A Simplified a Posteriori Error Estimation for a Consistent Atomistic-to-continuum Coupling Method in 2D

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Abstract

Atomistic-to-continuum coupling methods are a class of computational multiscale methods which combine the accuracy of the atomistic model and the efficiency of the continuum model for the computation of defects in crystal solids. Such methods can be efficiently implemented by adaptivity and achieve (quasi-)optimal balance between accuracy and efficiency. In this talk, we will present a simplified a posteriori error estimator for a consistent a/c coupling method in 2D. Such error estimator is essentially a simplified version of the residual based error estimator for the a/c method which avoids the computation of model error in the continuum bulk. We will show both analytically and numerically that the model error in the continuum region, which is expensive in computational due to the discrepency of the finite element mesh and the reference lattice, is of higher order compared with other sauce of error and thus can be omitted. Numerical experiments are also given to demonstrate the efficiency of the simplified error estimator compared with the classical residual based error estimator for the adaptive computation of crystal defects.

Keywords: atomistic-to-continuum coupling, coarse-graining, a posteriori error estimate, adaptive algorithm