1125-VC-337 **Tania Hazra*** (thazra@crimson.ua.edu), 1103 14th Street, Apt 26A, Tuscaloosa, AL 35401.
Stable Operator Splitting Method for Free Energy Calculation of One Atom Model. Preliminary report.

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. In a pseudo-transient continuation solution of the NPB equation, the nonlinear term is analytically integrated, so that the difficulties in direct treatment of the strong nonlinearity can be bypassed.

There are several methods to solve the NPB equations. We are interested in Alternating Direction Implicit (ADI) schemes and Locally-One Dimensional (LOD) schemes. The ADI methods are known to be conditionally stable, although being fully implicit. On the other hand, LOD scheme is computationally less expensive and LOD scheme based on implicit Euler integration is more stable than ADI schemes.

It has been observed that there is a noticeable difference between the linearized Poisson Boltzmann Equation result and ADI-based NPB results in steady state solutions. That motivated us to analyze the ADI schemes and later on LOD schemes to detect the factor for which the stability is getting affected. (Received August 27, 2016)