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An energy preserving finite difference scheme for the Poisson–Nernst–Planck system

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ABSTRACT

In this paper, we construct a semi-implicit finite difference method for the time dependent Poisson–Nernst–Planck system. Although the Poisson–Nernst–Planck system is a nonlinear system, the numerical method presented in this paper only needs to solve a linear system at each time step, which can be done very efficiently. The rigorous proof for the mass conservation and electric potential energy decay are shown. Moreover, mesh refinement analysis shows that the method is second order convergent in space and first order convergent in time. Finally we point out that our method can be easily extended to the case of multi-ions.

1. Introduction

The classical unsteady dimensionless drift–diffusion system which describes the evolution of positive and negative charged particles p, n, and electric potential ϕ is given as follows [1]

$$\begin{cases} p_t = \nabla \cdot (\nabla p + p\nabla\phi), \ \text{in } \Omega_T := (0,T] \times \Omega, \\ n_t = \nabla \cdot (\nabla n - n\nabla\phi), \ \text{in } \Omega_T, \\ -\Delta\phi = p - n, \ \text{in } \Omega_T, \end{cases} \tag{1}$$

where Ω is a bounded domain, $[0, T]$ is the time interval, the length scale is chosen as the Debye length, and the time scale is chosen as the diffusive time scale. Note that the Debye length is much smaller than the physical characteristic length in most cases. Thus, if the length scale is chosen as the physical characteristic length scale in these cases, there will be a small parameter in front of the electric potential term in the Poisson equation (1), which will result in a singular perturbation problem [2–5]. However, in this paper, we only consider the case that the characteristic length scale is the same order of the Debye length, which also has some applications. For example, inside the ion channel in the cell membrane, the characteristic length scale of the ion channel is the same order of the Debye length. In this situation, we could choose the Debye length as the length scale so that the dimensionless system (1) is meaningful. The above system is called Poisson–Nernst–Planck system, which was first formulated by Nernst and Planck to describe the potential difference in a galvanic cell. The system has lots of applications in electrochemistry [6], biology [7] and semiconductors [8–10]. Based on the analytical derivations for the energy and entropy laws, Schmuck theoretically proved the existence, and in some cases uniqueness of the weak

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solution for the more general context of the Navier–Stokes–Nernst–Planck–Poisson system [11]. In this paper, we focus on the numerical solution of the Poisson–Nernst–Planck system (1).

When numerically solving the PDEs, to keep the original physical feature is greatly important in constructing numerical schemes for different physical problems. For example, one successful and active research is to construct structure-preserving scheme for the ODE systems (see [12] and references therein). Only schemes that are carefully designed can preserve mass and energy conservative properties. For example, finite difference methods were developed for solving the Euler Equations and Burgers equations to preserve the discrete energy dynamics [13]. In [14], authors used a finite volume method for the shallow water equations which conserves the mass, momentum and energy of the system. A finite difference method was presented in [15] for solving the nonlinear Klein–Gordon equation which preserves the total energy. Qiao et al. [16] showed an unconditionally stable finite difference scheme for the dynamics of the molecular beam epitaxy, where the scheme preserves the energy decay rate exactly at discrete level. In [17], authors developed a general method of discretizing PDEs that preserving the energy using the average vector field method. Chiu et al. [18] developed a general mesh-free scheme for solving PDEs that can preserve the energy at discrete level. Chang et al. [19] discussed conservative and nonconservative properties of eight finite difference schemes for solving the generalized nonlinear Schrödinger equation. Chen et al. [20,21] proposed energy conservative finite difference schemes for solving the 2D and 3D Maxwell equations, respectively.

In the past several decades, there appears a wide range of literature on numerical methods for the Poisson–Nernst–Planck system, including finite difference method, finite element method, and finite volume method, see [22–31] and references therein. Here we just mention some of the recent work, Bessemoulin-Chatard [29] gave a conservative finite volume method for solving the drift–diffusion equation, where the entropy inequality is preserved. Flavell et al. [30] and Liu et al. [31] constructed two different conservative finite difference methods which satisfy the mass preserving, ion concentration positivity as well as total free energy dissipation numerically, where the total free energy is related to both electric potential and ion concentration, which is called entropy in [1]. And Prohl et al. [1] presented two different finite element methods which satisfy electric potential energy decay and entropy decay properties, respectively. Now we briefly illustrate the first part of the work in [1] as follows: under the following initial conditions and zero Neumann boundary conditions

$$p(0,\vec{x}) = p_0(\vec{x}) \geq 0,\ \ n(0,\vec{x}) = n_0(\vec{x}) \geq 0,\ \ \text{in } \Omega, \tag{2}$$

$$\frac{\partial \phi}{\partial \vec{n}} = \frac{\partial n}{\partial \vec{n}} = \frac{\partial p}{\partial \vec{n}} = 0,\ \ \text{on } \partial\Omega_T := (0,T] \times \partial\Omega. \tag{3}$$

It is well known [9] that the non-negative p, n is conserved in Ω_T, and the system (3) satisfies mass conservation, that is, for any $t \in (0, T]$,

$$M_p \equiv \int_\Omega p_0(\vec{x})d\vec{x} = \int_\Omega p(t,\vec{x})d\vec{x},\ \ M_n \equiv \int_\Omega n_0(\vec{x})d\vec{x} = \int_\Omega n(t,\vec{x})d\vec{x}, \tag{4}$$

where M_p, M_n are two positive constants which must be the same, since from (1) and (3) we have

$$M_p - M_n = \int_\Omega (p-n)dx = -\int_{\partial\Omega} \frac{\partial \phi}{\partial \vec{n}} ds = 0.$$

And it is also shown in [9,11] that the system satisfies the following energy law

$$E(t) + \int_0^t \int_\Omega ((p-n)^2 + (p+n)|\nabla\phi|^2)d\vec{x}dt = E(0), \tag{5}$$

where $E(t) = \frac{1}{2}\int_\Omega |\nabla\phi|^2 d\vec{x}$ is the electric potential energy. The above energy law (5) can be rewritten as

$$\frac{dE}{dt} = -\int_\Omega ((p-n)^2 + (p+n)|\nabla\phi|^2)d\vec{x}. \tag{6}$$

Prohl et al. [1] proposed a finite element method which can preserve the mass conservation (4), ion concentration positivity and electric potential energy decay (5) in [1]. However, the scheme in [1] is fully implicit, one has to solve a nonlinear system at each time step. In [1], a fixed point iteration method is used to solve the nonlinear system at each time step in order to get the rigorous physical quantities preserving results. In this paper, we present a simple semi-implicit finite difference method for the Poisson–Nernst–Planck system. For the new scheme, the unknown variables at next time step form a linear system which can be solved efficiently, no iteration is needed. Furthermore, the new scheme preserves mass conservation and electric potential energy identity numerically. Numerical results confirm the above properties. Mesh refinement analysis shows that the method is second order convergent in space and first order convergent in time. Finally, we point out that our method can be extended to the case of multi-ions without any difficulty.

The rest of the paper is organized as follows, Section 2 gives the detailed numerical scheme and its properties, Section 3 discusses the extension of the method for the case of multi-ions, Section 4 shows the numerical results, and conclusions and discussions are given in the final section.

2. Numerical method

In this section, we will develop a finite difference method which can guarantee the mass conservation (4) and energy decay (6) numerically.