Department of Mathematics

University of Houston

## Scientific Computing Seminar

Prof. Eliot Fried McGill University

## Self-propelled soft-core dumbbells for the simulation of active suspensions: application to self-motile bacterial suspensions

Thursday, Sep. 12, 2013 3:00 PM- 4:00 PM Room 646 PGH

## Abstract:

A simple model for simulating flows of active suspensions is presented. The approach is based on the dissipative particle dynamics framework. While the model is potentially applicable to a wide range of self-propelled particle systems, the specific class of self-motile bacterial suspensions is considered as a modeling scenario. To mimic the rod-like geometry of a bacterium, two dissipative particle dynamics particles are connected by a stiff harmonic spring to form an aggregate dissipative particle dynamics molecule. The bacterial motility is modeled through a constant self-propulsion force applied along the rod axis of each such aggregate molecule. The model accounts for hydrodynamic interaction forces between self-propelled agents through the pairwise dissipative interaction forces from the dissipative particle dynamics framework. Numerical simulations of this system are performed using a customized version of the open-source LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software package. Detailed studies of the influence of particle concentration, pairwise dissipative interaction forces, and Stokes drag forces on the statistics of the system are provided.

This seminar is easily accessible to persons with disabilities. For more information or for assistance, please contact the Mathematics Department at 743-3500.