# New Interdisciplinary Course Announcement for Spring 2012

# Multiscale Materials Modeling
# CBE 633
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Computational modeling now stands alongside experiment and theory as the third pillar of research. Materials modeling serves to develop fundamental relationships between the structure of a material and its thermophysical and transport properties. These structure/property relationships span a range of time and length scales. For each scale, there exists a set of appropriate computational tools. At the quantum scale, in which the distribution of electrons is the matter of interest, various density functional theory approaches exist to solve the Schrödinger equation. At the molecular scale, classical molecular dynamics or Monte Carlo simulations describe the distribution of atoms and molecules. At the mesoscale, coarse-grained models that still retain some aspects of the molecular nature of matter, allow tractable observations of systems over larger spatial and longer temporal scales. Finally, at the macroscale, Finite Element Methods solve continuum models describe the distribution of material, momentum and energy. Many of the most challenging materials modeling problems facing researchers today display behavior or exploit phenomena that span more than the one of the scales described above. Thus the generation of structure/property relationships requires multiscale materials modeling, or the clever integration of modeling techniques at different scales to yield a complete picture.

The course will be organized as follows. The first third of the course will involve the presentation of current, state-of-the-art techniques to explore each of the four scales alone. The second third of the course will examine emerging multiscale techniques bridge time and length scales. The final third of the course will involve student presentations and projects in which a particular multiscale materials modeling technique is applied to a problem of research interest to the student.

Single scale techniques surveyed in the first third of the course include density functional theory, classical molecular dynamics simulation, Monte Carlo simulation, Confined Random Walk simulation, Brownian Dynamics and the Finite Element Method. Multiscale techniques examined in the second third of the course include quantum mechanics/molecular mechanics simulation, reactive molecular dynamics, bridging through adaptive-resolution, coarse-graining through iterative Boltzmann inversion and integral equation theory, and continuum level modeling of the evolution of the pair correlation function.

This course will satisfy a “domain science” requirement of the Interdisciplinary Graduate Minor in Computational Science. The course will be structured to accommodate the skills and backgrounds of graduate students from all participating IGMCS departments. The course project will likely require programming in a language of the student’s choice or the use of publically available multiscale modeling software.