Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Analytical solutions of the Poisson-Boltzmann equation: biological applications ANDREW FENLEY, Virginia Tech (Physics Dept.), JOHN GORDON, ALEXEY ONUFRIEV, Virginia Tech (Computer Science Dept.) — Electrostatic interactions are a key factor for determining many properties of bio-molecules. The ability to compute the electrostatic potential generated by a molecule is often essential in understanding the mechanism behind its biological function such as catalytic activity, ligand binding, and macromolecular association. We propose an approximate analytical solution to the (linearized) Poisson-Boltzmann (PB) equation that is suitable for computing electrostatic potential around realistic biomolecules. The approximation is tested against the numerical solutions of the PB equation on a test set of 600 representative structures including proteins, DNA, and macromolecular complexes. The approach allows one to generate, with the power of a desktop PC, electrostatic potential maps of virtually any molecule of interest, from single proteins to large protein complexes such as viral capsids. The new approach is orders of magnitude less computationally intense than its numerical counterpart, yet is almost equal in accuracy. When studying very large molecular systems, our method is a practical and inexpensive way of computing bio- molecular potential at atomic resolution. We demonstrate the usefullnes of the new approach by exploring the details of electrostatic potentials generated by two of such systems: the nucleosome core particle (25,000 atoms) and tobacco ring spot virus (500,000 atoms). Biologically relevant insights are generated.

Andrew Fenley
Virginia Tech

Date submitted: 03 Dec 2005 Electronic form version 1.4