



复旦大学数学科学学院 数学综合报告会

报告题目: **Dynamic Implicit Solvent Model: Understanding Solvent Stokes Flow and Interface Dynamics for Biomolecules**

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报告时间: 12月28日星期三 10:00-11:00

报告地点: 光华东主楼 1801

摘要: The interface between protein solute and aqueous solvent exhibits complex geometries, and can undergo conformational changes by combined influences from electrostatic force, surface tension, and hydrodynamic force. To understand the role of solvent Stokes flow in this process, we develop a Dynamic Implicit Solvent Model (DISM). Based on this model, we first analytically study the linear stability of a cylindrical solute-solvent interface, where the asymptotic dispersion reveals a power law. Moreover, we develop a computational method to simulate the solvent Stokes flow and interface motion. The key components of our fluid solver are virtual node method, pressure Poisson equation, specially designed boundary condition, Schur complement and least square techniques. 3D numerical tests will demonstrate the convergence of our method, and show that this new approach can capture interesting dynamics of protein conformational change.

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