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An Energy-Preserving Discretization for the Poisson-Nernst-Planck Equations

The Poisson-Nernst-Planck (PNP) equations have recently been used to describe the dynamics of ion transport through biological ion channels besides being widely employed in semiconductor industry. This work is about the design of a numerical scheme to solve the PNP equations that preserves exactly (up to roundoff error) a discretized form of the energy dynamics of the system. The proposed finite difference scheme is of second-order accurate in both space and time. Comparisons are made between this energy dynamics preserving scheme and a standard finite difference scheme, showing a difference in satisfying the energy law. Numerical results are presented for validating the orders of convergence in both time and space of the new scheme for the PNP system.