Monte Carlo simulation of Brownian Motion

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Abstract

In this computational lab we model Brownian motion of pollen grains suspended in water. The simulation performed used a Markov chain Monte Carlo sampling method with a random walk in the velocity variable. Two models were simulated, the first of which produces incorrect results and leads to an unphysical increase of the mean squared velocity with the number of collisions experienced by the Brownian particle. In the second model this increase is corrected for by adding an approximation for the viscosity of the water is added to the model, thus producing a correct result for the mean square velocities and displacements for the Brownian particle.

Introduction

Brownian motion is the random motion attributed to small particles suspended in a liquid or gas that result from collisions of the particles with the fast moving molecules of the fluid.

In this report we attempt to model this motion for pollen particles suspended in water using Monte Carlo techniques. These methods of computational simulations rely on the repeated sampling of random numbers to solve potentially deterministic problems. Here specifically we are using a Markov chain Monte Carlo method with a random walk in the velocity variable. A Markov chain model describes a random process through time where the probability of the system moving from one state to another is only dependent on its current state, this property of 'memorylessness' is a key characteristic of a random walk process.

We will consider two models, the first which neglects the dependence of momentum transfer to the Brownian particle on its velocity before a collision, this leads to the average velocity increasing with the number of collisions.[1] In reality the mean squared velocity should approach a constant value due to frictional losses from the viscosity of the fluid. The second model approximates these losses to produce more realistic values for the final velocity and displacement of the particle.

Method

Model 1

We model Brownian motion as a series of random collisions in one dimension, where the probability of a collision occurring during a given time interval and the direction from which the bombarding particle comes are determined with the use of a normal distribution of pseudo-random numbers.[2]

By defining the velocity of the particle after N collisions as V_N and then supposing that each collision alters its velocity by one unit, either positive or negative the velocity of the Brownian particle can be written as

$$V_N = V_{N-1} + w \tag{1}$$

where $w = \pm 1$. Squaring (1) we obtain two equations depending on whether w is positive or negative. Then buy taking the average of the two equations we arrive at an expression for the mean square velocity[3]

$$\langle V_N^2 \rangle = \langle V_{N-1}^2 \rangle + 1 \tag{2}$$

by realising that $\langle V_1^2 \rangle = 1$ and iterating through the random walk we see that this mean squared value increases linearly with N

$$\langle V_N^2 \rangle = N \tag{3}$$

which is an unphysical result.

The displacement of the particle, X_N before a collision is given by

$$X_N = X_{N-1} + V_N \tag{4}$$

Here as with the velocity we have $\langle X_N^2 \rangle = 1$, we then arrive at an expression for the mean square displacement

$$\langle X_N^2 \rangle = (1/6)N(N+1)(2N+1) \tag{5}$$

for large values of N this equation reduces to

$$\langle X_N^2 \rangle \longrightarrow (1/3)N^3 \tag{6}$$

which is also an incorrect result and not in agreement with true Brownian motion.[1]

Model 2

A more realistic result for the velocity changes per collision can be obtained by taking conservation of momentum into account, we do this by introducing a factor ρ into the calculation of velocity for the particle. Where ρ is defined to be

$$\rho \equiv \frac{1 - m/M}{1 + m/M} \tag{7}$$

here m and M are the masses of the gas molecules and the Brownian particle respectively. This approximation is then applied to (1) giving

$$V_N = \rho V_{N_1} + w \tag{8}$$

By choosing a suitable value for ρ so that many collisions by the molecules are needed to produce a significant change in the velocity of the Brownian particle.[1]
We now perform the same procedure that led to (3), giving

$$\langle V_N^2 \rangle \longrightarrow \frac{1}{(1-\rho^2)} \tag{9}$$

as N becomes large. The expectation value for X_N is now given by

$$\langle X_N^2 \rangle \longrightarrow \frac{N}{(1-\rho)^2} \tag{10}$$

Thus we now have the mean square velocity value independent of the number of steps and the the mean square displacement of the particle increasing linearly with the number of steps.

Results & Discussion

Model 1

The simulation was run with 500 walks over 100k steps. The issues with this model are evident from Figure 1.

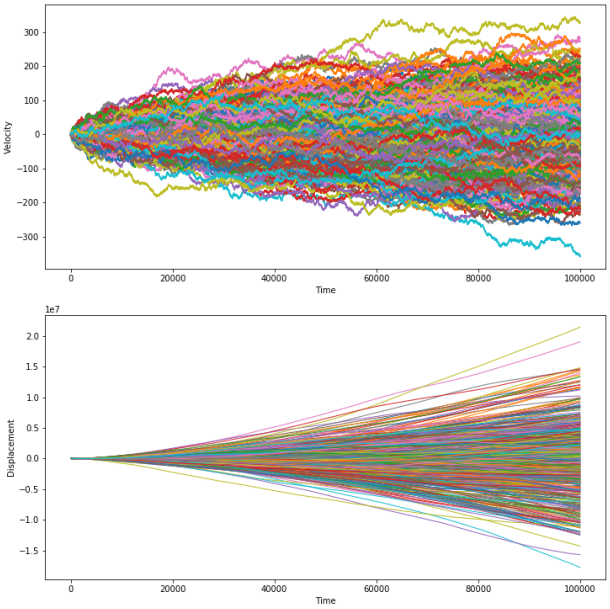

Figure 1: Results from 500 walks, $\rho = 1$

The final velocities are seen to increase with time, the final displacements also have unrealistic magnitudes at the ends of the walk, here they are on the order of 10^7 from the origin and display an unnatural smooth, constantly increasing trend.
When the velocities and displacements are squared and averaged we can clearly see from Figures 2 and 3 the agreement with Eqns.(3) and (6). That is, a linear increase in velocity with the displacement increasing with a cubic relationship.

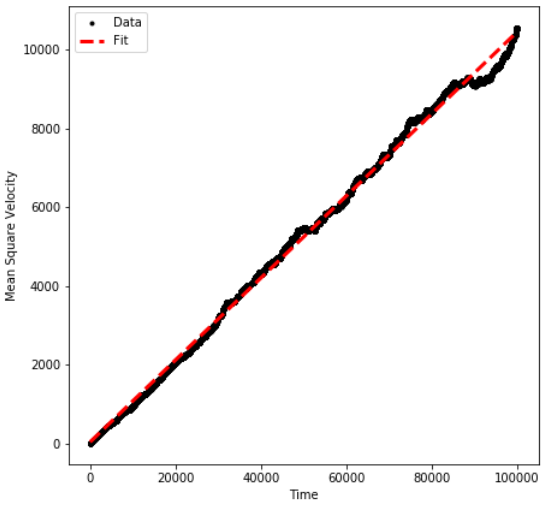

Figure 2: Mean Square Velocity, $\rho = 1$

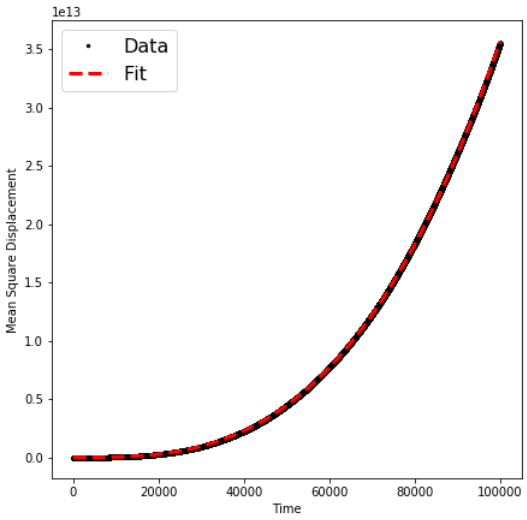

Figure 3: Mean Square Displacement, $\rho = 1$

Model 2

For the second model the momentum transfer approximation returns more realistic results as can be seen from Figure 4.

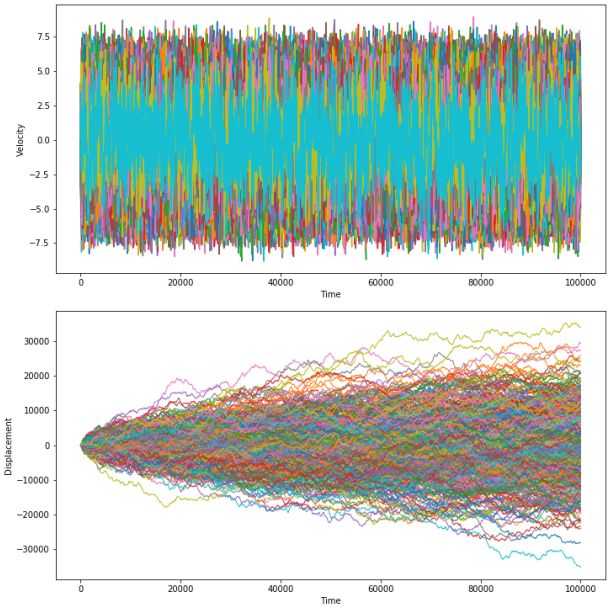

Figure 4: 500 walks, $\rho = 0.9$

The velocity approaches a constant value, this can be seem more clearly from the histogram in Figure 5. The mean value for velocity in this model was found to be 5.267 with a standard deviation of 0.452, this is in good agreement with the value of 5.263 obtained from (9) for $\rho = 0.9$.

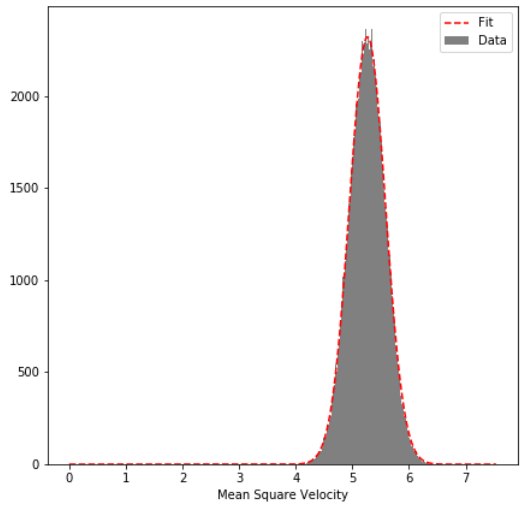

Figure 5: Mean Square Velocity, $\rho = 0.9$

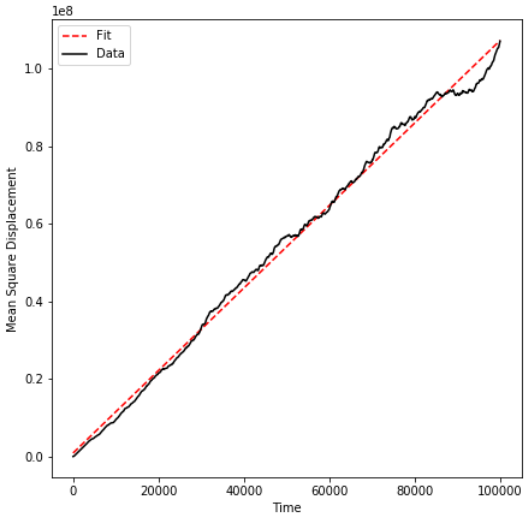

Figure 6: Mean Square Displacement, $\rho = 0.9$

Simulation Time

To obtain the a relationship between the mean square displacement and time taken for the simulation to run each simulation was run 10 times with a varying number of time steps. The results of these simulations are shown in Figures 7 and 8. Here we can see that the incorrect model has an exponential relation between the two variables while for the correct model we have a linear relationship.

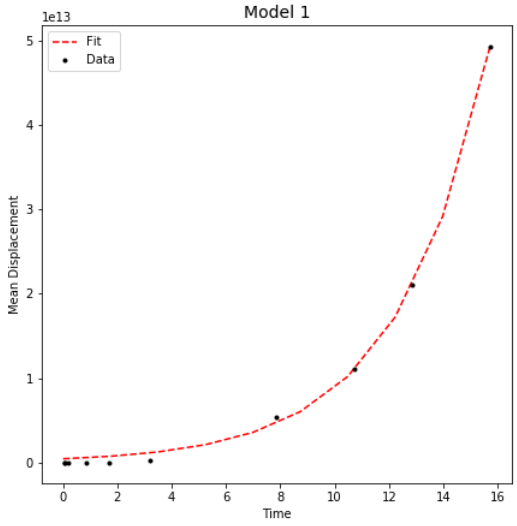

Figure 7: Time for Model 1 simulation

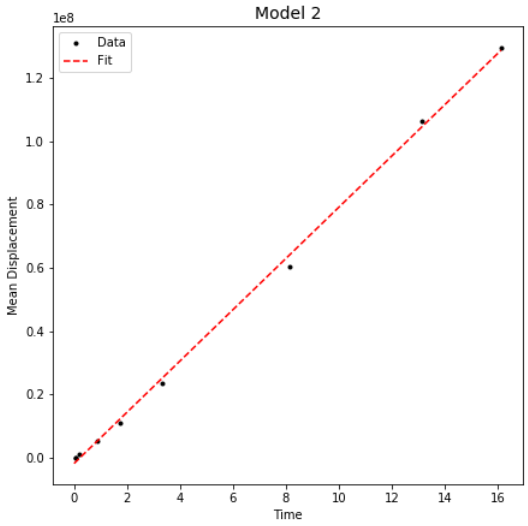

Figure 8: Time for Model 2 simulation

Conclusion

The differences in the results from the two simulations clearly show the incorrect assumptions in the first model. The velocity increase of the Brownian particle with time produces a displacement that is not in agreement with true Brownian motion. The momentum transfer approximation introduced in the second model produce more realistic results, this is seen in the lower plot in Figure 4.

In conclusion the simulations produced the desired results and are in agreement with the theory for both models. The mean velocities and displacements obtained for model 1 fit well with (3) and (6), while for the second model the mean velocity distribution obtained match the value predicted by (9) given a value 0.9 for ρ.

The second model could produce more accurate results if the w term in the velocity equations was defined more precisely and not restricting it to ± 1, the initial velocity could also be modified from its initial value of 0.

References

[1]L. Gunther and D. Weaver, "Monte carlo simulation of brownian motion with viscous drag", American Journal of Physics **46**, 543–545 (1978).

[2]C. Anger and J. Prescott, "A monte carlo simulation of brownian motion in the freshman laboratory", American Journal of Physics **38**, 716–719 (1970).

[3]R. P. Feynman, R. B. Leighton, and M. Sands, "The feynman lectures on physics; vol. i, pp. 6-5, 6-6", American Journal of Physics **33**, 750–752 (1965).