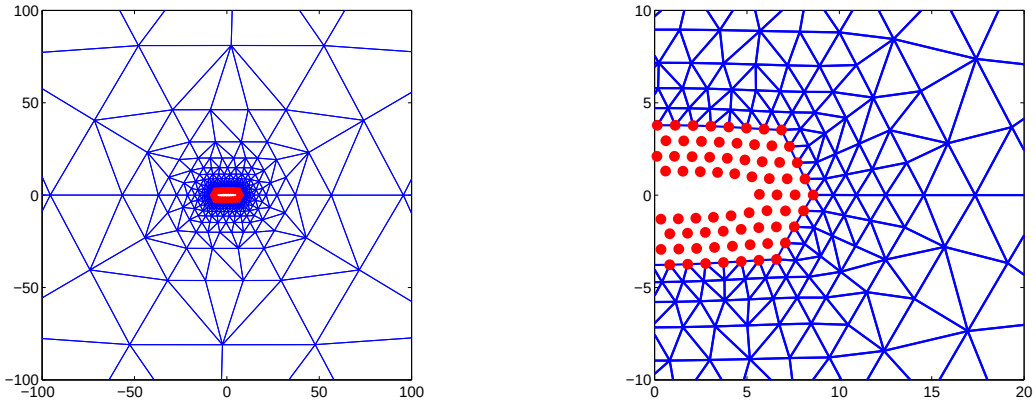

Figure 1: Micro-crack (deformed configuration in atomic units) in a 2D triangular lattice computed using an atomistic-to-continuum coupling method. The atomistic region represented by red points is coupled to the continuum region represented by blue finite element triangles

MATH 8450 Topics in Numerical Analysis
Multiscale Numerical Analysis for Materials

Mitchell Luskin
MWF 10:10 A.M. - 11:00 A.M.
Vincent Hall 364
(Time and room may be changed to accommodate student schedules. Please contact instructor.)

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-range 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 on the atomistic scale.

During the past several years, a mathematical structure has been given to the description and formulation of atomistic-to-continuum coupling methods, and corresponding numerical analysis has clarified the relation between the various methods and their sources of error. This course will begin by introducing the physical and mathematical background and then presenting the current state of numerical analysis for atomistic-to-continuum coupling methods.

Prerequisites are undergraduate numerical analysis and partial differential equations. All introductory material on continuum and atomistic modeling will be covered in the course.