Simulating Colloidal Interactions

Gilad Barlev '09 and Timothy Sullivan, Dept. of Physics, Kenyon College

Abstract

Our research built upon previous work done at Kenyon in simulating Brownian motion, expanding our model to simulate experiments that tracked the behavior of micron-sized polystyrene spheres suspended in highly deionized water and confined between two glass plates. Our end result was a program that successfully simulated experimental conditions and tracked the particle in up to three spatial dimensions. In additon, we were successful in completely automating the analysis of our data using a script written in *Origin C*. This analysis yielded agreement with experimental findings in the absence of external force and in the dimensions parallel to the constraining walls when force was applied, but in the presence of force, the simulations show a 25% discrepancy with experimental results in the direction perpendicular to the walls. This difference has yet to be accounted for.

Introduction

Previous experimental research developed a novel method of 3D tracking to examine the behavior of micron-sized polystyrene spheres suspended in highly de-ionized water and confined between two glass plates [1]. This research measured, among other things, how the diffusion coefficient of PS spheres depended on plate separation. The primary goal of our research was to create a working computer model that simulates our colleagues' experiments and thus produces data that can be analyzed and compared to experimental findings.

This research built upon previous work done at Kenyon in simulating Brownian motion—the seemingly random movements of a particle caused by it being buffeted by an enormous number of smaller particles—by applying a "random walk" to the simulated particle. Daniel Kiepfer and Benjamin Hildebrand ('03) wrote a program capable of simulating this "random walk" in the case of an unconstrained sphere.

The next step was thus to expand on this model to take into account forces and hydrodynamic drag, thus allowing us to simulate experimental conditions.

Adding Force

The authors of Ref. [1] were able to experimentally determine the potential of a particle at any given position within the cell. Graphs of these potentials were then fitted with an exponential function of the form:

$$\mathbf{U(z)/(kT) = Aexp(-\kappa z) + Bexp(-\kappa(z_0-z))}$$

where U is the potential, k the Boltzmann constant, T the absolute temperature, z = 0 is at one of the walls, z_0 is the wall separation, κ^{-1} corresponds to the screening length, and A and B are fitting parameters. Since $F=-{}^{dU}/_{dz}$ and the particle reaches its terminal velocity nearly instantaneously for our purposes (thus allowing us to use Stokes' Law), doing a bit of algebra and calculus, we find that the displacement of a particle over a timestep Δt can be approximated by

$$\mathbf{\Delta z = \kappa[Aexp(-\kappa z) - Bexp(-\kappa(z_0-z))]*D_0*\Delta t}$$

where D_0 represents the free diffusion coefficient.

References:

[1] C.H. Sow, T. Sullivan, et al., in preparation.
[2] Benjamin Hildebrand, et al., http://physics.kenyon.edu/people/sullivan/Research/BrownianMotion/index.html, viewed on 5 February, 2006.
[3] B. Lin, J. Yu, S. Rice, Physical Review E 62, 3 3909 (2000).
[4] J. Happel and H. Brenner, Low Reynolds Number Hydrodynamics (Kluwer, Dordrecht, 1991).

Methodology

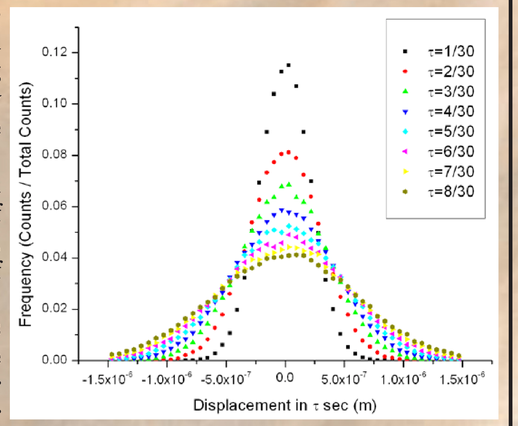
Our program, Colloid Simulator, written in C++, outputs several data files tracking the particle's position over the 80,000 timesteps (~45 minutes) of the simulation, recording the particle's displacement over a series of time periods τ (corresponding to between 1 and 8 timesteps) and binning these "delta" values so they can be imported into the Origin analysis program.

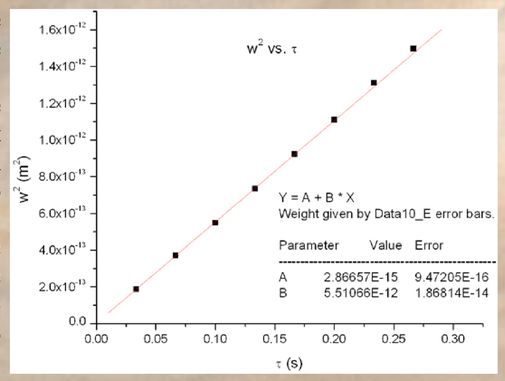
This binned data is then by plotted as a series of histograms (upper plot), and fitted with a version of the Gaussian.

The squares of the widths of these distributions are then plotted versus τ, (lower plot). The result is a linear trend, with the slope of the fit equal to eight times the diffusion coefficient [2].

All this analysis is done automatically using a script written in *Origin C*, a C-based language built into recent versions of Origin.

ColloidAnalysis.cperforms all the neccessary analysis on an entire set of simulations based on one of two experimental regimes.





Hydrodynamics

A particle moving in a fluid will create a flow in the fluid near the particle that will be modified by nearby objects, thus increasing drag on the sphere. In this case, as our PS sphere gets closer to a wall, its diffusivity drops. In the dimensions parallel to the walls, this *hydrodynamic drag* can be approximated by:

$$D_{x,y}(t) = D_o\left(1-\frac{9}{16}\frac{a}{z(t)}-\frac{9}{16}\frac{a}{[z_0-z(t)]}\right)$$

where D_0 is the free diffusion coefficient, a the radius of the sphere, z_0 the wall separation and z(t) the distance from one wall at time t [4].

In the dimension perpendicular to the walls, we see a different correction [4]:

$$D_z^{cal} = D_o \Big/ \lambda_z(z) + \lambda_z(z_o - z) - 1$$

$$\lambda_z(z) = \frac{4}{3}\sinh\alpha\sum_{n=1}^{\infty}\frac{n(n+1)}{(2n-1)(2n+3)} \times\left[\frac{2\sinh(2n+1)\alpha+(2n+1)\sinh 2\alpha}{4\sinh^2(n+1/2)\alpha-(2n+1)^2\sinh^2\alpha}-1\right]$$

$$\alpha = \cosh^{-1}(z/a)$$

D_x and D_y are easy enough to incorporate into the simulation, but D_z is given as an infinite series, and thus needed to be approximated.

Results & Conclusions

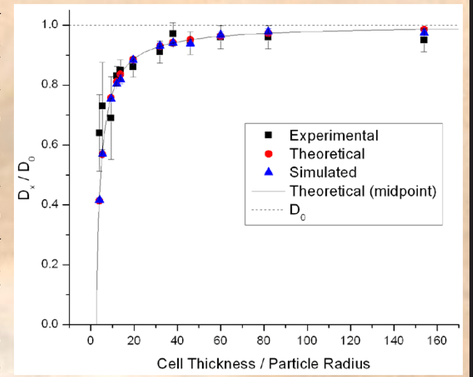
Our research successfully accomplished what we set out to do: the experimental data created by our collaborators can now be compared with simulated data from Colloid Simulator, which replicates experimental conditions by applying force and correcting for hydrodynamic drag.

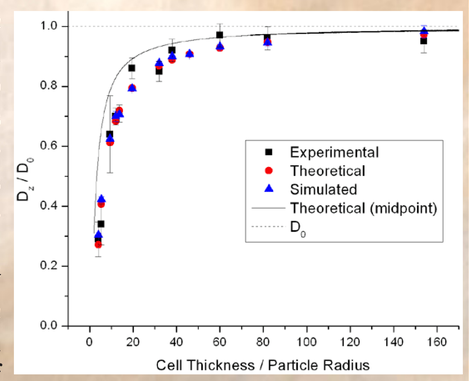
Colloid Simulator also modeled another experiment that looked at what happens to the diffusion coefficient of a small sphere trapped between two walls. These experimenters eliminated the effects of external forces so they could focus solely on the effects of hydrodynamic drag [3].

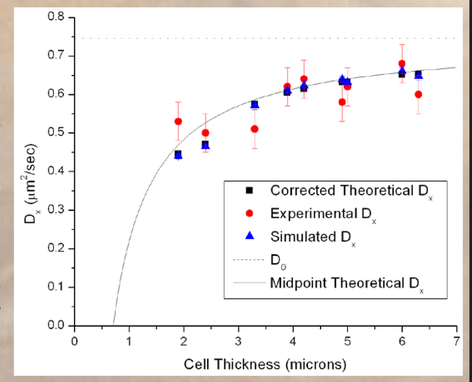
The data produced by Colloid Simulator in that case agrees with experimental data reported by the authors of Ref. [3] (top two).

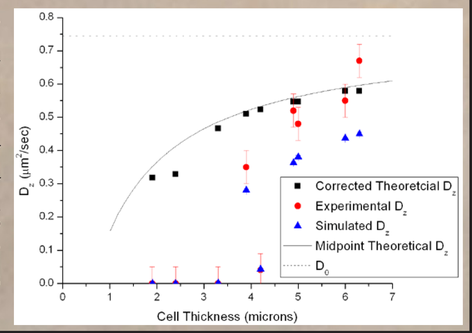
In addition, for our simulations that *did* take force into account, we saw agreement between simulated and experimental data in the dimensions parallel to the confining walls (second from the bottom).

However, when looking at the dimension perpendicular to the walls, our simulations showed a systematic discrepancy of about 25% when compared to experimental data (bottom). We have not yet been able to account for this difference. Future progress will rely on gaining access to the raw experimental data, thus allowing us to determine if the discrepancy is a result of, say, differences in analysis techniques.









Many thanks to Prof. Sullivan for his mentoring and guidance and to the Kenyon Summer Science Scholars program for funding my research.