MULTISCALE MODELING: NETWORK-CONTINUUM MODELS

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Recent advances in microelectronics, thin films, MEMS and nanotechnology have resulted in problems on a length scale which are too small to be modeled by conventional continuum mechanics and too large, computationally, to be described by accurate fine scale models. This has rendered multiscale modeling and simulations very important, which has been one of the fastest growing research areas in the past decade.

Multiscale modeling addresses a wide range of problems and takes a variety of mathematical forms. This method finds applications in modeling atomistic-continuum interfaces, granular materials, metallic foams and dislocation plasticity, to name a few. The simplest form of multiscale modeling involves models at two length scales viz. the fine scale and the coarse length scale, the coarse length scale usually being the effective continuum.

The primary question that arises is defining the coarse-scale variables in terms of the fine-scale ones such that it preserves the relevant physics of the fine-scale theory. The practical answer is provided by using appropriate boundary conditions in the small scale simulations. Solution techniques thus far have utilized periodic boundary conditions which have qualitative defects such as preventing strain localization and introducing spurious components with wavelength equal to the cell size in the solution fields. These defects are overcome by minimal boundary conditions which are imposed on a fine-scale computational cell as a constant derived from the coarse-scale model (Mesarovic, S. and Padbidri, J. 2005, *Phil. Mag.*, **85**(1), 65-78). These boundary conditions are termed minimal since they impose nothing but the desired constraint. These boundary conditions are based on the definition of the coarse strain as the volume average of the microscopic strain field (Bishop, J.F.W. & Hill, R, 1951, *Phil. Mag.*, **42**, 414-427). They have an integral form and yield a unique solution upon satisfying certain mathematical conditions.

The minimal boundary conditions are directly applicable to networks with local interactions. Metallic foams (in 2D) can be represented by a non-simplex network with beams as the basic elements at a fine-scale. The coarse-scale model is a special case of porous materials. Granular materials and concentrated suspensions of rigid particles in a viscous fluid can be represented by a discrete network approximation (Delaunay network of simplexes). The model includes a contact law, defined on the interactions between the particles. The minimal boundary conditions are applicable using the formulation of the discrete element method.