Radial Periodic Boundaries for Axi-Symmetric DEM Simulations: Development, Implementation and Validation

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Introduction

The ability of discrete element modelling (DEM) to provide useful information on the micro-scale parameters that underlie the observed macro-scale response of soil is now well established. Notable examples include the work of Thornton (2000) and Cheng et al (2003). In geotechnical laboratory testing the need to maintain a small ratio for the particle dimensions to the sample dimension is well established. The same consideration should be made when simulating element tests using discrete element simulations. One option is to consider an ideal, boundary free simulation environment using a rectangular periodic cell (e.g. Thornton, 2000). However where this approach, the simulations cannot easily be directly compared with physical tests for validation purposes. Furthermore, as demonstrated by Cui and O'Sullivan (2005) DEM simulations can provide insight into the non-uniformities present in real physical tests when the test boundary conditions are included in the DEM model. One limitation associated with particulate DEM simulations is their computational cost. Each particle is modelled as a rigid body, or a number of rigid bodies bonded together. Consequently of the number of degrees of freedom associated with the simulation of even a conventional triaxial laboratory test can easily be in the order of $10^5 – 10^6$. The simulations are also dynamic, requiring the dynamic equilibrium of each particle to be considered at discrete points in time. The inherent non-linearity of the particulate systems considered and conditional numerical stability of the central difference time integration algorithm used in DEM limit the time step that can be used in the simulations, further adding to the computational cost. While there is potential to improve DEM simulation run-times by efficient coding, careful compiler selection and parallel processing, there is also merit in exploring the possibility to reduce the number of particles or degrees of freedom present in the system by taking advantage of symmetry considerations where possible.

This paper proposes a framework for simulating only one segment of the system for DEM simulations of geometrically axi-symmetric assemblies of particles, reducing the number of particles that need to be analysed while preserving the three dimensional contact force network. Axi-symmetry is encountered in a variety of systems of interest in geomechanics, most notably the samples tested in the commonly used triaxial test are cylindrical and the applied stress field is axi-symmetric. The concept of the system is firstly proposed, followed by a description of the analytical and laboratory validation of the approach. The evolution of the approach for 90^o segments has been described in prior publications (e.g. Cui et al (2007), O'Sullivan et al (2008) and O'Sullivan and Cui (2009)). The objective of the current paper is to describe the generalized formulation for the approach and a coherent documentation of the key findings from the completed validation study.

Description of Boundary Conditions

The use of rectangular periodic boundaries for DEM simulations of boundary free element tests has been described by numerous DEM analysts (including Thornton (2000)). In that approach rectangular samples are used the particle coordinates and contact force information is translated to the opposite

boundary to maintain an infinite continuous network of interparticle contact forces. For axi-symmetric simulations this concept can be adapted by rotating the particle coorindates and contact force information to maintain a continuous network about the central vertical axis in a triaxial test simulation. Figure 1 illustrates this concept for a 90° segment, where a quarter of the system is considered and two orthogonal, vertical radial period boundaries bound the quadrant. Particles A and B are both adjacent to these boundaries. The coordinates of particle B are rotated for the purposes of contact detection. The magnitude of the interparticle force between particle A and B is calculated using the rotated particle coordinates. This force is then applied directly to particle A and rotated for application to particle B as illustrated. For ease of implementation of the system the z axis should be taken to act along the centre of symmetry of the sample and the x axis should form one of the circumferential boundaries, the second periodic boundary is then inclined at an angle θ to the x axis, where $\theta \leq 90^{o}$. Then for general implementation of the system the coordinates of B (x_B, y_B, z_B) are mapped to the point B' ($x_{B'}$, $y_{B'}$, $z_{B'}$) using the following orthogonal rotation:

$$\begin{pmatrix} x_B \\ y_B \\ z_B \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_{B\prime} \\ y_{B\prime} \\ z_{B\prime} \end{pmatrix}$$

The contact force coordinates are then mapped back to the original particle B using the inverse of this transformation matrix. This approach was implemented into a modified version of the TRUBAL DEM code (Cundall and Strack, 1979) initially only for $\theta = 90^{o}$ segment, and then extended to the general case of $\theta \leq 90^{o}$ as described by Barreto Gonzalez (2009).

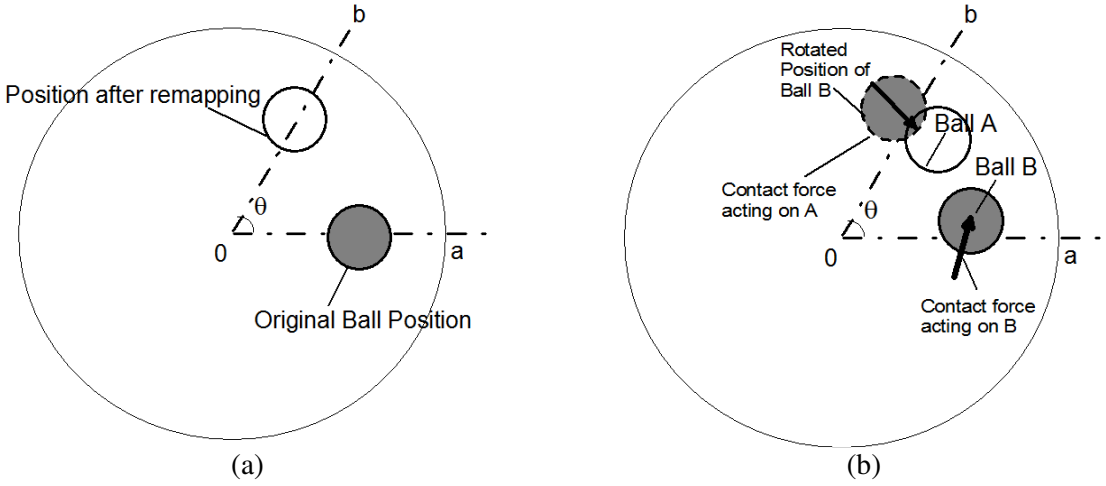
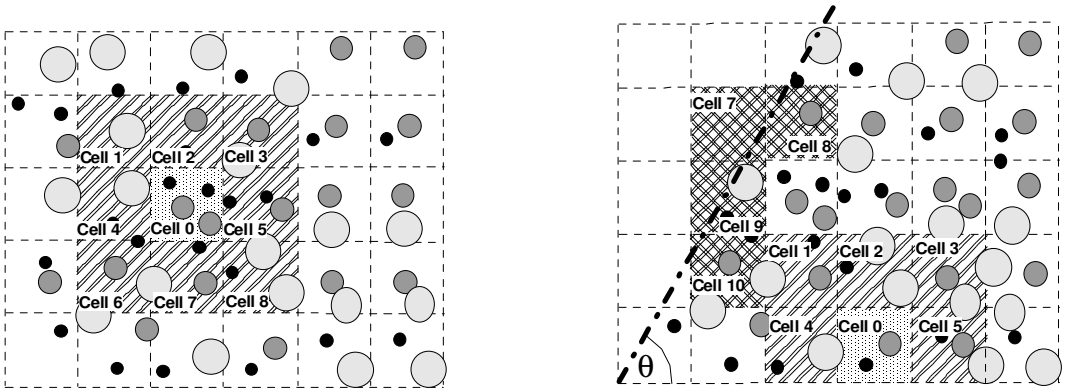


Figure 1 Illustration of circumferential periodic boundaries (a) Mapping of ball to new equivalent position. (b) Rotation of contact forces along boundaries

An additional challenge regarding the general implementation of the axi-symmetric periodic boundary system is the contact detection algorithm. Typically in a DEM simulation testing for contact between a given particle and every other particle in the system is both computationally expensive and unnecessary. From geometrical considerations any one particle can potentially contact only those particles that are close to it. The most common approach to identifying particles that are close is to adopt a binning algorithm. In this approach the entire system of particles is overlain with a regular grid, with each grid cell having dimensions (in 3D) $\Delta x \times \Delta y \times \Delta z$, with n_x, n_y and n_z being the number cells in the x, y, and z directions respectively. Using this information a simple calculation can be used to map each particle to a cell in the grid and a list of the particles mapped to each grid cell

can be generated. Then, as illustrated in Figure 2(a) for a simple cartesian system, the adjacent cells (housing potential contacting particles) can be simply identified. In contrast, for the axi-symmetric system where a particle is adjacent to the periodic boundary geometrical considerations increase the number of cells housing potential contacting particles along the other periodic boundary.

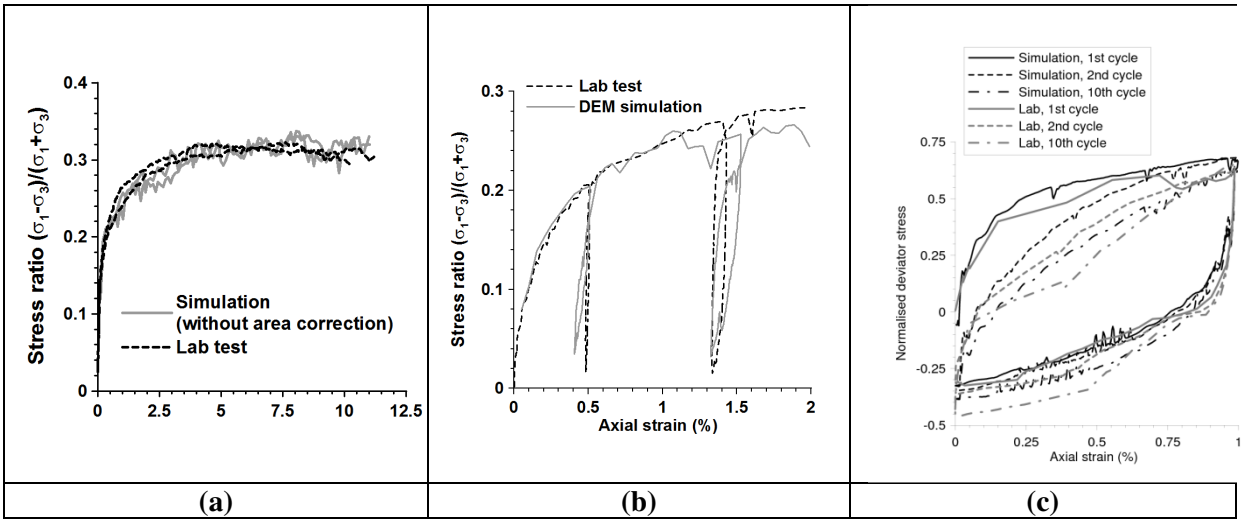


(a) (b)

Figure 2 Illustration of contact detection challenges for axisymmetric system

Validation

The axi-symmetric periodic boundary environment was validated both analytically and experimentally. As discussed by O'Sullivan (2002) amongst others, consideration of the response of uniform disks and spheres with lattice packing configurations is useful for validation of DEM simulations. The first phase of the validation of the axi-symmetric considered uniform spheres with a face-centered-cubic (FCC) packing configuration and a comparison was made with the analytical solution proposed by Thornton (1979). A quantitative match between the simulation results and the analytical results was achieved (within 5% error). The experimental validation of the algorithm considered the response of specimens of steel spheres in vacuum confined triaxial tests. The testing and simulation program considered both uniform (mono disperse) and non-uniform (poly disperse) triaxial tests. The samples were subject to simple, strain controlled monotonic triaxial tests, tests involving pre-peak load reversals and strain controlled cyclic tests. As illustrated in Figure 3 a good agreement was obtained between the physical tests and numerical simulations in for all three test series.



(a) **(b)** **(c)**

Figure 3 Validation results (a) Monotonic triaxial tests (b) Monotonic triaxial tests including pre-peak load reversals (c) Cyclic triaxial tests.

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