The nanofluidics and biology group

The projects in this group draw on the considerable experience at CTR in using advanced algorithms and large-scale simulation used to analyze turbulence related phenomena. This group applied these capabilities to two new areas: nanofluidics and biological flows.

Nanofluidics plays an important role in biodetectors, tribology, and diffusion through porous media, and anywhere that non-continuum or discrete molecular effects play a significant role. Two projects studied nanofluidics. Walther, Jaffe, Halicioglu, and Koumoutsakos studied the interaction of water with carbon nanotubes, whose size and unique physical and electrical properties make them attractive building blocks for nanostructures. They have been proposed as ultra-fine tips for atomic force microscopes for probing complex molecules and for use in biosensors, both of which involve interactions with water. Yet their interaction with water is not well understood. Atomistic simulations were used to determine conditions for two nanotubes suspended in water to attract and to study their general hydro-phobic/-phyllic properties.

Similar atomistic simulation techniques were used by Freund to examine the details of electro-osmotic flow in a nanometer-scale channel. In electro-osmosis, an applied electric field pulls counter ions distributed above a charge surface to induce a net flow. This pumping mechanism is used in present-day micron-scale devices, often for biosensor application. However, the flow is driven by a near-wall nanometer-scale layer which is small enough to be studied atomistically. This project simulated the electro-osmotic flow of a aqueous solution of Cl^- in a 50Å wide channel. Differences were found between the present simulation results and standard theories that assume infinitesimal ions and constant dielectric properties.

In addition to studies of these physical systems, considerable progress was made in developing and implementing efficient algorithms for atomistic simulations. Walther, Jaffe, Halicioglu, and Koumoutsakos discuss a new formulation of the P^3M method for computing long-range electrostatic interactions. Freund and Darve implemented an efficient P^3M algorithm for a $1/r^6$ inter-atomic force potential which is being used in ongoing surface tension research. Some of the computer codes used in these studies have also been transferred to researchers in the Astrobiology Branch of NASA Ames for studying molecular biophysics. Collaboration with this group is ongoing.

Ghosal, Rogers, and Wray examined the role of turbulence in the life cycle of phytoplankton, which affect global ecology and sustain oceanic food chains. In the short term, phytoplankton impact people via the health of fisheries; in the long term, since their carbon uptake counters carbon-dioxide emissions from the burning fossil fuels, their response to increased carbon in the atmosphere and warmer seas will impact global climate. Because many phytoplankton are non-swimming and actually sink, turbulence is essential in transporting them and maintaining healthy populations in the sunlit upper layers of bodies of water. This project used population models in conjunction with simulation data to study the role of turbulence in their population dynamics.

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