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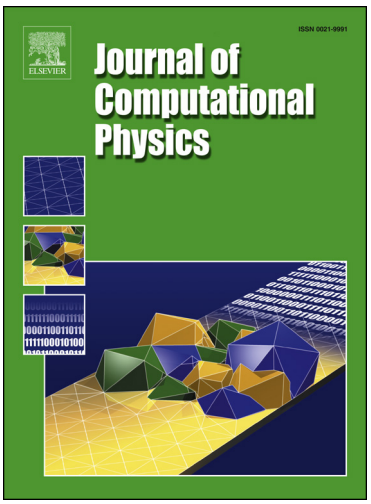

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Hailiang Liu, Zhongming Wang

PII: S0021-9991(16)30502-2
DOI: http://dx.doi.org/10.1016/j.jcp.2016.10.008
Reference: YJCPH 6886

To appear in: *Journal of Computational Physics*

Received date: 22 July 2016
Revised date: 18 September 2016
Accepted date: 3 October 2016

Please cite this article in press as: H. Liu, Z. Wang, A free energy satisfying discontinuous Galerkin method for one-dimensional Poisson–Nernst–Planck systems, *J. Comput. Phys.* (2016), http://dx.doi.org/10.1016/j.jcp.2016.10.008

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ACCEPTED MANUSCRIPT

A FREE ENERGY SATISFYING DISCONTINUOUS GALERKIN METHOD FOR ONE-DIMENSIONAL POISSON–NERNST–PLANCK SYSTEMS

HAILIANG LIU† AND ZHONGMING WANG‡

Abstract. We design an arbitrary-order free energy satisfying discontinuous Galerkin (DG) method for solving time-dependent Poisson-Nernst-Planck systems. Both the semi-discrete and fully discrete DG methods are shown to satisfy the corresponding discrete free energy dissipation law for positive numerical solutions. Positivities of numerical solutions are enforced by an accuracy-preserving limiter in reference to positive cell averages. Numerical examples are presented to demonstrate the high resolution of the numerical algorithm and to illustrate the proven properties of mass conservation, free energy dissipation, as well as the preservation of steady states.

1. Introduction

In this paper, we develop an arbitrary-order free energy satisfying numerical method for solving the initial boundary value problem of the Poisson–Nernst–Planck (PNP) system,

$$\partial_t c_i = \nabla \cdot (\nabla c_i + q_i c_i \nabla \psi) \quad x \in \Omega,\ t > 0 \tag{1.1a}$$

$$-\Delta \psi = \sum_{i=1}^{m} q_i c_i + \rho_0(x), \quad x \in \Omega,\ t > 0, \tag{1.1b}$$

$$c_i(0, x) = c_i^{\text{in}}(x), \quad x \in \Omega, \tag{1.1c}$$

$$\frac{\partial \psi}{\partial \mathbf{n}} = \sigma, \quad \frac{\partial c_i}{\partial \mathbf{n}} + q_i c_i \frac{\partial \psi}{\partial \mathbf{n}} = 0, \qquad x \in \partial\Omega,\ t > 0, \tag{1.1d}$$

where $c_i = c_i(t, x)$ is the local concentration of i^{th} charged molecular or ion species with charge q_i $(1 \le i \le m)$ at the spatial point x and time t, $\Omega \subset \mathbb{R}^d$ denotes a connected closed domain with smooth boundary $\partial\Omega$, $\psi = \psi(t, x)$ is the electrostatic potential governed by the Poisson equation subject to the Neumann boundary data σ and the charge density that consists of both fixed charge ρ_0 and mobile ions, the latter being a linear combination of all the concentrations c_i. Here $\mathbf{n}$ is the unit outward normal vector on the domain boundary $\partial\Omega$. In this system, the diffusion coefficient, the thermal energy and the dielectric coefficient have been normalized in a dimensionless manner.

The side conditions are necessarily compatible, i.e.,

$$\int_\Omega \left(\sum_{i=1}^{m} q_i c_i^{\text{in}}(x) + \rho_0(x) \right) dx + \int_{\partial\Omega} \sigma ds = 0, \tag{1.2}$$

for the solvability of the problem.

The PNP system is a mean field approximation of diffusive molecules or ions, and consists of Nernst-Planck (NP) equations that describe the drift and diffusion of ion species, and the Poisson equation that describes the electrostatics interaction. In the process of charge transport

1991 *Mathematics Subject Classification.* 35K40, 65M60, 65M12, 82C31.

Key words and phrases. Poisson-Nernst-Planck equation, free energy, discontinuous Galerkin methods.

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