

# Center for Applied Mathematics and Center for Biocomplexity Colloquium

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***“Multiscale Modeling of Biomolecular Systems”***

**Monday September 29, 2008**

**4:00pm**

**129 Hayes-Healy Center**

***\*Tea at 3:30pm\****

Under physiological conditions, most biological processes, such as signal transduction and protein folding, occur in water, which consists of 65-90 percent human cell weight. The behavior of solvent and synergy of solvent-solute are important to the quantitative understanding of biological processes. Explicit calculations of biomolecules in the solvent remain prohibitively expensive. The Poisson-Boltzmann equation (PBE) based multiscale model marries a microscopic discrete description of biomolecules with a macroscopic continuum treatment of the solvent. Solvation free energy, pKa, electrostatic potential and molecular dynamics of large biomolecules are obtained from this model.

In this talk, we report two new developments in this multiscale model. First, new geometrical flow equations are introduced for the formation and evolution of solvent-solute interfaces. These equations take account for not only intrinsic geometric forces, such as mean curvature forces, but also potential forces from solvent-solute interactions. Our geometric flow approach significantly improves the solvation prediction of large biomolecules. Second, a high-order accurate elliptic interface method, the matched interface and boundary (MIB) method, is developed and implemented in conjugation with the Green's function formalism to solve the PBE and provide the most accurate and highly efficient calculations of electrostatic potentials and solvation free energies for biomolecules. An MIB based molecular dynamics method has also been developed for protein folding. Our MIB based methods dramatically improve the accuracy, stability and reliability of the current state of the art in the PBE based implicit solvent model.