数学与系统科学研究院 计算数学所学术报告

(系列讲座)

报告人: 卢本卓副研究员(ICMSEC)

系列讲座题目:

Continuum modeling of biomolecular systems (I, II, III)

报告题目: (讲座之一)

Continuum Modeling I:

Poisson-Boltzmann electrostatics (I)

--Boundary integral formulations for the PBE

报告时间: 2008年12月8日(周一)

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:

A brief introduction is given to some biophysical backgrounds, computational approaches, continuum electrostatics and the Poisson-Boltzmann model. Following this, I' ll talk about boundary element methods for solution of the linearized PB equation. Different boundary integral forms are shown. In particular, for non-smooth mesh from the surface discretization, the geometry-corrected integral equations and the strong- and hyper-singular integrals are derived and discussed, which has not been completely accomplished and implemented.

欢迎大家参加!