

**The Hong Kong Polytechnic University
Department of Applied Mathematics**

Colloquium

**A positivity preserving, energy stable and convergent numerical scheme for the
Poisson-Nernst-Planck system**

By

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Abstract

A finite difference numerical scheme is proposed and analyzed for the Poisson-Nernst-Planck equation (PNP) system. To understand the energy structure of the PNP model, we make use of the Energetic Variational Approach (EnVarA), so that the PNP system could be reformulated as a non-constant mobility, conserved gradient flow, with singular logarithmic energy potentials involved. To ensure the unique solvability and energy stability, the mobility function is explicitly treated, while both the logarithmic and the electric potential diffusion terms are treated implicitly, due to the convex nature of these two energy functional parts. The positivity-preserving property for both concentrations is established at a theoretical level. This is based on the subtle fact that the singular nature of the logarithmic term around the value of 0 prevents the numerical solution reaching the singular value, so that the numerical scheme is always well-defined. In addition, an optimal rate convergence analysis is provided in this work, in which many highly non-standard estimates have to be involved, due to the nonlinear parabolic coefficients. The higher order asymptotic expansion (up to third order temporal accuracy and fourth order spatial accuracy), the rough error estimate (to establish the discrete maximum norm bound), and the refined error estimate have to be carried out to accomplish such a convergence result. In our knowledge, this work will be the first to combine the following three theoretical properties for a numerical scheme for the PNP system: (i) unique solvability and positivity, (ii) energy stability, and (iii) optimal rate convergence. A few numerical results are also presented in this talk, which demonstrates the robustness of the proposed numerical scheme.

Date: 10 May 2021 (Monday)

Time: 11:00-12:00 (Hong Kong Standard Time GMT +8)

Venue: Online Talk via Zoom (Meeting ID: 948 2411 7810)

Speaker: Prof. Cheng Wang, University of Massachusetts Dartmouth

Host: Dr. Xiao Li, The Hong Kong Polytechnic University

Click to join:

<https://polyu.zoom.us/j/94824117810?pwd=cU9OWEkwTlFtd3FFYzJ6eHFqdnM4dz09>



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