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On preconditioning the treecode-accelerated boundary integral (TABI) Poisson–Boltzmann solver

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ABSTRACT

We recently developed a treecode-accelerated boundary integral (TABI) solver for solving Poisson–Boltzmann (PB) equation [1]. The solver has combined advantages in accuracy, efficiency, memory, and parallelization as it applies a well-posed boundary integral formulation to circumvent many numerical difficulties associated with the PB equation and uses an $O(N \log N)$ treecode to accelerate the GMRES iterative solver. However, as observed in our previous work [2], occasionally when the mesh generator produces low quality triangles, the number of GMRES iterations required to solve the discretized boundary integral equations $Ax = b$ could be large. To address this issue, we design a preconditioning scheme using preconditioner matrix M such that $M^{-1}A$ has much improved condition while $M^{-1}z$ can be rapidly computed for any vector z. In this scheme, the matrix M carries the interactions between boundary elements on the same leaf only in the tree structure thus is block diagonal with many computational advantages. The sizes of the blocks in M are conveniently controlled by the treecode parameter N_0, the maximum number of particles per leaf. The numerical results show that this new preconditioning scheme improves the TABI solver with significantly reduced iteration numbers and better accuracy, particularly for protein sets on which TABI solver previously converges slowly. In addition, this preconditioning scheme potentially can improve the condition number of various multipole method accelerated boundary elements solvers in scattering, fluids, elasticity, etc.

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1. Introduction

In biomolecular simulations, electrostatic interactions are of paramount importance due to their ubiquitous existence and significant contribution in the entire force fields. However, computing these nonbonded interactions is challenging since they are pairwise at cost of $O(N^2)$ and long range [3]. To reduce the degree of freedom of the system in terms of electrostatic interactions, implicit solvent Poisson–Boltzmann (PB) model is used [4], in which the water molecules are treated as continuum and the dissolved electrolytes are approximated using the statistical Boltzmann distribution. The PB model has broad application in biomolecular simulations such as protein structure [5], protein–protein interaction [6,7], chromatin packing [8], pKa [9–12], membrane [13,14], binding energy [15–17], solvation free energy [18,19], ion channel profiling [20], etc.

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The PB equation is an elliptic interface problem with several numerical difficulties such as discontinuous dielectric coefficients, singular source, complex interface, and infinity boundary condition. Standard finite difference discretization in solving PB equation is efficient and robust thus popular [21–24], however it may suffer from accuracy reduction due to discontinuity of the coefficients, non-smoothness of the solution, singularity of the sources, and truncation of the domains, unless special interface and singularity treatments are applied [25,26] at the price of more complicated discretization scheme and possibly reduced convergence speed in iteration. Meanwhile, boundary integral methods are effective alternatives, which analytically circumvent above-mentioned difficulties. In addition, due to the structures hidden in the linear algebraic system after the discretization of the boundary integral and molecular surface, the matrix-vector product in each iteration can be accelerated by fast methods such as fast multipole methods (FMM) and treecode [27,28]. Our recently developed treecode-accelerated boundary integral (TABI) Poisson–Boltzmann solver is such an example [1] combining the advantages of both boundary integral equation and multipole methods. The TABI solver uses the well-posed derivative form of the Fredholm second kind integral equation [29] and the $O(N \log N)$ treecode [28] combined to solve the PB equation efficiently and accurately. It also has advantage in memory use and parallelization [1,30]. The TABI solver has been used by many computational biophysics/biochemistry groups and it has been disseminated standalone or as a contributive module of the popular APBS software package [31,32].

A bottleneck that hinders the efficiency of the TABI solver, which only uses the simplest diagonal or Jacobi preconditioning is at the mesh quality for triangulating the large and complex molecular surfaces. Our numerical tests previously showed that although the adopted integral formulation is well-posed [29], the mesh quality for triangulating the complex molecular surface affects the convergence speed of GMRES [1,2]. Currently our choice of the triangular mesh generator is the MSMS package developed by Sanner et al. [33], which is very efficient in generating triangular meshes for given biomolecules. However, due to the complexity of the molecular surface, the produced triangles could be irregularly shaped e.g. small in size, large in angle ($\approx \pi$), or in some other shapes which might affect the iterative convergence but cannot be filtered by our preprocessing subroutines. To resolve these issues, on one hand we are seeking better choices for molecular surface triangulation, and on the other hand we are trying to find solution to reduce the effect of mesh quality.

In the present work, we provide a newly designed preconditioning scheme, which cancels the slow-down effects caused by the mesh quality, while the added computational cost due to preconditioning is negligibly small. Our numerical simulation shows that for many tested proteins on which the TABI solver used to converge slowly now converges rapidly with this update. In addition, we believe this preconditioning scheme can benefit many multipole methods accelerated boundary integral Poisson–Boltzmann solvers such as [34–44]. The similar ideas can also be used to accelerate solving boundary integral equations from other areas such as scattering, fluids, elasticity, etc.

We next provide theories and algorithms related to the TABI solver and its preconditioning, followed by numerical results and discussion. This paper ends with a concluding remark section.

2. Theory and algorithms

In this section, we briefly describe the Poisson–Boltzmann (PB) implicit solvent model, review the current PB solvers, and introduce our recently developed treecode-accelerated boundary integral (TABI) PB solver, followed by our preconditioning scheme.

2.1. The Poisson–Boltzmann (PB) model for a solvated biomolecule

The PB model for a solvated biomolecule is depicted in Fig. 1(a) in which the molecular surface Γ separates the solute domain Ω_1 from the solvent domain Ω_2. Fig. 1(b) is an example of the molecular surface Γ as the triangulated surface of protein barnase [6]. In domain Ω_1, the solute is represented by N_c partial charges q_k located at atomic centers $\mathbf{r}_k$ for $k = 1, \cdots, N_c$, while in domain Ω_2, a distribution of ions is described by a Boltzmann distribution and we consider a linearized version in this study. The solute domain has a low dielectric constant ϵ_1 and the solvent domain has a high dielectric constant ϵ_2. The modified inverse Debye length $\bar{\kappa}$ is given as $\bar{\kappa}^2 = \epsilon_2 \kappa^2$, where κ is the inverse Debye length measuring the ionic strength; $\bar{\kappa} = 0$ in Ω_1 and is nonzero only in Ω_2. The electrostatic potential $\phi(\mathbf{x})$ satisfies the linear PB equation,

$$-\nabla \cdot \epsilon(\mathbf{x}) \nabla \phi(\mathbf{x}) + \bar{\kappa}^2(\mathbf{x}) \phi(\mathbf{x}) = \sum_{k=1}^{N_c} q_k \delta(\mathbf{x} - \mathbf{x}_k), \tag{1}$$

subject to continuity conditions for the potential and electric flux density on Γ,

$$[\phi] = 0, \quad [\epsilon \phi_\nu] = 0, \tag{2}$$

where $[f] = f_1 - f_2$ is the difference of the quantity f across the interface, and $\phi_\nu = \partial \phi / \partial \nu$ is the partial derivative in the outward normal direction ν. The model also incorporates the far-field boundary condition,

$$\lim_{\mathbf{x} \to \infty} \phi(\mathbf{x}) = 0. \tag{3}$$