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摘要
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A FINITE DIFFERENCE SCHEME FOR SOLVING THE NONLINEAR POISSON-BOLTZMANN EQUATION MODELING CHARGED SPHERES

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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.

Key words Nonlinear Poisson-Boltzmann equation Electrostatic interaction Irregular domain Monotone iterative method Multigrid solver.

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