Construction and Analysis of Consistent Energy Based Atomistic/Continuum Coupling Methods

Lei Zhang

Institute of Natural Sciences, Shanghai Jiao Tong University

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].

References

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

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

[3] C. Ortner, L. Zhang, *Implementation of Geometric Reconstruction Based Atomistic-to-Continuum Coupling*, 2013, Submitted