数学与系统科学研究院

计算数学所学术报告

(系列讲座)

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系列讲座题目：
Continuum modeling of biomolecular systems (I, II, III)

报告题目： (讲座之三)
Continuum Modeling III:

III. Fully continuum modeling of electro-diffusion-reaction processes in realistic biomolecular systems

报告时间： 2008 年 12 月 17 日(周三)
下午 3:00—4:00

报告地点： 科技综合楼三层 311
计算数学所报告厅

Abstract:

The continuum model is being used by a growing number of researchers to simulate multiscale processes within biological systems. The Poisson–Nernst–Planck equation is used to model fully–continuum diffusion–reaction processes, and appears to be a framework to study even more general molecular solvation effects. We'll discuss our recent developments in PNP methodologies, including the finite element solution, mesh generation, regularization of the nonlinear Poisson–Boltzmann equation, and PNP model extensions. Some math issues are raised as well. The work is applied to both simple model systems and the neurotransmitter consumption by an enzyme in the synapse. The intricate interplay of electrostatics, diffusion, ionic/molecular sizes and other properties is shown in observations of the calculated reaction rate coefficients and ionic density profiles.

欢迎大家参加！