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Parallel Smoothed Aggregation Multilevel Schwarz Preconditioned Newton-Krylov Algorithms for Poisson-Boltzmann Problems

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Abstract. We study a multilevel Schwarz preconditioned Newton-Krylov algorithm to solve the Poisson-Boltzmann equation with applications in multi-particle colloidal simulation. The smoothed aggregation-type coarse mesh space is introduced in collaboration with the one-level Schwarz method as a composite preconditioner for accelerating the convergence of a Krylov subspace method for solving the Jacobian system at each Newton step. The important feature of the proposed solution algorithm is that the geometric mesh information needed for constructing the multilevel preconditioner is the same as the one-level Schwarz method on the fine mesh. Other components, such as the definition of the coarse mesh, all the mesh transfer operators, and the coarse mesh problem, are taken care of by the Trillinos/ML packages of the Sandia National Laboratories in the United States. After algorithmic parameter tuning, we show that the proposed smoothed aggregation multilevel Newton-Krylov-Schwarz (NKS) algorithm numerically outperforms than smoothed aggregation multigrid method and one-level version of the NKS algorithm with satisfactory parallel performances up to a few thousand cores. Besides, we investigate how the electrostatic forces between particles for the separation distance depend on the radius of spherical colloidal particles and valence ratios of cation and anion in a cubic system.

AMS subject classifications: 65F08, 49M15, 65M55, 68W10
Key words: Poisson-Boltzmann equation, domain decomposition, Newton-Krylov-Schwarz algorithm, smoothed aggregation, parallel computing.

1. Introduction

This work aims to develop a parallel efficient and scalable computational tool for simulating the colloidal phenomena modeled by the Poisson-Boltzmann equation (PBE) [4, 6, 18, 19]. Another popular computational technique is based on the Monte

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Carlo simulation [24, 25, 27]. For a review of the recent developments in numerical solution algorithms and numerical schemes for PBEs, see [12–14, 26]. A colloidal system [15] is a mixture of several different kinds of molecules dispersed among each other, and can be roughly classified into two phases: One is a dispersed phase, and the other one is a continuous phase. In general, the particles in the dispersed phase, referred to as the colloidal particles, are usually larger than the ones in the continuous phase. The colloidal particles may be in a molecule or conglomerated into several molecules, and they range in size from one nanometer to ten micrometers. For example, in milk, the continuous medium is water and the dispersed phase contains other substances such as lactose and proteins. Although the colloidal particles are rather small, they have a very high surface-area-to-volume ratio due to their small diameters. The nature of interface plays a significant role in the interaction of colloidal systems. Otherwise, some colloids have the appearance of solutions such as polystyrene sulfate dispersed in deionized water. The polystyrene sulfate is synthesized with a large number of ionizable sulfate salt groups bonded to polystyrene spheres surfaces in a chemical. The sulfate groups dissociate in water, leaving negative charges bound to its sphere surface and positively charged counterions in the solution.

Hwang et al. [10] studied a parallel one-level Newton-Krylov-Schwarz (NKS) algorithm [3] for solving the large, sparse, nonlinear system of equations derived from PBE with applications in the numerical simulation of the two colloidal particles interaction in the symmetrical 1:1 electrolytes. The idea of the NKS algorithm is to find a search direction and then update the solution along that direction with a proper step size. The method repeats these two key steps until an acceptable approximate solution is found. As a Newton-type method, the search direction is determined by solving the corresponding Jacobian system with a Krylov subspace method, such as the generalized minimal residual method (GMRES) [17] or flexible GMRES [16] in conjunction with Schwarz type preconditioners. Their numerical results showed that the one-level PBE solver is scalable up to 128 computing cores on the distributed-memory system. As the follow-up paper to [10], the main contribution of this work is three-fold. First, we generalize our PBE solver that can handle the case of an asymmetrical electrolyte. Secondly, we develop a multilevel version of the PBE solver by adding the smoothed aggregation type of coarse grid space [2, 22] to improve the algorithmic scalability of the PBE solver further. As shown in the numerical results section, the overall computing time is reduced by a half or more when compared to the one-level version of the PBE solver. Also, our multilevel PBE solver exhibited satisfactory parallel performance up to thousands of cores for the test problems with 40 million unknowns. Related research work include Holst and Saied [9] who applied the algebraic multigrid method to linearized PBE arising from biophysics application and showed numerically that this approach outperformed some other alternatives, including an incomplete Cholesky dexomposition, and a family of preconditioned conjugate gradient methods. Womack et al. [23] developed a scientific software package, called DL_MG which was based on a geometric multigrid method and implemented by using the hybrid MPI and OpenMP parallel programming and their PBE solver was successfully applied to the electronic