1048-65-144 **Jingfang Huang*** (huang@amath.unc.edu), CB # 3250, Phillips Hall, Department of Mathematics, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3250, and **Benzhuo Lu**, **Xiaolin Cheng** and **J. Andrew McCammon**. *An adaptive fast multipole algorithm for electrostatic interactions in biomolecular systems.*

Poisson-Boltzmann (PB) electrostatics is a well established model in biophysics, however its application to the study of large scale biosystem dynamics such as the protein-protein encounter is still limited by the efficiency and memory constraints of existing numerical techniques. In this talk, we present an efficient and accurate scheme which incorporates recently developed novel numerical techniques to further enhance the present computational ability. In particular, a boundary integral equation approach is applied to discretize the linearized Poisson-Boltzmann (LPB) equation; the resulting integral formulas are well conditioned and are extended to systems with arbitrary number of biomolecules; the solution process is accelerated by the Krylov subspace methods and an adaptive new version of fast multipole method (FMM); and in addition to the full electrostatic interaction energy, the forces and torques can be computed in a post-processing procedure. The Adaptive Fast Multipole Poisson-Boltzmann (AFMPB) solver will be released under open source license agreement. (Received February 04, 2009)