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Asymptotic Preserving scheme and Gradient-flow structure for Multiscale Poisson-Nernst-Planck system

Thursday, 12 February 2026 14:50 (25 minutes)

In this talk, we further develop the multiscale model introduced in Astuto, Raudino and Russo (2023) by deriving a gradient-flow structure that incorporates the time-dependent boundary condition obtained therein. The model describes a drift-diffusion equation for ion transport in the presence of a trapping potential, focusing on surface traps whose attraction range, denoted by δ, is much smaller than the characteristic length scale of the problem. The multiscale formulation is derived via an asymptotic expansion with respect to this small parameter, leading to an effective boundary condition that captures the ion adsorption process at the surface. Using the same asymptotic framework, we derive the associated free energy and show that, at steady state, the ionic concentration concentrates on the trap surface in the sense of measures, giving rise to a Dirac-type contribution. This observation naturally motivates the study of the time evolution of the concentration in the space of positive measures. Numerical results for the drift-diffusion and the multiscale models are compared in one spatial dimension.

In the second part of the talk, we extend the multiscale approach to a Poisson-Nernst-Planck (MPNP) system, accounting for the correlated dynamics of positive and negative ions and for Coulomb interactions. In the regime of very small Debye lengths, the quasi-neutral limit reduces the system to an effective diffusion equation for a single carrier. While this simplification facilitates the analysis, it may fail to capture relevant behaviors close to the quasi-neutral regime. To overcome this limitation, we develop and validate an Asymptotic Preserving numerical scheme that remains stable as the Debye length tends to zero, without imposing restrictive time-step constraints.

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