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：

Construction and analysis of consistent energy based atomistic/continuum coupling methods

邀请人： 崔涛 博士

报告时间：2014 年 8 月 29 日（周五）

上午 10:00-11:00

报告地点： 科技综合楼三层 **311**

计算数学所报告厅

Abstract：

We discuss the construction and numerical analysis of energy based atomistic/continuum coupling methods (A/C Coupling) for modeling crystalline solids with defects, in particular, the issues of consistency (so-called 'ghost force removal') and stability of the coupling method. For general multi-body interactions on the 2D triangular lattice, we show that ghost force removal (patch test consistent) a/c methods can be constructed for arbitrary interface geometries[1]. Moreover, we prove that all methods within this class are first-order consistent at the atomistic/continuum interface and second-order consistent in the interior of the continuum region. The convergence and stability of the method is analyzed and justified with numerical experiments[2,3]. Development of optimal implementation for consistent methods is dicussed [3，4].

References:

[1] Construction and sharp consistency estimates for atomistic/continuum coupling methods with general interfaces: a 2D model problem, C. Ortner, L. Zhang, SIAM Numerical Analysis. Volume 50, Issue 6, pp. 2940-2965 (2012).

[2] (In-)Stability and Stabilisation of QNL-Type Atomistic-to-Continuum Coupling Methods, C. Ortner, A. Shapeev, L. Zhang, 2013, Accepted by SIAM Multiscale Model. Simul.

[3] Implementation of Geometric Reconstruction Based Atomistic-to-Continuum Coupling, C. Ortner, L. Zhang, 2013, Accepted by Computer Methods in Applied Mechanics and Engineering

[4] Atomistic/Continuum Blending with Ghost Force Correction，C. Ortner, L. Zhang, 2014, arXiv:1407.0053

欢迎大家参加！