1145-VC-980 **Sheik Ahmed Ullah*** (saullah@crimson.ua.edu) and **Shan Zhao**. *A new ADI method for the Poisson-Boltzmann equation with a two-component regularization.* Preliminary report.

The Poisson Boltzmann Equation (PBE) is a well-established implicit solvent continuum model for the electrostatic analysis of solvated biomolecules. The solution for the nonlinear PBE is still a challenge due to its strong singularity by the source terms, dielectrically distinct regions, and exponential nonlinear terms. In this paper, a new alternating direction implicit method (ADI) is proposed which inherits all the advantages of the two-component regularization and the time-dependent PBE with ADI method, while possessing a novel approach to combine them. A modified version of the ghost fluid method has been introduced to incorporate the jump conditions into the new ADI method. The proposed scheme produced better accuracy than previous ADI methods for a benchmark problem and simpler to implement. Though this scheme can use larger time increments than the previous ADI methods, it still blows up for some special cases. Later to improve the stability, Locally One Dimensional (LOD) method has been used to replace the ADI method. Finally, to test the ability of this newly proposed ADI-GFM and LOD-GFM method, we have evaluated the solvation free energy for a collection of 24 proteins with various sizes and the salt effect on the protein-protein binding energy of the complex 1beb. (Received September 23, 2018)