数学与系统科学研究院

计算数学所学术报告

报告人：　Dr. Huan Lei

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报告题目：

Mesoscopic modeling of complex fluid system with molecular fidelity

邀请人：　卢本卓 研究员

报告时间：2015 年 9 月 3 日（周四）

下午 15:00-16：00

报告地点：　数学院南楼九层

902 会议室

Abstract:

Many macroscopic dynamic processes such as transport, reactive flow, directed assembly, manifest themselves on the scale of collective behavior of atomistic interaction, commonly referred to as mesoscale. This scale is characterized by the emergence of fluctuation, interface and heterogeneity; a fundamental challenge to model and understand these emergent phenomena roots in the multiscale and multifaceted nature of such processes. In this talk, I will present my work on mesoscale modeling of complex fluid with molecular fidelity to probe the governing principles for the non-equilibrium properties of complex physical systems. In micrometer scale, we establish the mesoscale formulation directly from microscopic model (Phys. Rev. E., 81, 026704, 2010) and extend the framework to model in vivo microcirculation under blood disease (sickle cell anemia). We show that specific flow pattern incurring vaso-occlusion crisis can be accurately captured from model (PNAS, 110, 11326, 2013). Toward nanoscale, complex fluid systems are governed by both interfacial surface tension and thermal fluctuation. Our mesoscopic model with molecular fidelity accurately captures interfacial fluctuation (capillary wave spectrum), solvation energy (Lum-Chandler-Weeks theory) and rare event transition between the metastable states (J. Chem. Phys., 142, 194504, 2015).

biosketch: Huan Lei is a research scientist in Pacific Northwest National Laboratory. He received his Ph.D. on Applied Mathematics from Brown University in 2012 and his advisor was Prof. George Karniadakis. After that, he worked as a postdoctoral associate with Dr. Nathan Baker at Pacific Northwest National Laboratory. His research work is mainly on developing mesoscale models and numerical methods applicable to multiphysical systems beyond equilibrium; in particular, non-equilibrium dynamic processes and intrinsic transition between the metastable states.

欢迎大家参加！