**140c Microscopic Mechanisms of Molecule Migration in Nanochannels**

*Rajesh Khare, Michael Graham, and Juan De Pablo*

The development of micro and nanofluidic devices for biological molecule manipulation has fueled significant interest in understanding transport phenomena at the nanoscale. Traditionally, flow fields have been extensively used for manipulating molecules in these devices. Our recent work has showed that thermal gradients can also be used to effectively control transport phenomena at the nanoscale.

We use molecular simulations to investigate the effect of shear flow and thermal gradients on molecule migration in fluids confined to nanochannels. Two types of systems are studied: a simple fluid mixture and a dilute polymer solution. Polymer chains are represented using a bead-spring model and a coarse grained model is used for the solvent. Non-bonded interactions are represented using either a WCA or a full Lennard-Jones potential. Diffusion and hydrodynamic effects are determined by the intermolecular interactions in such a model system.

Simulations are used to identify the conditions (strength of the shear field and the thermal gradients) that cause molecule migration both towards and away from the channel walls. The results of simulations are compared with experimental data and with predictions from Brownian dynamics simulations and kinetic theory. These results are explained on the basis of kinetic and thermodynamic driving forces.