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：

Sampling problems in molecular dynamics

邀请人： **周爱辉研究员**

报告时间： **2010 年 1 月 15 日(周五)**

下午 4:00—5:00

报告地点： **科技综合楼三层 311**

计算数学所报告厅

Abstract：

One aim of molecular dynamics is to compute some macroscopic quantities from microscopic

models, through means of some relevant observables in an appropriate thermodynamic ensemble. These calculations are typically difficult because the measure to sample is multimodal, which makes classical Markov Chain Monte Carlo algorithms very slow to converge. We review some classical methods which are used in molecular dynamics to deal with this problem, with an emphasis on adaptive importance sampling methods. Applications of the method to other field (like in Bayesian statistics) are mentioned.

欢迎大家参加！