数学与系统科学研究院

计算数学所学术报告

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报告题目：

Numerical Methods for a Poisson-Nernst-Planck-Fermi Model of Biological Ion Channels

邀请人：　卢本卓 研究员

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下午 15:00-16:00

报告地点：　数学院南楼九层

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Abstract:

Numerical methods are proposed for an advanced Poisson-Nernst-Planck-Fermi (PNPF) model for studying ion transport through biological ion channels. This model accounts for the steric effect of ions and water molecules with different sizes and interstitial voids, the correlation effect of crowded ions with different valences, and the polarization effect of water molecules in an inhomogeneous aqueous electrolyte. The steric energy is shown to be comparable to the electrical energy under physiological conditions, demonstrating the crucial role of the excluded volume of particles and the voids in the natural function of channel proteins. Water is shown to play a critical role in both correlation and steric effects in the model. We extend the classical Scharfetter-Gummel (SG) method for semiconductor devices to include the steric potential for ion channels, which is a fundamental physical property not present in semiconductors. Together with a simplified matched interface and boundary (SMIB) method for treating molecular surfaces and singular charges of channel proteins, the extended SG method is shown to exhibit important features in flow simulations such as optimal convergence, efficient nonlinear iterations, and physical conservation. The generalized SG stability condition shows why the standard discretization (without SG exponential fitting) of NP equations may fail and that divalent Ca2+ may cause more unstable discrete Ca2+ fluxes than that of monovalent Na+. Two different methods—called the SMIB and multi-scale (atomic-macroscopic) methods—are proposed for different types of channels such as gramicidin A (GA), L-type calcium, NCX (sodium/calcium exchanger), KcsA (potassium), and TRPV (transient receptor potential vanilloid) channels. GPU (graphic processing unit) algorithms for solving the PF model will be briefly illustrated to tackle large-scale simulations of ion channels. The PNPF currents are in accord with the experimental I-V (V for applied voltages) data of GA and TRPV, and I-C (C for bath concentrations) data of the calcium channel with 108-fold bath concentrations that pose severe challenges in theoretical simulations. We also present the results of NCX exchange mechanism, KcsA selectivity, and GPU computing.

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