数学与系统科学研究院

计算数学所学术报告

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报告题目：

Coarse-graining molecular dynamics using Galerkin method

邀请人：　明平兵研究员

报告时间：**2011** 年 **11** 月 **24** 日（周四）

下午 **16：00-17：00**

报告地点：　科技综合楼三层 **311**

计算数学所报告厅

Abstract:

We consider molecular dynamics (MD) model as a microscopic description of mechanical properties of a solid system. It is written as a Hamiltonian system for the position and momentum of the atoms. Many complicated material processes can in principle be understood at the atomic level using MD. However, a realist system often consists of a huge number of atoms, and the computation is too large for numerical simulations.

This talk will present a method to reduce the dimension, i.e., the number of atomic degrees of freedom, associated with the MD model. The method is motivated by traditional Galerkin projection for linear and nonlinear wave equations. Then we generalize this approach by introducing a set of auxiliary variables to extend the approximation to a larger subspace. The latter approach is similar to moment closure methods for kinetic equations. In addition to the numerical methods, we will present some error analysis along with some numerical experiments on the simulation of material defects.

欢迎大家参加!