1046-65-1472 **Stephen D Bond*** (sdbond@illinois.edu), Department of Computer Science, University of Illinois, 201 N Goodwin Ave, Urbana, IL 61801, and **Burak Aksoylu**, **Eric C Cyr** and **Michael J Holst**. *Goal-Oriented Error Estimation and Multilevel Preconditioning for the Poisson-Boltzmann Equation.*

The computation of "free energy" has been described as one of the most important and challenging problems in computational chemistry. Free energy is the thermodynamic state function which describes the macroscopic properties of a system and, hence, plays an integral role in multiscale modeling and coarse-grained simulation. One of the most popular coarse-graining methods approximates the solvent (e.g., water) interactions by a dielectric continuum as described by the Poisson-Boltzmann equation (a nonlinear elliptic PDE). To calculate the "solvation free energy" for the coarse grained system, one must evaluate a linear functional of the solution to this PDE. In this talk, we show how one can calculate the solvation free energy using an adaptive finite element approximation to the solution of the Poisson-Boltzmann equation. In our scheme, the mesh refinement is driven by goal-oriented error estimation based on the free energy functional. Hierarchical basis methods are used to precondition the resulting algebraic systems arising in the multilevel finite element discretization. (Received September 15, 2008)