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Unconditional Positivity-Preserving and Energy Stable Schemes for a Reduced Poisson-Nernst-Planck System

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Abstract. The Poisson-Nernst-Planck (PNP) system is a widely accepted model for simulation of ionic channels. In this paper, we design, analyze, and numerically validate a second order unconditional positivity-preserving scheme for solving a reduced PNP system, which can well approximate the three dimensional ion channel problem. Positivity of numerical solutions is proven to hold true independent of the size of time steps and the choice of the Poisson solver. The scheme is easy to implement without resorting to any iteration method. Several numerical examples further confirm the positivity-preserving property, and demonstrate the accuracy, efficiency, and robustness of the proposed scheme, as well as the fast approach to steady states.

AMS subject classifications: 65N08, 65N12, 92C35

Key words: Biological channels, diffusion models, ion transport, positivity.

1 Introduction

Biological cells exchange chemicals and electric charge with their environments through ionic channels in the cell membrane walls. Examples include signaling in the nervous system and coordination of muscle contraction, see [6] for a comprehensive introduction. Mathematically the flow of ions can be modeled by drift-diffusion equations such as the Poisson-Nernst-Planck (PNP) system, see e.g. [5,7,8,12].

In this investigation we design, analyze and numerically validate positivity-preserving algorithms to solve time-dependent drift-diffusion equations. As a first step, in this paper we focus on a reduced model derived by Gardner et al. [12] as an approximation to the full three dimensional (3D) PNP system. Let us first recall the full model and its reduction.

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1.1 Mathematical models

The general setup in [12] is a flow of positive and negative ions in water in a channel plus surrounding baths in an electric field against a background of charged atoms on the channel protein. The distribution of charges is described by continuum particle densities $c_i(\mathbf{x},t)$ for the mobile ions (such as K^+,N_a^+,C_a^{++},$\cdots$). The flow of ions can be modeled by the PNP system of m equations

$$\begin{aligned}&\partial_t c_i=-\nabla\cdot J_i,\quad i=1,\cdots,m;\ \mathbf{x}\in\Omega\subset\mathbb{R}^3,\ t>0,\\&J_i=-(D_i\nabla c_i+z_i\mu_i c_i\nabla\psi),\\&-\nabla\cdot(\epsilon\nabla\psi)=\sum_{i=1}^{m}q_i c_i-e\rho,\end{aligned}\tag{1.1}$$

where J_i is the flux density, in which D_i is the diffusion coefficient, μ_i the mobility coefficient which is related to the diffusion coefficient via Einstein's relation $\mu_i=\frac{D_i}{k_B T_0}$, where k_B is the Boltzmann constant and T_0 is the absolute temperature [6]. In the Poisson equation, ϵ is the dielectric coefficient, q_i the ionic charge for each ion species i, $\rho=\rho(\mathbf{x})$ the permanent fixed charge density, and e the proton charge.The coupling parameter $z_i=q_i/e$. In general, the physical parameters ϵ, μ_i and D_i are functions of $\mathbf{x}$. Let us mention that the case of no permanent charge does not pertain to biological channels. Even channels without permanent charge (in the form of so called acid and base side chains) have large amounts of fixed charge in their (for example) carbonyl bonds (see, e.g., [17] and references therein).

The derivation of the Nernst-Planck equation typically follows two steps, namely, using the energy variation to obtain the chemical potential and then using Fick's laws of diffusion to attain the Nernst-Planck equation (see e.g. [2]). In the charge dynamics modeled by the traditional NP equation, mobile ions are treated as volume-less point charges. In order to incorporate more complex effects such as short-range steric effect and long range Coulomb correlation, modifications of the PNP equations were derived (see, e.g., [23] and references therein). Nonetheless, the scheme methodology proposed in this paper can well be adapted to solve such modified PNP systems.

The 3D geometry of the ion channel can be approximated by a reduced problem along the axial direction x, with a cross-sectional area $A(x)$ [29,30]. Subject to a further rescaling as in [13], the corresponding PNP system (1.1) reduces to the following equations

$$\begin{aligned}&\partial_t c_i=\frac{1}{A(x)}\partial_x(A(x)D_i(\partial_x c_i+z_i c_i\partial_x\psi)),\quad x\in\Omega=[0,\,1],\quad t>0,\\&-\frac{1}{A(x)}\partial_x(\epsilon A(x)\partial_x\psi)=\sum_{i=1}^{m}z_i c_i-\rho(x),\quad x\in\Omega,\quad t>0.\end{aligned}\tag{1.2}$$

For ionic channels, an important characteristic is the so-called current-voltage relation, which can characterize permeation and selectivity properties of ionic channels (see [1]