Shaozhong Deng\* (shaodeng@uncc.edu), Department of Mathematics and Statistics, UNC at Charlotte, Charlotte, NC 28223. Efficient methods of images for hybrid explicit/implicit solvent simulations.

Electrostatic interactions are well-known to provide crucial contributions to the structure, dynamics and function of bio-macromolecules; as such, they remain as major objects of computational biology. In this talk, we will discuss our past results as well as recent efforts in the development of multiple-image-based reaction-field methods for calculating electrostatic interaction in hybrid explicit/implicit bio-molecular dynamics simulations. Some preliminary results of molecular dynamics simulation of liquid water by using the multiple image methods are also to be presented. (Received February 09, 2009)