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Some Random Batch Particle Methods for the Poisson-Nernst-Planck and Poisson-Boltzmann Equations

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Abstract. We consider in this paper random batch interacting particle methods for solving the Poisson-Nernst-Planck (PNP) equations, and thus the Poisson-Boltzmann (PB) equation as the equilibrium, in the external unbounded domain. To justify the simulation in a truncated domain, an error estimate of the truncation is proved in the symmetric cases for the PB equation. Then, the random batch interacting particle methods are introduced which are $\mathcal{O}(N)$ per time step. The particle methods can not only be considered as a numerical method for solving the PNP and PB equations, but also can be used as a direct simulation approach for the dynamics of the charged particles in solution. The particle methods are preferable due to their simplicity and adaptivity to complicated geometry, and may be interesting in describing the dynamics of the physical process. Moreover, it is feasible to incorporate more physical effects and interactions in the particle methods and to describe phenomena beyond the scope of the mean-field equations.

AMS subject classifications: 35Q92, 35Q84, 65N75

Key words: Interacting particle systems, Coulomb interaction, reflecting stochastic differential equation, charge reversal phenomenon, singular-regular decomposition.

1 Introduction

The charge distribution in dilute ionic solution around some charged surfaces is important for a wide range of applications in electrochemistry [9, 22], biophysics [13, 29] and

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colloidal physics [14, 59]. In the so-called implicit solvent model, the solvent is modeled by a continuum while the ions can be either modeled by charged particles or continuum distributions. When one models the ions using continuum distributions, some partial differential equations (PDEs) can be proposed. Regarding the ion transport, the Poisson-Nernst-Planck (PNP) equations [15,18,32,47] have been used to describe the non-equilibrium processes in the dilute regime. The Poisson-Boltzmann (PB) equation, proposed by Gouy [22] and Chapman [9] independently, can be viewed as the equilibrium of the PNP equations. The PB equation is a typical implicit solvent model to describe the distribution of the electric potential in dilute solution at equilibrium state when an object with free charges inside is immersed into an ionic solution. Various numerical methods have been proposed for the PNP and PB equations based on the PDE descriptions in literature [8,49], such as the finite difference method (FD) [11,18,20], finite element method (FEM) [3,10] and boundary element/integral method [6,48].

While the continuum descriptions of the charge distributions can capture some mean-field behaviors, the numerical simulations based on particles, or molecular dynamics (MD) simulations, can potentially give more physics and give some dynamical properties of the systems [19]. The MD simulations with electrostatic Coulomb interactions are usually challenging due to the long-range nature. A lot of efforts have been made to efficiently approximate the pair-wise interactions between charges in an electrolyte, such as the fast multipole method (FMM) [23], the Ewald method [17], particle mesh Ewald (PME) [12] and particle-particle particle mesh Ewald (PPPM) [50]. Recently, a stochastic method, the Random batch Ewald (RBE) method [37], was proposed to simplify particle simulations with Coulomb interaction. FMM can reduce the cost to $\mathcal{O}(N)$ per time step but the implementation is nontrivial and the efficiency can be observed when the number of particles is large. The Ewald-based methods like PPPM or RBE methods can reduce the cost to $\mathcal{O}(N\log N)$ or $\mathcal{O}(N)$ per time step, but the simulations take place in a box with periodic boundary conditions (BCs). Another popular method for plasma simulations is the particle-in-cell (PIC) method [58]. The PIC method considers the interaction between particles by computing the electric field on a deterministic grid and coupling the charged particles to the field, which has a cost of $\mathcal{O}(N\log N)$ using FFT. The collision-field method [41] can be viewed as an improved version of PIC. It treats the inter-species collisions in deterministic grid like PIC, while treats the intra-species collisions through the Langevin equation. This method can ensure momentum and energy conservation exactly using velocity corrections.

In this work, we would like to seek some particle methods for the PNP and PB equations using the random batch idea. In our particle methods, we simulate the overdamped Langevin equations which are the microscopic descriptions corresponding to the PNP equations so that the distributions in large time will solve the PB equation. In the simulation, each particle will interact with the others through the long-range Coulomb interaction. Note that solving the PDEs using particle methods with interaction is often expensive and the accuracy is lower compared with solving the PDEs directly. We emphasize the advantages of using particle methods in several aspects. On the one hand,