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Efficient, positive, and energy stable schemes for multi-D Poisson-Nernst-Planck systems

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In this work, we design, analyze, and numerically validate positive and energy dissipating schemes for solving the time-dependent multi-dimensional system of Poisson-Nernst-Planck (PNP) equations, which has found much use in the modeling of biological membrane channels and semiconductor devices:

$$\partial_t \rho_i = \nabla \cdot \left[D_i(x) \left(\nabla \rho_i + z_i \rho_i \nabla \phi \right) \right], \quad x \in \Omega \subset \mathbb{R}^d, \quad t > 0, \tag{1a}$$

$$-\nabla \cdot (\epsilon(x) \nabla \phi) = f(x) + \sum_{i=1}^{s} z_i \rho_i, \tag{1b}$$

subject to initial data $\rho_i(x,0) = \rho_i^{in}(x) \geq 0$ $(i = 1, \cdots, s)$ and appropriate boundary conditions. Here $\rho_i = \rho_i(x,t)$ is the charge carrier density for the i-th species, and $\phi = \phi(x,t)$ the electrostatic potential. $D_i(x)$ is the diffusion coefficient, z_i is the rescaled charge. In the Poisson equation, $\epsilon(x)$ is the permittivity, $f(x)$ is the permanent (fixed) charge density of the system, s is the number of species. The equations are valid in a bounded domain Ω with boundary $\partial\Omega$ and for time $t \geq 0$.

The semi-implicit time discretization based on a reformulation of the system gives a well-posed elliptic system, which is shown to preserve solution positivity for arbitrary time steps. The first order (in time) fully-discrete scheme is shown to preserve solution positivity and mass conservation unconditionally, and energy dissipation with only a mild O(1) time step restriction. The scheme is also shown to preserve the steady-states. For the fully second order (in both time and space) scheme with large time steps, solution positivity is restored by a local scaling limiter, which is shown to maintain the spatial accuracy. These schemes are easy to implement. Several three-dimensional numerical examples verify our theoretical findings and demonstrate the accuracy, efficiency, and robustness of the proposed schemes, as well as the fast approach to steady states.

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References

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