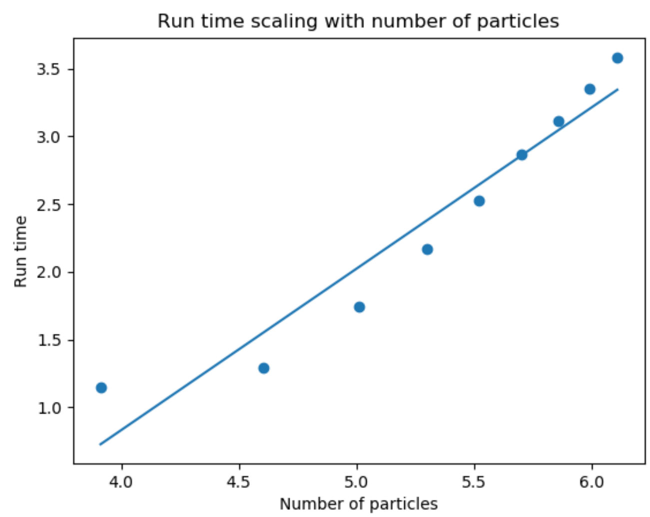


Fig. 6 - The run-time of the program scales with the number of particles squared.

# 5 Future Plans

This project will be extended to further model the motion of a colloidal particle in a variety of environments. In order to do this well it is important that the dynamics of the nano-particles in the baths be constructed so that the energies of the different environments can be compared in a meaningful way. While it is easy enough to adjust the energy or speed of the nano-particles in each of the environments it is not obvious how to compare the energy of the Brownian bath with that of the Ballistic bath. Before moving forward to analyzing the motion of particles in more complex geometries, like mazes [5], or introducing potentials to the bath it seems important that a quantitative method for comparing the different nano-particle environments be developed.

In the long-term, this model will be extended to model self-propelled particles (SPP) such as E. Coli. This well require introducing non-circular particles to the nano-particle bathes. It would also be interesting to model a non-spherical larger particle in the bath.

# 6 References

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[2] Berg, H. C. Random walks in biology. (Princeton Univ. Press, 1983).

[3] 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).

[4]Elgeti, J., Gompper, G. (2015). Run-and-tumble dynamics of self-propelled particles in confinement. EPL (Europhysics Letters), 109(5), 58003. doi:10.1209/0295-5075/109/58003

[5]Khatami, M., Wolff, K., Pohl, O., Ejtehadi, M. R., Stark, H. (2016). Active Brownian particles and run-and-tumble particles separate inside a maze. Scientific Reports, 6(1). doi:10.1038/srep37670