1145-VN-1551 **Tania Hazra*** (thazra@misericordia.edu) and **Shan Zhao**. *A super-Gaussian Poisson-Boltzmann model for electrostatic solvation energy calculation: EDC Analysis and Application on Protein Cavities.* Preliminary report.

Understanding the mechanism of many biological systems requires the calculations of electrostatic potential and solvation energy of macromolecules. In the classical implicit solvent Poisson-Boltzmann (PB) model, the macromolecule and water are modeled as two-dielectric media with a sharp border. However, the dielectric property of interior cavities and ion-channels is difficult to model realistically in a two-dielectric setting. In fact, whether there are water molecules or cavity-fluid inside a protein cavity remains to be an experimental challenge. Physically, this uncertainty affects the subsequent solvation free energy calculation. In order to compensate this uncertainty, a novel super-Gaussian dielectric PB model is introduced in this work, which devices an inhomogeneous dielectric distribution to represent the compactness of atoms and characterizes empty cavities via a gap dielectric value.

Mathematically, an effective dielectric constant (EDC) analysis is introduced in this work to benchmark the dielectric model and select optimal parameter values. Computationally, a pseudo-time alternative direction implicit (ADI) algorithm is utilized for solving the super-Gaussian PB equation, which is found to be unconditionally stable in a smooth dielectric setting. (Received September 23, 2018)