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:

A Nonlocal Modified Poisson-Boltzmann Equation and Finite Element Solver for Computing Electrostatics of Biomolecules

邀请人: 卢本卓 研究员

报告时间: 2016年6月21日(周二)

上午 10:00-11:00

报告地点: 数学院南楼六层

602 会议室

Abstract:

The nonlocal dielectric approach has been studied for more than forty years but only limited to water solvent until the recent work (SISC, 35(6):B1267-1284, 2013). As the development of this recent work, we proposed a nonlocal modified Poisson-Boltzmann equation (NMPBE) to incorporate nonlocal dielectric effects into the classic Poisson-Boltzmann equation (PBE). In this talk, I will introduce NMPBE present an efficient finite element algorithm and a related software package for solving NMPBE.

欢迎大家参加!