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TRANSITION BETWEEN MODELS IN MULTISCALE SIMULATIONS: CONTINUUM AND GRANULAR MODELS

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ABSTRACT

Multiscale modelling addresses problems on a scale too small to be modelled by traditional continua, yet too large to be economical for more accurate fine scale models. We consider two-scale problems: the fine-scale model and the coarse-scale continuum. Sequential simulations for such models give rise to the key question: *How are the coarse-scale fields to be passed on to the fine scale computational cell*? The mathematical conditions that answer this question are called minimal boundary conditions (MBC) [1]. They are *minimal* in the sense that, nothing but the desired constraint is imposed – unlike periodic BC, which (i) introduce superficial cell-size wavelengths in the solution fields, (ii) allow localization only on specific planes, and, (iii) prevent response with higher order gradients, common, for functionally graded materials.

Kinematic MBC for fine scale continua have been discussed [1], and implemented into the finite element framework based on the definition of the coarse strain, as the volume average of the microscopic strain field, $\mathbf{e}(\mathbf{x})$:

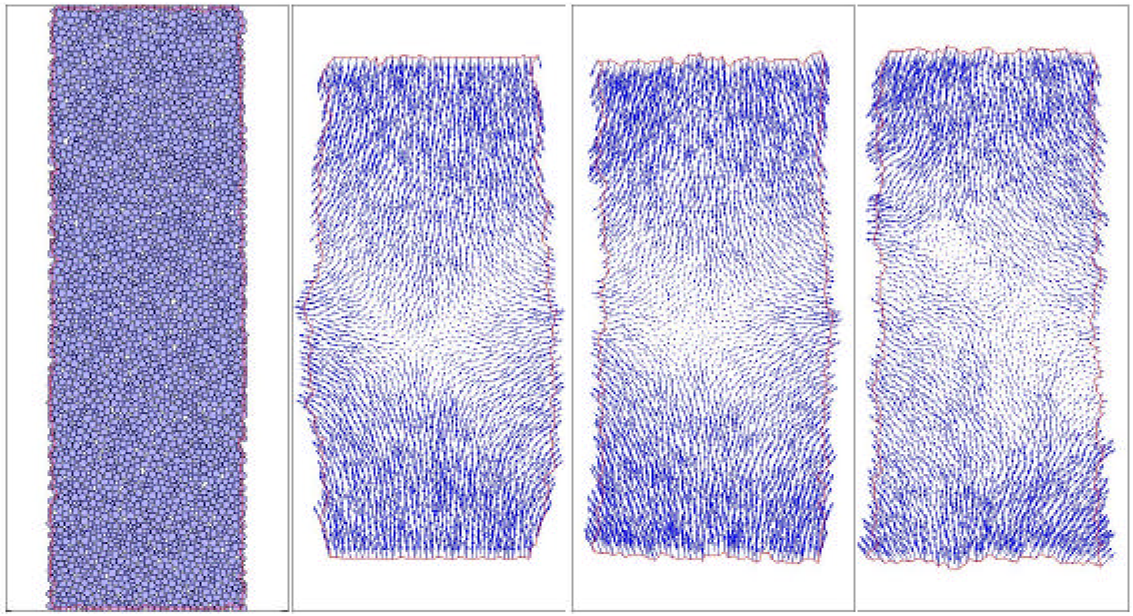
$$\mathbf{E} = \frac{1}{V}\int_V \mathbf{e}(\mathbf{x})\, dV = \frac{1}{2V}\int_S (\mathbf{un} + \mathbf{un}) dS \qquad (1)$$

where $\mathbf{u}(\mathbf{x})$ is the displacement vector, and $\mathbf{n}$ is the unit normal to the surface. Compared to periodic BC, the MBC show superior accuracy and computational economy [1]. Here, the application to fine-scale continuum models to fine-scale discrete models with local interactions – granular materials, is addressed.

The key to this application is the equivalent representation of kinematics of granular flow using the Delaunay network, the complementary graph to the Dirichlet (or Voronoi) tessellation [2]. To create an equivalent fine-scale continuum for granular statics, we use the cell-based description of strain in granular materials [2, 3, 4], which defines an effective C^0 continuum, formally equivalent to a set of constant strain finite elements (CSFE). Thus, the implementation for quasistatic problems, is identical to the one used in the fine-scale continuum model.

Dynamic, explicit integration algorithms, such as those used for granular materials, enable efficient parallelization and so, should be preserved. A direct implementation of integral MBC (1, 4) would couple all degrees of freedom on the boundary and would result in

inefficient computations. Hence, we implement these boundary conditions by means of the penalty method [5]. The penalty is imposed on the violation of the prescribed strain rate rather then strain, since computing strain requires re-tessellation in each increment.



(a) (b) (c) (d)

Figure 1. (a) After hydrostatic pressure (b) Displacement vectors from (a) to 17% strain for BiAxial case (c) Displacement vectors from (a) to 17% strain for MBC (d) Displacement vectors from 12.5%-15% strain for MBC.

We consider an assembly of discs with uniform size distribution between ½ and 1 and apply hydrostatic pressure using the interpretation of Delaunay cells as CSFE (Fig. 1a). Then, axial strain is applied (Fig. 1b, c). The top and bottom rigid plate boundary (Fig. 1b) induces a wedge shaped block-like motion near the boundary and consequently, barrelling, and persistent shear bands, while the MBC (Fig. 1c) shows no such boundary effects. However, MBC do allow temporary strain localisation on an inclined plane (Fig. 1d), not achievable with periodic BC. Using MBC, any component or combination of strains can be prescribed to any shape of the computational cell.

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