Towards controlled nanoscale propulsion and maneuverability

Title of the dissertation: Dynamics of diffusive and driven nanoparticles in fluids

Contents of the dissertation: The ability to make measurements and manipulate matter at micrometer and nanometer scales will have far-reaching applications. In the past decade, significant progress has been made in developing microscale and nanoscale motors that can be used for targeted delivery. These advances are not without complications, however, such as those brought about by thermal effects which are more apparent at the nanoscale.

Modeling microscale and nanoscale objects that interact with a fluid requires a fluid model that is quantitatively accurate and can capture macroscopically observed quantities without any adjustable parameters to make quantitative predictions of the dynamics. In this thesis, we have modeled diffusive and driven systems through the use of a recently developed numerical multiscale simulation method—a coupled fluctuating lattice-Boltzmann and molecular dynamics (LBMD) method—to study thermal effects on driven systems.

The diffusion coefficients of simple shapes and complex aggregate clusters obtained from the LBMD method were first shown to be quantitatively consistent. The LBMD method was then used to study the diffusive and driven dynamics of magnetic helices. The magnetic helices, which interact with an external rotating magnetic field, rotate and propel in the fluid. In the presence of thermal fluctuations, spatial and temporal control of these nanohelices may be achieved. We also show that the self-propelled systems can also be modeled using this method.

Field of the dissertation: Engineering physics

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