The University of Chicago

Departments of Computer Science,
Mathematics, and Statistics

Scientific and Statistical Computing Seminar

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Atomistic-to-Continuum Coupling Methods for Solids

FRIDAY, November 18, 2011, at 3:30 PM

133 Eckhart Hall, 5734 S. University Avenue (unless announced otherwise).

ABSTRACT

Many materials problems require the accuracy of atomistic modeling in small regions, such as the neighborhood of a crack tip. However, these localized defects typically interact through long ranged elastic fields with a much larger region that cannot be computed atomistically. Materials scientists have proposed many methods to compute solutions to these multiscale problems by coupling atomistic models near a localized defect with continuum models where the deformation is nearly uniform. During the past several years, we have given a mathematical structure to the description and formulation of atomistic-to-continuum coupling methods, and corresponding theory has clarified the relation between the various methods and the sources of error. This theory has guided the development of more reliable and efficient coupling methods.

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