CONCURRENT ATOMISTIC TO CONTINUUM COUPLING AND ADAPTIVE MODEL SELECTION FOR MULTISCALE PROBLEMS

By

Mohan Nuggehally

An Abstract of a Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the Degree of

DOCTOR OF PHILOSOPHY

Major Subject: Mechanical Engineering

The original of the complete thesis is on file
in the Rensselaer Polytechnic Institute Library

Examining Committee:

Mark S Shephard, Thesis Adviser

Catalin R Picu, Thesis Adviser

Jacob Fish, Member

Rahmi Ozisik, Member

Rensselaer Polytechnic Institute
Troy, New York

June 2007
(For Graduation August 2007)

ABSTRACT

A concurrent Atomistic to Continuum (AtC) coupling method is presented. The problem domain is decomposed into an atomistic sub-domain where fine scale features need to be resolved, a continuum sub-domain which can adequately describe the macroscale deformation and an overlap interphase sub-domain that has a blended description of the two. The problem is formulated in terms of equilibrium equations with a consistent blending between the continuum stress and the atomistic force in the interphase. Coupling between the continuum and the atomistics is established by imposing constraints between the continuum solution and the atomistic solution over the interphase sub-domain in a weak sense. The formulation is subjected to patch tests to demonstrate its ability to represent the constant strain modes and the rigid body modes.

An adaptive method for the selection of models in a concurrent multiscale approach is presented. Different models from a hierarchy are chosen in different sub-domains of the problem domain adaptively in an automated problem simulation. Two error indicators are used for the hierarchy of models consisting of a linear elastic model, a nonlinear elastic model and an Embedded Atom Method (EAM) based atomistic model. A nonlinear indicator η_{NL-L}, which is based on the relative error in the energy between the nonlinear model and the linear model is used to select or de-select the nonlinear model sub-domain. Atomistic indicator is a stress gradient based criterion to predict dislocation nucleation, which was developed by Miller and Acharya [61]. A material specific critical value associated with the dislocation nucleation criterion is used in selecting and de-selecting the atomistic sub-domain during an automated simulation. An adaptive strategy uses limit values of the two indicators to adaptively modify the sub-domains of the 3 different models. Example results are illustrated to demonstrate the adaptive methods and its applicability to solve some material science problems.