Title: Using computer simulations to understand flow-induced structures

Abstract: The role of flow and its ability to induce and change structures in materials is important in a wide range of applications. In this talk, I will discuss two examples in which we have used computer simulations to better understand how flow induces these structures. In the first example, the flow is externally imposed on a solution of polymers and nanoparticles. We have used a coarse-grained Brownian Dynamics method to examine the structures that form in flow. For some values of concentration, interaction strengths, and flow strengths, the flow can induce a collapse of the polymer and nanoparticles into a globule state. We have analyzed the formation as a barrier hopping process in a free energy landscape. For small shear rates, the flow acts to alter the first passage process across the barrier. At higher shear rates, the flow causes a hopping back and forth between the two states. In the second example, the flow is generated by the system itself. As a microorganism swims through a fluid, it causes a flow disturbance which affects other microorganisms. I will discuss our theoretical and simulation approaches to understanding how these hydrodynamic interactions can lead to large-scale collective behavior of groups of organisms. In particular, we have found that correlations of the orientations of neighboring organisms play an important role even for very dilute systems. We have also examined how non-Newtonian fluids impact the ability of the organisms to coordinate. We will discuss possible implications of these results on fluid mechanical barriers to infection.

Patrick T. Underhill
Assistant Professor
Rensselaer Polytechnic Institute
Dept. of Chemical & Biological Engineering Ricketts Building, Room 132
110 8th St
Troy, NY 12180
(518)276-3032
http://www.rpi.edu/~underp3