PHYSICAL MATHEMATICS SEMINAR

TRANSITION BETWEEN THE MODELS IN MULTI-SCALE MODELING AND SIMULATIONS

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ABSTRACT:

Consider two different models with two characteristic length scales – the fine and the coarse scale. The fundamental problem of (multiscale) modeling is the definition of the coarse-scale variables in terms of the fine-scale variables.

The fine-scale variables are usually not uniquely defined from the coarse-scale ones. Nevertheless, if the coarse-scale variables are prescribed, the fine-scale variables must satisfy certain conditions. The computational setup of a fine-scale simulation with prescribed coarse-scale variables is the fundamental problem in multi-scale simulations.

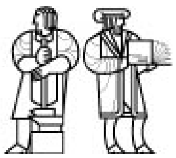
To address these problems, we first develop a mathematical classification of multi-scale problems, focusing primarily on the problems arising in mechanics of materials. The classification is based on those physical features of the models that separate the models mathematically: (dis)similarity of the models, (non-)equilibrium, (non-)locality, and, Eulerian vs. Lagrangean formulation.

We begin with kinematic variables and quasi-static (equilibrium) problems. The kinematic inter-scale transition can be considered independently provided that the models in question are characterized by local interactions. We take the coarse model to be the classical continuum. We develop the minimal kinematic boundary conditions (MKBC) for fine-scale simulations based on the rigorous definition of the coarse strain, and, implement them within the framework of the finite element method. When applied to a material with disordered microstructure, the MKBC are superior to the traditional periodic boundary conditions. Interestingly, the MKBC lead to a unique solution for a broad class of problems with pointwise positive definite fine-scale stiffness. The examples include polycrystals, metallic foams and granular materials.

The models with non-local interactions (e.g., molecular statics) require additional non-kinematic conditions. The theoretical basis for such conditions is discussed.

TUESDAY, MAY 3, 2005
2:30 PM
Building 2, Room 338

Refreshments at 3:30 PM in Building 2, Room 349.



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