Accelerating BEM in macromolecular electrostatics computing

†*B.Z. Lu

Academy of Mathematics and Systems Science, Institute of Comput Math, Chinese Academy of Sciences, Haidian, Beijing 100190, China,

*Presenting author
†Corresponding author: bzlu@lsec.cc.ac.cn

Abstract

Our software package AFMPB (adaptive fast multipole Poisson-Boltzmann) adopting a BEM is developed for rapid evaluation of electrostatic interaction in biomolecular systems modeled by the linearized Poisson-Boltzmann equation. It achieves a nearly optimal O(N) performance by introducing a number of techniques. The solver utilizes a well-conditioned boundary integral equation (BIE) formulation, a node-patch discretization scheme, a Krylov subspace iterative solver package with reverse communication protocols, an adaptive new version of fast multipole method in which the exponential expansions are used to diagonalize the multipole-to-local translations, and a parallelism with Cilk-Plus. As an example, the current software is able to solve the PBE with a generated linear system of twenty millions of freedoms for a huge virus molecular structure with a million of atoms. The program and its description, as well as several closely related libraries and utility tools are available at http://lsec.cc.ac.cn/~lubz/afmpb.html.

Keywords: Node-patch BEM, Fast algorithm, Biomolecule, Poisson-Boltzmann electrostatics.

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