

数学与系统科学研究院  
**计算数学所学术报告**

**报告人: Prof. Claude Le Bris**  
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**报告题目:**

**Coarse Graining Atomistic Systems at  
Positive Temperature: A Mathematical  
Approach for Materials Science**

**邀请人: 周爱辉研究员**

**报告时间: 2008年5月28日(周三)**  
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:**

**We present a possible approach for the computation of free energies and ensemble averages in the context of one-dimensional coarse-grained models in materials science. The approach is based upon a thermodynamic limit process, and makes use of ergodic type theorems and large deviation theory. In addition to providing a possible efficient computational strategy for ensemble averages, the approach in particular allows for assessing the validity and the accuracy of some basic assumptions of the finite-temperature quasicontinuum method. This is joint work with X. Blanc (Paris 6) and F. Legoll (ENPC-LAMI).**

**欢迎大家参加！**