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Transitioning Models in Multiscale Simulation for Continua and Granular Materials

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Summary

While multiscale materials simulations are one of the fasting growing areas of computational research, commonly used rigid and periodic boundary conditions introduce additional and often times unrealistic constraints. Minimal kinematic boundary conditions (MKBC) result in a unique solution for the linear elastic case, and simulations indicate that this representation is applicable to a representative volume element (RVE) of any shape. Computed response behavior is superior to other BC's, in that they give more realistic overall behavior, reduce the required size of the RVE providing a natural multiscale linkage, and eliminate the superficial size dependent effects, ubiquitous in simulations with other boundary conditions.

Multiscale modeling and simulations have been one of the fastest growing research areas during the last decade. Nanomaterials, microelectronics, and ultrathin films have brought to light the problems on scales that are too small to be modeled by traditional continua, yet too large to be efficiently treated by more accurate fine scale models. When these models are invoked sequentially and information is passed from one scale to another, the key question related to simulation of the fine-scale cell becomes: *How are the coarse-scale fields to be passed onto the fine scale?*

Mathematical conditions that address this question are called ***minimal boundary conditions*** (MBC). The attribute *minimal* signifies that such conditions impose no additional restrictions on the fine-scale computational cell (other then the desired coarse-scale field). Practitioners have usually bypassed this question with a series of clever manipulations, including the popular periodic boundary conditions. Consider the problem of the mechanical response of a granular material to an applied shear stress. The drawbacks of periodic boundary conditions (Figure 1) are:

- Introduction of superficial cell-size wavelengths, requiring large computational cells,
- Localization on specific planes,
- Preventing response with higher order gradients–commonly encountered in functionally graded materials.

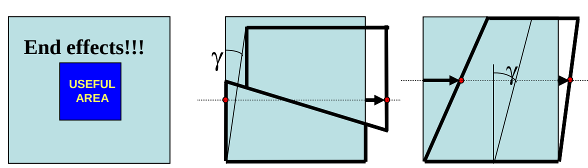

Figure 1. Impossible solutions under periodic boundary conditions: finite size correlation effects (left), shear localization on an inclined plane (middle), and, strain gradient (e.g., in functionally graded material) (right).

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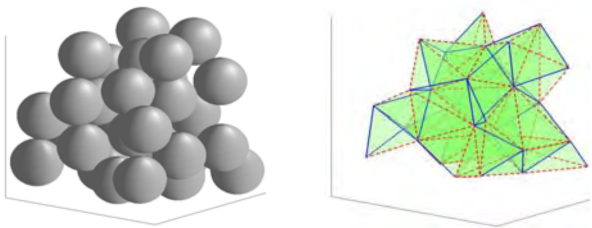

Figure 2. (left) A cluster of particles. (right) Contact graph (blue, solid lines), complementary graph (red, dashed lines) and Delaunay (all lines). Graphs corresponding to the packing sample.

An alternate and more efficient means to address this problem is to describe the topological evolution of a granular material using *Delaunay* and *contact graphs* for the geometric representation. The Delaunay graph is the set of lines that connects the centroids of the nearest neighbors. The contact graph consists of the lines between centroids of particles that are in contact, and are a subset of the Delaunay graph. A small particle cluster and its Delaunay and contact graphs are shown in Figure 2.

Minimal boundary conditions can then be imposed on a fine-scale computational cell as a constraint derived from a coarse-scale model. Recently, Mesarovic & Padbidri formulated minimal kinematic boundary conditions for equilibrium, continuum-continuum problems, and implemented them into a computational finite element (FE) framework. The coarse scale strain can be expressed as the volume average of the microscopic strain field $\varepsilon(x)$, by:

$$\mathbf{E} = \frac{1}{V}\int_V \boldsymbol{\varepsilon}(\mathbf{x})\,dV = \frac{1}{2V}\int_S (\mathbf{un} + \mathbf{un})\,dS$$

where $\mathbf{u}(\mathbf{x})$ is the displacement vector, and $\mathbf{n}$ is the unit normal to the surface. The implementation for quasistatic discrete element methods with implicit integration is direct. Kinematic and static continua defined by linear interpolation of the discrete model are formulated in a manner completely analogous to boundary conditions for constant strain finite elements. These conditions are 'minimal'-nothing but the desired coarse strain constraint is imposed. To study more realistic 3D configurations, we have developed a parallelized implementation with Delaunay and boundary detection. The resulting models provide greater accuracy with fewer numbers of elements allowing for greater ranges of dynamic simulations.

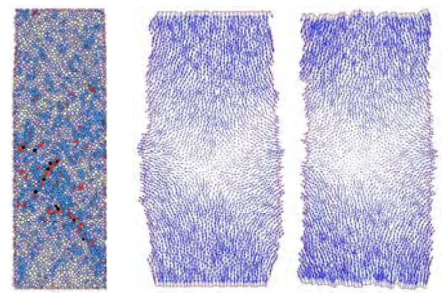

Figure 3. (left) 2D particle packing under isostatic pressure. (middle) Velocity vector plot during deformation when vertical strain is imposed by means of top and bottom rigid plates. Note the marked diagonal (X) shear bands. (right) Velocity vector plot during deformation when axial strain is imposed as minimal kinematic boundary condition. Note uniform lateral swelling and absence of shear bands.

Related Publications

Mesarovic, S.Dj. 2005 Energy, configurational forces and characteristics lengths, associated with the continuum description of geometrically necessary dislocations. *Int. J.Plast.* **21**, 1855.

Mesarovic, S. Dj. & Padbidri, J, 2005, Minimal kinematic boundary conditions for simulations of disordered microstructures, Phil. Mag., 85, n1, 65-78.

Mesarovic, S.Dj. & Padbidri, J. 2007 Transition between the models in multiscale simulations. Continuum and network models. Proc. Multiscale and Functionally Graded Materials, Oahu, 2006.

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