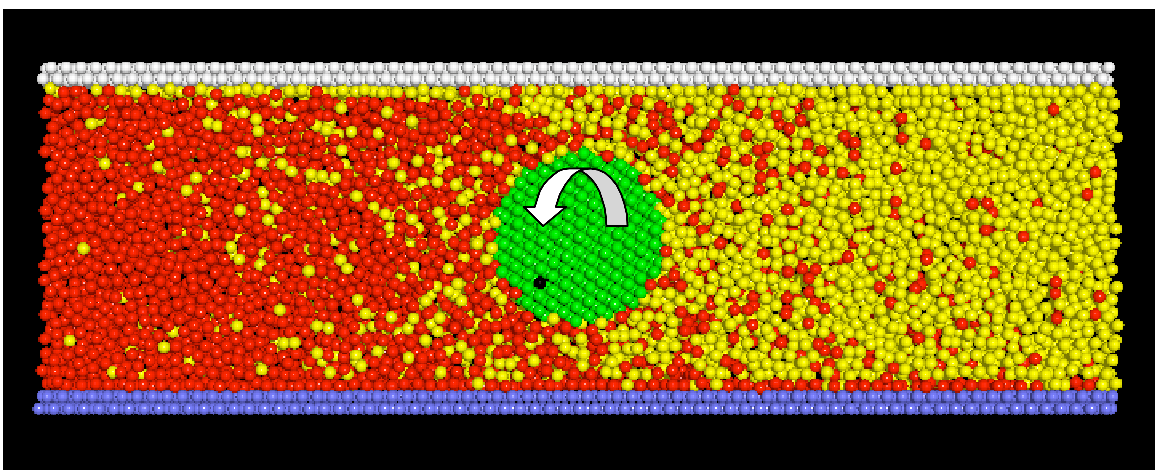
NIRT Highlight (Theory, Modeling and Simulation)

Entropy driven Nano-motors and Nano-pumps

Imagine being able to manipulate atto-litre volumes of fluid in nano-sensors or employ massively parallel chemical testing devices that scan many mixtures to identify one ideal combination. As one works with smaller and smaller volumes of fluids, surface forces at solid-fluid interfaces start to become comparable or even larger than bulk forces, such as pressure gradients. Interfacial effects are poorly understood, and often frustrate designs based on macroscopic devices. Recently, researchers at Johns Hopkins University have been working to understand these forces and harness them to drive flow. They have demonstrated, using simulations of molecular models, how an understanding of surface forces can be used to make nano-pumps and nano-motors.

Multicomponent mixtures and other complex fluids have many degrees of freedom associated with their internal structure and composition. This introduces variations in interfacial properties that can be manipulated, both spatially and temporally. A simple example is described in Ref. 1 and illustrated below. The walls have different interactions with the two constituents of a miscible binary fluid. This coupled with a concentration gradient can drive fluid flows between the walls. We have constructed a quantitative model of this effect and demonstrated its use in the construction of the entropy driven nano-motor shown in Figure 1 (Ref. 2). A nano-pump is created if both walls favor the same fluid. This material is based upon work supported by the National Science Foundation under Grant No. 0083286.



A snapshot of a molecular dynamics simulation of a nanomotor. A miscible binary fluid (red and yellow molecules) is confined between two solid walls (blue and white molecules). A concentration gradient is maintained by a reservoir of red at the left end of the channel and a reservoir of yellow at the right. The yellow atoms are attracted more strongly to the top wall and red atoms to the bottom wall. The solid cylinder (green) has intermediate properties. The combination of the concentration gradient and the asymmetric wall interactions results in a spontaneous shear flow that causes a counter-clockwise rotation of the cylinder. The simulation is three-dimensional and extends indefinitely into the page.

References:

1. "Molecular and Continuum Boundary Conditions for a Miscible Binary Fluid", C. Denniston and M. O. Robbins, Physical Review Letters **87**,178302 (2001).
2. Quicktime movie at http://www.pha.jhu.edu/~colin/movies.html.

NSF award 0103408, Mark O. Robbins and Colin Denniston, Johns Hopkins University