

数学与系统科学研究院

计算数学所学术报告

报告人: 杨志坚 教授

(武汉大学)

报告题目:

**Derivation of Continuum Models
from Atomistic Models**

邀请人: 崔俊芝 院士

报告时间: 2013 年 4 月 10 日 (周三)

上午 10:00

报告地点: 科技综合楼三层 301

计算数学所小报告厅

Abstract:

In this talk, I will introduce how to derive continuum models from atomistic ones. For static problems, I will discuss the Cauchy-Born rule and its generalizations. For dynamic problems, continuum mechanics quantities can be computed from molecular dynamics (MD) models based on the classical Irving-Kirkwood (IK) formalism. Practical implementations of IK formulas involve a spatial averaging using a smooth kernel function. The obtained results usually need to be further processed to reduce the fluctuation, e.g., by ensemble or time averaging. I will discuss the extension of the IK formalism to systematically incorporate both spatial and temporal averaging into the expression of continuum quantities.

欢迎大家参加!