PhD Dissertation Defense Announcement Mechanical and Aerospace Engineering Department University of Texas at Arlington

ANALYSIS OF A NANOPARTICLE'S MOTION IN AN OPTICAL TWEEZER

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<u>Abstract</u>

This work presents a simulation and experimental analysis of a nanoparticle's motion in an optical tweezer. Specifically, different simulation and analysis techniques are developed to investigate a suspected regime change in the dynamics of the micro/nano particles from overdamped to underdamped motion as the particle size reduces to submicron scale. Moreover, the simulation techniques developed here provide accurate prediction of the particle dynamics along with low computation time. Finally, the experimental setup developed here provides new experimental data that help answer the question of the regime change with increased certainty.

Micro- and nano- scale systems, such as an optical tweezer, require a longer time to simulate because of the disproportionality that exists between fluid and inertia forces. This problem is resolved by the use of a multiscale approach that relies on the method of multiple scales, which scales the forces such that they are similar in proportion. The scaling approach has been used previously with two- and three- dimensional models, where the laser forces were computed by discretizing the laser beam into a finite number of rays. However, this method of calculating laser forces starts to fall apart as the particle size becomes smaller than the wavelength of the laser. This work presents a three-dimensional model that relies on the Generalized Lorenz-Mie Theory (GLMT) to calculate laser forces.

An online constraint embedding method has been used in the past to enforce the normality constraint of the Euler parameters in the rotational dynamics of the 3D model. However, this method requires the integrator to be stopped in order to change the dependent Euler parameter. This work provides a novel elimination approach that does not require the definition of the dependent Euler parameter. Moreover, this approach does not require extra equations to be solved during the integration, which results in lower computation time.

The numerical solvers used to integrate the Equations of Motion (EOMs) change both the type of result and the computational requirement. A micro- or nano- particle observes forces due to the Brownian motion in the surrounding fluid. The inclusion of such forces makes the EOMs of the particle stochastic differential equations (SDEs) instead of the ordinary differential equations (ODEs). Moreover, the disproportionality in the inertia and fluid forces makes these equations stiff in nature. Thus, the stiff SDE solvers from the Julia programming language are used here to tackle both of these scenarios. The use of these solvers along with the scaling technique helps achieve further reduction in computation time.

The inclusion of Brownian motion force and the use of stochastic differential equation solvers allow the analysis of the problem in the frequency domain. It is common practice with optical trapping experiments to measure the trap stiffness with the use of Power Spectral Density (PSD) analysis. This work develops a theoretical equation of the PSD of the nanoparticle's position along with scaling. This helps estimate the PSD of the nanoparticle that would show the underdamped behavior in the experiments.

Finally, a completely new experimental setup is prepared to investigate the claim of regime change from previous experiments in further detail. The experimental setup is designed to achieve easy and repeated trapping of the nanoparticle along with high frame rate recording of its trajectory. Software for all the necessary hardware, i.e. the high-speed camera, laser shutter and the back illumination system, is developed in-house to automate performing the experiments.