

Biophysical Applications of the Adaptive Cartesian Grid Poisson-Boltzmann Equation Software Package

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The Poisson-Boltzmann equation (PBE) is one of the most widely used implicit solvent models to describe electrostatic interactions of biomolecules in ionic solutions. The commercial Adaptive Cartesian Grid (ACG) Poisson-Boltzmann equation solver was tested extensively over a number of years by performing PBE calculations on biomolecular systems of varying size and charge density (A. H. Boschitsch & M. O. Fenley, *Journal of Chemical Theory and Computation* 7:1524-1540 (2011)). In this talk, popular biophysical applications of the ACG PBE solver will be reported with the goal of highlighting unique features of ACG. These ACG features include the low CPU cost and high accuracy for PBE calculations of large-scale and highly charged biomolecular systems (*e.g.*, ribosomes) on conventional computer platforms.