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Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver

Bo Zhang[1], Benzhuo Lu[2], Xiaolin Cheng[3], Jingfang Huang[4,*], Nikos P. Pitsianis[1,5], Xiaobai Sun[1] and J. Andrew McCammon[6]

[1] *Department of Computer Science, Duke University, NC 27708, USA.*
[2] *Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100910, China.*
[3] *Center for Molecular Biophysics, Oak Ridge National Laboratory, TN 37831, USA.*
[4] *Department of Mathematics, University of North Carolina, Chapel Hill, NC 27599, USA.*
[5] *Department of Electrical and Computer Engineering, Aristotle University, Thessaloniki, 54124, Greece.*
[6] *Department of Chemistry & Biochemistry, Center for Theoretical Biological Physics, Department of Pharmacology, Howard Hughes Medical Institute, University of California, San Diego, CA 92093, USA.*

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Abstract. This paper summarizes the mathematical and numerical theories and computational elements of the adaptive fast multipole Poisson-Boltzmann (AFMPB) solver. We introduce and discuss the following components in order: the Poisson-Boltzmann model, boundary integral equation reformulation, surface mesh generation, the node-patch discretization approach, Krylov iterative methods, the new version of fast multipole methods (FMMs), and a dynamic prioritization technique for scheduling parallel operations. For each component, we also remark on feasible approaches for further improvements in efficiency, accuracy and applicability of the AFMPB solver to large-scale long-time molecular dynamics simulations. The potential of the solver is demonstrated with preliminary numerical results.

AMS subject classifications: 45B05, 65Y05, 68W10, 90B10, 92C05, 92C40

Key words: Biomolecular system, electrostatics, Poisson-Boltzmann equation, fast multipole methods, mesh generation, directed acyclic graph, dynamic prioritization, parallelization.

*Corresponding author. *Email addresses:* zhangb@cs.duke.edu (B. Zhang), bzlu@lsec.cc.ac.cn (B. Lu), chengx@ornl.gov (X. Cheng), huang@email.unc.edu (J. Huang), Nikos.P.Pitsianis@duke.edu (N. P. Pitsianis), xiaobai@cs.duke.edu (X. Sun), jmccammo@ucsd.edu (J. A. McCammon)

1 Introduction

In the past three decades, the Poisson-Boltzmann (PB) continuum electrostatic model has been adopted in many simulation tools for theoretical studies of electrostatic interactions between biomolecules such as proteins and DNAs in aqueous solutions. Various numerical techniques have been developed to solve the PB equations and help elucidate the electrostatic role in many biological processes, such as enzymatic catalysis, molecular recognition and bioregulation. Existing simulation packages or PB solvers use the finite difference method, such as in DelPhi [1], GRASP [2, 47], MEAD [13], UHBD [3, 46], PBEQ [35, 36], PB solver [32] in AMBER [18], ZAP [27] and MIBPB [62], or use the finite volume/multigrid method, such as in the Adaptive Poisson-Boltzmann Solver (APBS) [4]. In a circumstance where the linearized PB is applicable, the partial differential equations can be reformulated into a set of surface integral equations (IEs) by using Green's theorem and potential theory. The unknowns in the IEs are located on the molecular surface only, and the resulting discretized linear system can be solved efficiently and accurately with certain fast convolution algorithms, in particular, the fast Fourier transform (FFT) and the fast multipole method (FMM).

The main purpose of this paper is to introduce the adaptive fast multipole Poisson-Boltzmann (AFMPB) solver, in the aspects of mathematical theories, numerical properties and computational components. The numerical components of the AFMPB are mostly based on previously published results, by some of the authors and other researchers. We give a brief summary and provide certain references, not exhaustively, to the precursor work. Certain computational components, especially for algorithmic parallelization and parallel scheduling, are recently developed by the authors. We introduce them briefly. We emphasize that even when each component is well studied and understood, a coherent integration of these components still calls for special attention and efforts. The success of a mathematical software is ultimately measured by its applicability and the extent of its applications. The rest of the paper is organized into two sections. In Section 2, we describe the PB model, the boundary integral equation (BIE) reformulation, the surface mesh generation, a node-patch discretization approach, the Krylov subspace methods, the new version of FMMs, and a dynamic prioritization technique for parallelization. We comment on each topic certain feasible strategies or active efforts for further improvements in efficiency and accuracy. In Section 3, we present numerical results from preliminary experiments and demonstrate applicability and performance of the AFMPB solver.

2 Theoretical foundations and computational elements

2.1 Continuum Poisson-Boltzmann electrostatics model

The electrostatic force is considered to play an important role in the interactions and dynamics of molecular systems in aqueous solution. In the Poisson equation model, when the charge density that describes the electrostatic effects of the solvent outside the