数学与系统科学研究院

计算数学所学术报告

报告人：肖立 副研究员

(中科院计算所)

报告题目：

Multi-resolution model for biomolecular simulation

邀请人：　卢本卓研究员

报告时间：**2017** 年 **12** 月 **22** 日（周五）

上午 **10:00--11:00**

报告地点：　数学院南楼七层

714 会议室

报告摘要：

Atomistic simulation has become an

important tool for studying the structures, dynamics, and functions of biomolecular systems. Nevertheless efficient atomistic simulation of large and complex biomolecular systems is still one of the remaining challenges in computational molecular biology. The computational challenges in atomistic simulation of biomolecular systems are direct consequences of their high dimensionalities. Indeed biomolecules are highly complex molecular machines with thousands to millions of atoms. What further complicates the picture is the need to realistically treat the interactions between biomolecules and their surrounding water molecules that are ubiquitous and paramount important for their structures, dynamics, and functions.

Since most particles in biomolecular simulations are to represent water

molecules solvating the target biomolecules, an implicit treatment of water molecules allows greatly increased simulation efficiency. Indeed, implicit solvation offers a unique opportunity for more efficient simulations without the loss of atomic-level resolution for biomolecules. Advance in implicit solvation, coupled with developments in sampling algorithms, classical force fields, and quantum approximations, will prove useful to the larger biomedical community in a broad range of studies of biomolecular structures, dynamics and functions.

This talk reports the authors' work on developing multi-scale models for biomolecule simulation with implicit treatment of water. Specifically:

1) a math framework to compute electrostatic forces in implicit solvent model is derived;

2) a charge central interpolation method is implemented to efficiently compute electrostatic forces with high accuracy;
3) a multi-scale model with automatic pore regions detection is applied on membrane system to compute solvation energy;
4) a physical model of multi-scale model is proposed and a fluid dynamics algorithm solver is developed; and
5) the fluid dynamics algorithm is incorporated with the Amber molecular mechanics simulation engine to conduct atomistic simulations of biomolecules in the continuum solvent models.

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