11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

A POSTERIORI ERROR ESTIMATES FOR QUASICONTINUUM APPROXIMATIONS

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Key words: *Quasicontinuum Method, Atomistic/Continuum Coupling, A Posteriori Error Control, Adaptive Mesh Refinement*

This talk focuses on the rigorous a posteriori error estimates of and their applications to different quasicontinuum (QC) methods[1, 2, 4], which are a class of computational methods for the coupling of atomistic and continuum models for micro- or nano-scale materials.

This talk consists of three parts.

In the first part, we establish a general frame work for the a posteriori error estimates of the QC methods which can be formulated in an abstract variational formulation. The a posteriori error analysis is based on the computation of the residual and the stability of the QC solution under the atomistic energy functional. We will show in an abstract level that how the residual can be bounded under certain Sobolev norms using certain techniques in analysis such as integration by parts and the trace inequality and obtained in the optimal order.

In the second part, we will apply the frame work to estimate the a posteriori error of a recently developed consistent atomistic/continuum coupling method in [4]. Detailed formulation as well as the analysis will be given for this method in a two dimensional setting. The application of the Bond-Density Lemma [4], which essentially reformulate the residual in a stress-strain form so that the general frame work can be applied, will be presented. Stability analysis is also given in this section.

In the third part, the numerical experiment will be presented to illustrate the result of our analysis. Adaptive mesh refinement techniques, which can be applied to general QC mesh generation and refinement, are also discussed.

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