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A FINITE DIFFERENCE SCHEME FOR SOLVING THE NONLINEAR POISSON-BOLTZMANN EQUATION MODELING CHARGED SPHERES [*1)]

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Dedicated to the 70th birthday of Professor Lin Qun

Abstract

In this work, we propose an efficient numerical method for computing the electrostatic interaction between two like-charged spherical particles which is governed by the nonlinear Poisson-Boltzmann equation. The nonlinear problem is solved by a monotone iterative method which leads to a sequence of linearized equations. A modified central finite difference scheme is developed to solve the linearized equations on an exterior irregular domain using a uniform Cartesian grid. With uniform grids, the method is simple, and as a consequence, multigrid solvers can be employed to speed up the convergence. Numerical experiments on cases with two isolated spheres and two spheres confined in a charged cylindrical pore are carried out using the proposed method. Our numerical schemes are found efficient and the numerical results are found in good agreement with the previous published results.

Mathematics Subject Classification: 65N06, 65B99.
Key words: Nonlinear Poisson-Boltzmann equation, Electrostatic interaction, Irregular domain, Monotone iterative method, Multigrid solver.

1. Introduction

The interactions between colloidal particles control the operation of many important industrial processes and also determine the properties of the final products. The nonlinear Poisson-Boltzmann equation has been used for the description of the distribution of electrostatic potential in colloidal dispersions, see, e.g., [20, 22]. Knowing the electrostatic potential, one can calculate the force of particle-particle interaction. Features of interparticle interaction are of great importance for the stability of colloidal dispersions.

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The problem of obtaining numerical solutions of the nonlinear Poisson-Boltzmann equation has a long history. In 1956, Hoskins and Levine [11] made the first such attempt for identical spheres interactions under constant surface potential. Their calculations were based on a second-order finite difference scheme and were carried out on a relatively small grid $(8 * 16)$. In [4], Bowen and Sharif considered the axi-symmetric situations of the Poisson-Boltzmann problem. While the problem is defined in the three-dimensional (3D) space, they can reduce it to a problem in two space dimensions using the geometrical symmetry. Their work used an adaptive finite element method for two interacting charged spheres enclosed in a charged cylindrical capillary. In their 1998 *Nature* paper [3], the authors found that in the absence of the charged capillary wall the two particles repelled one another over the whole range of particle separations, while in the presence of the charged wall a long range attractive force arose. However, their results were questioned by several authors, see, e.g., [14, 21]. In another *Nature* paper [9], the calculations in [3] were repeated and it was found that although the particle-particle interactions were reduced by the presence of a wall, no attraction was found.

Due to its practical importance, the problem of the long-range electrostatic attraction between like-charge spheres has recently been studied numerically by many authors, see, e.g., [1, 2, 6, 7, 8, 10]. Among these numerical schemes, few are related to the finite difference approach. This is mainly due to the difficulty given by the presence of a multi-connected domain. To overcome the difficulty, a conformal mapping approach may be used in some special cases to transform the multi-connected domain to a rectangular one. One can then solve the transformed Poisson-Boltzmann equation by using finite difference methods on the rectangular domain with a regular grid, see, e.g., [6]. In the present work, we will propose another type of finite difference scheme useful for handling general multi-connected domains. The goal is to solve the problem under consideration on the original multi-connected domain with a uniform Cartesian grid, while maintaining the simplicity of the finite difference scheme and the second-order approximation accuracy. The proposed method is flexible for complex domains on which the conformal mappings are not available. Since a uniform Cartesian grid on the domain is used, the method is simple and there is almost no extra cost in the grid generation. Moreover, our approach also allows to use the fast Poisson solvers based on multigrid methods. The method will be used to solve the Poisson-Boltzmann equation describing the long-range electrostatic attraction between like-charge spheres.

This paper is organized as follows. In Section 2, we give a description of the problem. In Section 3, a monotone iterative strategy useful for a class of semi-linear PDEs of elliptic type will be discussed. This strategy will be useful for linearizing the nonlinear Poisson-Boltzmann equation. In Section 4, a modified central finite difference scheme is introduced. Special attention is given to handle the irregular interface inside the rectangular domain. In Section 5, the proposed numerical scheme is applied to solve the nonlinear Poisson-Boltzmann equation for two identical charged spherical particles immersed in a symmetric univalent electrolyte and for two spheres confined in a like-charged cylindrical pore. We also compare our results with those available in the literature. Some concluding remarks are provided in the final section.

2. The Description of the Problem

We consider the nonlinear Poisson-Boltzmann equation

$$\Delta\Psi = \sinh\Psi, \tag{2.1}$$

where Ψ is the electrostatic potential. Usually, the above equation is defined in a 3D space, but for two isolated like-charged spherical particles immersed in a symmetric univalent electrolyte or like-charged spheres confined in a long, charged cylindrical pore, because of the symmetry of the geometry, we can rewrite the nonlinear Poisson-Boltzmann equation (2.1) as the following