1135-VN-444 **Tania Hazra*** (thazra@crimson.ua.edu), 1103 14th Street, Apt 26A, Tuscaloosa, AL 35401, and **Shan Zhao** (szhao@ua.edu), 345 Gordon Palmer Hall, Box 870350, Tuscaloosa, AL 35487-0350.

Stable ADI Scheme with Super-Gaussian Dielectric Distribution and Minimal Molecular Surface.

The work explores the stability impact of the novel unconditionally stable operator splitting methods for solving the time dependent nonlinear Poisson-Boltzmann (NPB) equation for the electrostatic analysis of solvated biomolecules. We start solving the NPB equation using conditionally stable method, namely Alternating Direction Implicit (ADI) scheme. Our goal is to make the existing ADI schemes stable. Now, for modeling protein electro-statics using implicit methods, we require dielectric properties of the system to be known, in particular, the value of the dielectric constant of protein. In our work, we have applied the Gaussian dielectric constant distribution to ADI scheme. Also we have used the minimal molecular surface (MMS), that minimizes the surface free energy of the macromolecule in the aquatic environment and it is typically free of geometric singularities. Combination of Gaussian dielectric constant distribution and MMS makes the ADI scheme unconditionally stable. By raising the content of the exponent to a higher power (super-Gaussian dielectric constant distribution) ADI scheme can produce more accurate solvation energy for proteins. (Received September 03, 2017)