数学与系统科学研究院

计算数学所学术报告

报告人：　Prof. Dexuan Xie

（ *Department of Mathematical Sciences, University of Wisconsin-Milwaukee* ）

报告题目：

Recent Advances in Calculation of Biomolecular Electrostatics

邀请人：　卢本卓 研究员

报告时间：2018 年 12 月 19 日（周三）

上午 10:00-11:00

报告地点：　数学院南楼六层

602 教室

Abstract:

Calculation of electrostatics for biomolecules such as proteins in an ionic solvent is a fundamental task in computational biology, biochemistry, and biophysics. The Poisson-Boltzmann equation (PBE) is one commonly used dielectric continuum model for such a task. It has been applied to protein study, rational drug design, and many other bioengineering applications. To reflect polarization correlation among water molecules and ionic size effects, we recently developed new variants of PBE, called the size modified PBE (SMPBE), nonlocal modified PBE (NMPBE), and nonlocal Poisson-Fermi (NPF) models, along with their fast finite element algorithms and software packages. In this talk, I will report these recent advances. I will also introduce our new SMPBS (Size Modified Poisson-Boltzmann Solvers) web server (smpbs.math.uwm.edu), which was published on the Journal of Computational Chemistry last year. SMPBS will be demonstrated as a useful tool for computing the electrostatic solvation free energy of a protein in an ionic solvent. Our research projects were partially supported by the National Science Foundation, USA, through grants DMS-0921004 and DMS-1226259.

欢迎大家参加！