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An Adaptive Conservative Finite Volume Method for Poisson-Nernst-Planck Equations on a Moving Mesh

Xiulei Cao[1] and Huaxiong Huang[1,2,*]

[1] *Department of Mathematics and Statistics, York University, Toronto, ON M3J 1P3, Canada.*
[2] *Fields Institute for Research in Mathematical Sciences, Toronto, ON M5T 3J1, Canada.*

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Abstract. In this paper, we present a finite volume method for solving Poisson-Nernst-Planck (PNP) equations in one spatial dimension. To reduce computational cost, an adaptive moving mesh strategy is employed in order to resolve thin Debye layers near the boundary. In addition to the standard monitor functions, we propose two new ones for the moving mesh partial differential equations to improve the accuracy of the numerical solution. The method guarantees the strict mass conservation. We have proved that the scheme maintains positivity on the adaptive moving mesh which has not been done for PNP.

AMS subject classifications: 65N08, 68U20

Key words: Poisson-Nernst-Planck, finite volume method, adaptive moving mesh, mass conservation.

1 Introduction

The Poisson-Nernst-Planck (PNP) system is a mathematical model for studying ion transport. The applications of PNP equations include colloid chemistry, electro-hydrodynamics and electro-kinetics in semiconductor devices and biological systems [10, 23, 29, 36, 37].

In the mathematical literature, well-posedness and stability analysis of PNP can be found in [3, 12, 33]. Singular perturbation approach has been used to obtain solutions of steady-state PNP systems in [2, 28, 38, 41]. There different numerical approximations for the steady state Poisson-Nernst-Planck equations can be found in [1, 4, 22, 30]. Numerical studies of the PNP system using finite difference discretizations, discontinuous

*Corresponding author. *Email addresses:* `xlcao@yorku.ca` (X. Cao), `hhuang@yorku.ca` (H. Huang)

Galerkin method were reported in [11, 14, 26, 27], which satisfies the mass preserving, ion concentration positivity as well as total free energy dissipation numerically. In [11], a one dimension finite difference method for solving PNP equations was proposed, which ensures the correct rates of energy dissipation. On irregular domains, Mirzadeh et al. [32] presented a conservative hybrid finite-difference/finite volume method, where several strategies to generate quadtree adaptive grids were proposed. In [16,34], linearized finite element schemes that preserve electric energy decay and entropy decay properties were discussed. Chainais-Hillairet et al. [5, 6] introduced a finite volume scheme for multi-dimensional drift-diffusion equations and proved the convergence of the scheme.

One of the challenges for solving PNP equations numerically is to capture the thin boundary layer near the boundary without excessive computational cost when the Debye layer is much thinner than the length scale of the problems. A related issue is the strict mass conservation of ionic species, which needs to be ensured to avoid large error in the computed electric potential due to the near singular nature of the Poisson equation.

In this paper, we adapt moving mesh methods to solve PNP equations. Adaptive moving mesh methods have important applications for a variety of physical and engineering areas, since they greatly outperform the uniform mesh methods. There has been important progress in developing mesh methods for PDEs. In [44], an adaptive moving mesh finite difference method is presented to solve two types of equations with dynamic capillary pressure effect in porous media. The authors in [25] have studied the anisotropic mesh adaptation for linear finite element solution of 3D anisotropic diffusion problems. An efficient AMG preconditioning strategy is applied to solve the unsteady Navier-Stokes equations with moving mesh finite element method in [43].

In this work, we present a conservative finite volume scheme which keeps computational cost low while maintaining solution accuracy. We achieve this by using an adaptive moving mesh strategy and carefully choosing monitor function for the moving mesh partial differential equations to obtain desirable mesh distribution. In addition, we show that the scheme maintain positivity on dynamically adaptive moving mesh.

The rest of the paper is structured as follows. In Section 2, we introduce the mathematical model and the PNP system. In Section 3, we present the finite volume scheme and show that, at each time step, the fully discrete scheme poses two key properties: the positivity of the numerical solutions and strict mass conservation. In Section 4, moving mesh method is presented and two different monitor functions are tested. We conclude the paper with numerical results and a brief discussion of future directions.

2 Mathematical model

We consider the transport of mobile ions in a one dimensional domain $\Omega=(-L,L)$ $(L>0)$. The motion of ions is governed by the Nernst-Planck equations [9, 13]:

$$\frac{\partial c_i}{\partial t}=\nabla\cdot(D_i\nabla c_i+b_iz_iec_i\nabla\phi),\quad i=1,2,\cdots,N, \tag{2.1}$$