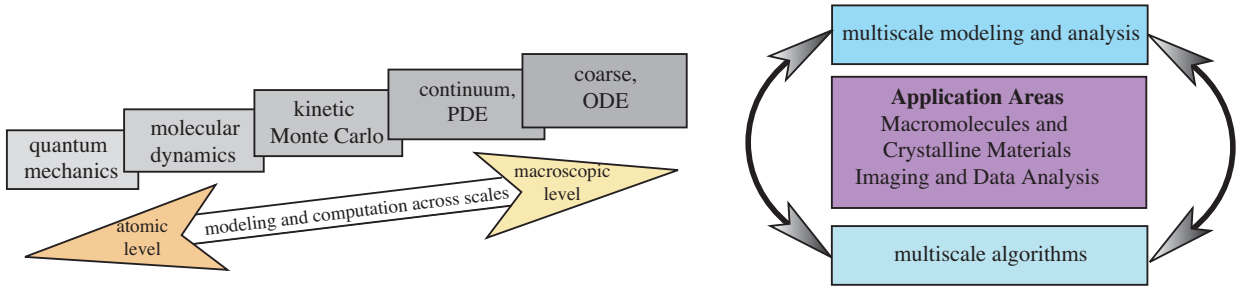
MMS: Multiscale Modeling and Simulation

This NSF/ITR funded project focuses on the need for accurate and reliable modeling, analysis, and simulation of multiscale systems. The research is being carried out in the context of CIMMS, the *Center for Integrative Multiscale Modeling and Simulation*, an interdisciplinary, multi-department, research center at Caltech. The Center integrates activities of researchers from Caltech, as well as those from other Universities, Government Laboratories and Industry to carry out its mission.

Research. The research will be organized around two main themes: ***modeling and analysis across scales*** and ***multiscale algorithms***. These themes will be implemented in several main application areas, such as ***macromolecules and crystalline materials*** and ***imaging and data analysis***. The first of the themes focuses on the mathematical modeling and analysis of multiscale physical systems, while the second focuses on the computational algorithms that are very relevant to this endeavor, and scientific computation and information technology more broadly. One of our main objectives is to bring these two main areas closer together in an interactive way and to prove the efficacy of doing this in the context of the two concrete and important application areas.



A broad range of scientific and engineering problems depend crucially on behavior at multiple scales, including the dynamics of biomolecules, the microstructure of materials, image and data analysis, earthquake physics and atmospheric and oceanic dynamics. The multiscale nature of these problems is enormously challenging from both the modeling and computational perspectives.

Recently, there have been some exciting, but problem specific, advances that have focused our attention on a special intellectual opportunity. These advancements include the quasicontinuum and weak-convergence methods in materials, new models in averaged fluid dynamics, new multiscale computational techniques for PDEs and image analysis, and new methods for addressing stochastics, uncertainty, and model validation. There are also examples where the two themes of modeling and algorithm development have been unified in solving outstanding problems, such as multiresolution methods and subdivision surfaces in thin shell computations that led to great progress in the problem of element locking. In this proposal, we identify challenging multiscale problems that are ideally suited for the collaborative interdisciplinary environment of CIMMS. The intention is to uniquely bridge the gaps in research, education and knowledge transfer between mathematics, computer science, engineering, biology and other disciplines.

A Unique Multidisciplinary Infrastructure. CIMMS has a special infrastructure for the proposed activities through its regular group meetings, workshops, conferences, and journal. This interdisciplinary setting fosters the kind of joint research that is essential to promote substantial progress on our targeted problems. The research team for this proposal has an excellent track record of accomplishment in mathematical and computational multiscale methods and their application to specific problems of national importance.

Education and Human Resources. This project helps to support a setting for multidisciplinary research for graduate students and postdoctoral fellows. The benefit of interaction with multiple research disciplines in multiscale modeling and information science will help train a new generation of scientists in this important area. To help accomplish this goal, new courses on multiscale science will be created and undergraduates engaged through summer programs. In addition, CIMMS has established very useful industrial contacts, (such as with the United Technology Research Center) that foster valuable student, postdoc and faculty exchanges.