数学与系统科学研究院 计算数学所学术报告

报告人: Dr. Ray Luo

(University of California, Irvine)

报告题目:

Scaling in Biomolecular Solvation: Are Proteins Large?

邀请人: 陈志明研究员

报告时间: 2008年7月9日(周三)

上午10:00—11:00

报告地点: 科技综合楼三层 311

计算数学所报告厅

Abstract:

In this talk geared towards a mathematician audience, I will discuss the mathematical and computational challenges in biomolecular simulations, i.e. the balance of accuracy and efficiency in different levels of abstraction. Specifically I will go over the continuum representation of the biomolecular simulation protocol. The pros and cons of this reduced representation, and our recent investigations into its quality and scalability using realistic biomolecular systems as test cases. If time permits, I will go over our recent efforts in adapting the continuum representations in biomolecular dynamics simulations.

欢迎大家参加!