Finite volumes for a generalized Poisson–Nernst–Planck system with cross-diffusion

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Modeling concentrated ion mixtures in solvents like water is a complex research area with key applications in biology (e.g., ion transport through protein channels) and electrochemistry (e.g., batteries).

In this talk, I will present a finite volume scheme for modeling the diffusion of ions in constrained geometries using a degenerate Poisson-Nernst-Planck system with size exclusion yielding cross-diffusion. The proposed method utilizes a two-point flux approximation and is part of the exponentially fitted scheme framework. The scheme is shown to be thermodynamically consistent, as it ensures the decay of some discrete version of the free energy. Classical numerical analysis results - existence of discrete solution, convergence of the scheme as the grid size and the time step go to 0 - follow. The long-time behavior of the scheme is also investigated, both from a theoretical and numerical point of view. Numerical simulations confirm our findings, but also point out some possibly very slow convergence towards equilibrium of the system under consideration.

This is a joint work with Clément Cànces and Maxime Herda.