CHAPTER

4

A guide to modeling the geotechnical behavior of soils using the discrete element method

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Introduction

The discrete element method (DEM) originally developed by Cundall and Strack (1979) for the analysis of rock mechanics problems is significantly popular. Its use is widespread across multiple disciplines (e.g., Fleissner, Gaugele, & Eberhard, 2007; Horabik & Molenda, 2016; Ketterhagen, am Ende, & Hancock, 2009; O'Sullivan, 2011; Richards, Bithell, Dove, & Hodge, 2004; Sarhosis, Bagi, Lemos, & Milani, 2016), the number of publications has also exponentially increased (O'Sullivan, 2011), and open-source and commercial DEM codes are widely available. There is a large body of existing research using DEM, as well as a number of detailed publications on the use of DEM (e.g., O'Sullivan, 2011; Rapaport, 2004; Thornton, 2015). The usefulness of DEM is recognized; however, it is not easy for the novice user to understand in detail its capabilities, limitations, and potential pitfalls. This chapter is aimed to provide a concise source of information that may be of use for anyone interested in using DEM for the simulation of geotechnical problems, but who has limited or no experience or knowledge of the topic.

This article/chapter starts by describing the DEM algorithm. Consequently, the steps required are used as a template for the following sections. Boundary types, particle types, specimen generation, as well as some details on contact detection, force calculation, and numerical

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integration procedures are therefore described. Subsequently, an introduction to the common data analysis required for DEM simulations is presented in terms of macro- and micro-variables. While most of the information on the initial sections refers to specimens of spheres, this information provides a theoretical background to then discuss how more realistic granular material simulations can be performed. Particle shape, crushing, fluid coupling, and clay behavior are briefly discussed. The chapter is then concluded with some practical considerations required for running good DEM simulations.

DEM algorithm

The essence of DEM is that individual particle movements (i.e., translation and rotation) and their interaction with other particles can be quantified in detail. The first step of any DEM simulation is to define its geometry. This typically involves providing the locations of all boundaries and particles as well as defining the physical and geometrical properties to adequately represent their behavior. Then, the following steps are followed sequentially:

1. Identify interparticle and boundary-particle contacts.
2. Calculate contact forces using an appropriate contact model (force-displacement law).
3. Calculate the acceleration of particles using Newton's second law of motion.
4. Integrate the particle accelerations twice to obtain particle velocities and displacements, respectively.
5. Update particle and boundary positions.
6. Advance simulation time by a time-step increment and repeat steps 1–6 until the simulation is complete.

The following sections follow this order to describe important issues of the implementation and the appropriate use of DEM algorithms. Rather than focusing on the detail, the emphasis is on the principles while providing references for readers to deepen their knowledge.

Boundary types

In most DEM simulations, three different boundary types may be used, namely, rigid, flexible, and periodic (Fig. 1). Although DEM is a strain/displacement-based algorithm, all boundary types can be stress-controlled by servo-control algorithms and are generally modeled with no mass/inertia.

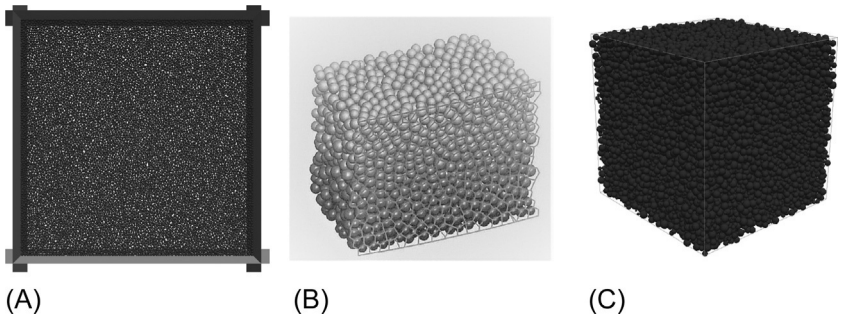

FIG. 1 (A) Rigid, (B) flexible, and (C) periodic boundaries.

Rigid boundaries can take any shape, from a cylindrical/rectangular plate typically seen in geotechnical element tests (i.e., direct shear box, triaxial), and such as those illustrated in Fig. 1A, for a two-dimensional biaxial compression simulation. Rigid boundaries can also represent more complex geometries such as funnels, rotating drums, comminutors, etc. These boundaries are generally specified as a collection of planes and/or triangular facets or sets of glued/bonded particles.

Flexible boundaries (see Fig. 1B) may be used to represent stress-controlled membranes such as the latex membranes surrounding soil specimens in a triaxial device. In this case, implementations are varied and include movable rigid/plate boundaries (e.g., Kuhn, 1995), elasticity-based models (e.g., Qu, Feng, Wang, & Wang, 2019), bonded particles (e.g., Wang & Leung, 2008), or Voronoi/Delaunay approaches (e.g., Cheung & O'Sullivan, 2008). The approach by Kuhn (1995) uses triangular plates connecting the centroids of particles in contact with the membrane, and to which an equivalent force corresponding to the stress required is applied. On the other hand, Voronoi/Delaunay approaches do not directly model the flexible boundary (see Fig. 1B); they simply use Delaunay triangulation and/or Voronoi tessellation approaches to calculate areas with centroids coinciding with the particle centroids. In this way, a force can be applied to each particle according to the required stress level. Each of these approaches has its own advantages and disadvantages. While the implementation of these approaches is not complex, particular attention must be given to provide the regular updates of the geometry of the boundary which increases the computational cost of the DEM simulation.

A challenge when using rigid boundaries (e.g., Fig. 1A), which is also present in physical laboratory experiments and boundary-value problems, is that stress and strain nonuniformities may occur. In other words, the stresses/strains measured in the neighborhood of a rigid boundary may not be the same as those measured far from them. To reduce the effect of these nonuniformities, the geometry of the simulation should be

carefully considered, and as a result, a significantly large number of particles may be required. An alternative method commonly adopted is to use periodic boundaries. They provide a means to avoid boundary effects and are the equivalent of single element simulations in finite element analyses. As such, it is then possible to simulate a uniform and infinite strain field using a significantly smaller number of particles than that required to simulate the same soil behavior using rigid boundaries. Implementation details for the use of periodic boundaries are clearly described by O'Sullivan (2011).

Particle types

In its simplest form, DEM involves the simulation of individual spheres (3D) and discs (2D). These particles provide an efficient means to quantify micro-mechanics, but they are an over-simplification of reality. However, any shape can be simulated using various approaches. One of the most common methods employed to replicate more realistic particle shapes is the use of clumps of individual particles (see Fig. 2A). Any particle shape can be represented for a DEM simulation using this method. Care is, however, needed if there is an overlap between the individual clump particles because the inertia of the clump needs to be adjusted. An approach to avoid this is described by Ferellec and McDowell (2010). Also, the more spheres are used to model each particle, the more accurate its representation, but this also increases the computational effort required for the simulation. To a certain extent, even particle surface roughness could be modeled in this way, albeit at a significant computational expense.

Sphero-simplices (Pournin, 2005) are other convenient means to simulate differing particle shapes while benefiting of the computational efficiency related to the simulation of spheres. Their modeling consists of lines and/or polygons across which a sphere can be moved to recreate a particle shape with rounded corners (see Fig. 2B). Superquadric equations are an extension from ellipses and spheres to represent more complex particle shapes using a limited number of mathematical parameters (Fig. 2C) that have been used widely (e.g., Cleary, 2004; Podlozhnyuk, Pirker, & Kloss, 2018; Soltanbeigi et al., 2018). Polyhedra and other simple geometries, such as cylinders and ellipses, are also commonly used in DEM simulations (Gan & Yu, 2020; Lin & Ng, 2004; Lu, Third, & Müller, 2015; Xie, Song, & Zhao, 2020; Zhao, Kruyt, & Millet, 2020) as those illustrated in Fig. 2D. In reality, any curve (or surface) in space can be described by analytical/mathematical expressions. As such, potential surfaces and other 'avatar' approaches are often used (e.g., Harkness, 2009; Kawamoto, Andò, Viggiani, & Andrade, 2018), which can accurately replicate more realistic particle shape.

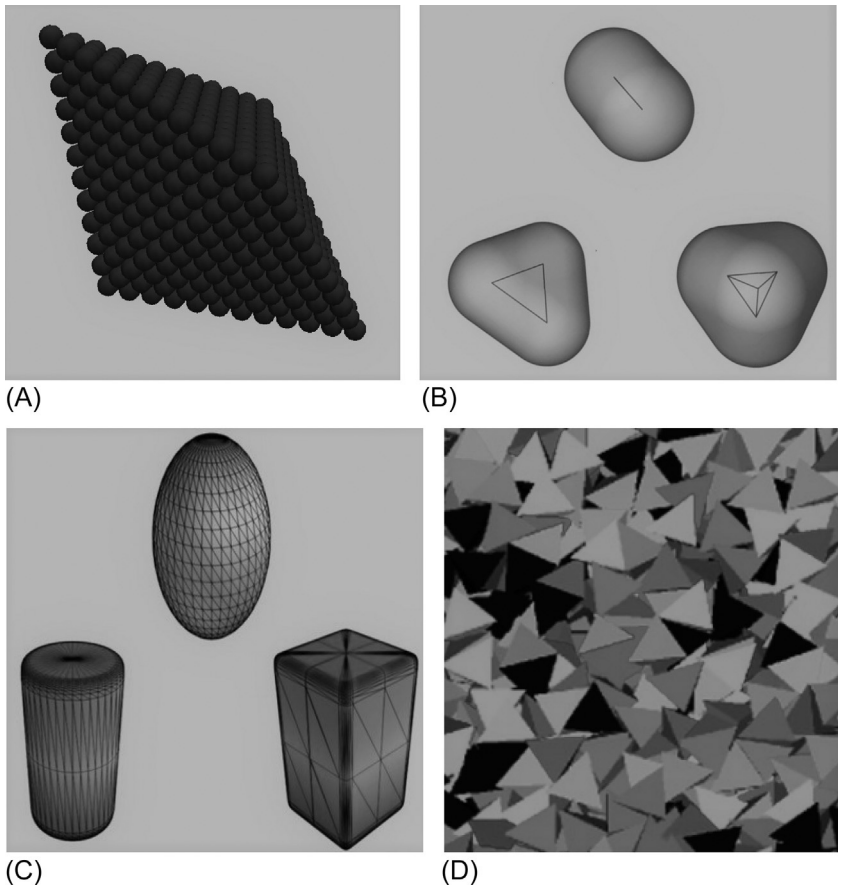

FIG. 2 (A) Spheres and clumps, (B) sphero-simplices, (C) superquadrics, (D) polyhedra.

Specimen generation

Having defined the geometry of individual particles as well as the boundary types required, an assembly of particles enclosed by the boundaries that adequately represent reality needs to be generated. To do this, various approaches may be used including random generation, radial expansion, gravitational deposition, or other approaches. In many DEM simulations, random generation is usually the first stage. Here, a number of particles are generated within the boundaries while ensuring that there are no interparticle or boundary-particle contacts. There are several approaches to achieve this, but it is common to first (randomly) locate the largest particles and then try several times to fill the spaces between them with the smaller particles. At this point, the particles may have

the same shape, but not necessarily the same mean diameter as the real soil. If that is the case, the radial expansion method is used to incrementally increase the particle size while the DEM simulation is run. This approach provides some control over the final density of the specimen, but not its resulting confining stress. Furthermore, the resulting particle size distribution may just be a scaled version of the real one. A real particle size distribution's shape and size can be defined from the outset using the random method, and then servo-control algorithms can be used to achieve the desired stress state. As an alternative, geometrical/sequential specimen generation methods can also be used, but these are generally only applicable to simple particle shapes (e.g., Cui & O'Sullivan, 2003). Since the aim of most DEM simulations is that of replicating reality, the gravity deposition method is worthy of consideration. After random generation, body forces can be switched on during a simulation. This provides weight to individual particles, and therefore, they move in the gravitational direction as cycling progresses. Typically, a significant number of cycles are required for all particles to settle and attain a state of equilibrium.

Whatever the method used, control of the initial density of DEM specimens is relatively easy. When interparticle friction is small, particles can slide against each other and accommodate with ease and thus achieving very dense particle assemblies. On the other hand, high interparticle friction restricts interparticle movement and hence results in DEM specimens with low density. Note that it is possible to change the value of the coefficient of interparticle friction during the specimen generation stage to further control the density. However, care must be taken to achieve a stable structure after friction reductions as they may produce excessive interparticle sliding and consequently density increases. However, the effect of interparticle friction on specimen density is nonlinear, and it reduces as the value of interparticle friction increases. Furthermore, it is not commonly recognized that superfluous increases in the shear stiffness of specimens may occur when using high friction values.

Another important aspect of specimen generation approaches is their effect on fabric (i.e., the geometric configuration of the particles). Radial and random generation approaches provide specimens with isotropic fabric (i.e., contacts orientations distributed equally in all directions). On the other hand, gravitational deposition methods generate preferred contact orientations in the direction of the gravitational force and therefore, an anisotropic fabric. The use of particle shape beyond spheres or discs also affects fabric anisotropy, particularly when gravity is used because the major particle axis tends to align perpendicularly to the direction of gravity. It is important to be aware of these effects because it is well recognized that fabric anisotropy and specimen preparation affect the mechanical response of granular materials (e.g., Vaid, Sivathayalan, & Stedman, 1999)

Contact detection

To calculate interparticle forces, contacts between individual particles need to be identified. A key assumption of DEM simulations is that although particles are assumed to be rigid, they are allowed to overlap to account for some degree of deformation that would occur in physical experiments. Consequently, contact between two spheres simply occurs when the distance between particle centroids is equal or smaller than the sum of their radii. The process of contact detection is one of the most time-consuming stages in DEM simulations. As a result, there are several implementations of contact detection algorithms aiming to increase computational efficiency. The simplest and most inefficient way is of course to test the existence of contacts between each particle and every other particle in the simulation.

There are, however, more efficient ways to detect interparticle contacts that include: (i) neighboring cell approaches, (ii) nearest neighbor approaches, and (iii) bounding box (sweep and prune) approaches, among others. To understand the differences between these approaches is convenient to consider the case of interparticle contacts between discs (Fig. 3).

When using neighboring cell approaches (see Fig. 3A), the spatial domain is divided into smaller individual "cells" (boxes in 3D). Normally, a list of particles for each cell is compiled which can be then updated periodically. The gain in efficiency is made because for each particle contact, checks are only made with particles within the same cell and the neighboring cells. Cell size of course then needs to be related to particle size.

Nearest neighbor approaches (see Fig. 3B) define a neighborhood for each particle (discontinuous line) and then a list of near-neighbors (i.e., lighter particles) is maintained and periodically updated for each particle. Contacts are then only checked between neighbors. Care must also be taken when considering the size of the neighborhood in relation to the particle size distribution.

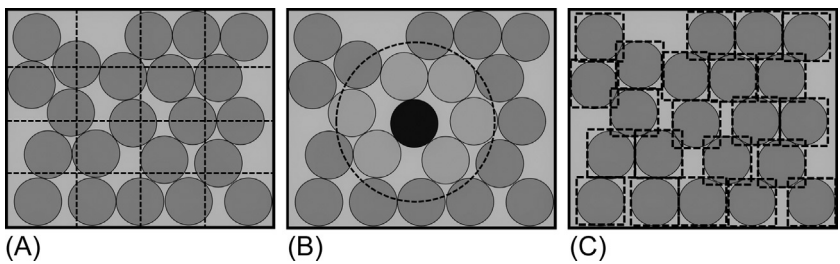

FIG. 3 Contact detection algorithms using (A) neighboring cell, (B) nearest neighbor, and (C) bounding box approaches.

The principle behind bounding box approaches is that each particle has a bounding box (with discontinuous lines) with edges aligned with the global axes (see Fig. 3C). Contacts between particles can only occur if the boxes overlap in the two (or three, for 3D) coordinate directions. Hence first, a sweep is first done to find overlapping bounding boxes and a second round of finer contact detection (i.e., pruning) between overlapping boxes.

If particle shapes other than spheres are considered, the approaches described above can still be used. They are, however, used first as "coarse" contact detection approaches using bounding spheres (or boxes) as illustrated in Fig. 3C. A fine detection is then required because several contact types may be found that add to the complexity of the calculations (e.g., point-surface, point-edge, or surface-surface contact types when using polyhedral particles). Accuracy in contact detection is important because the nature of the contacts also determines the magnitude of contact forces as described in the next section.

The computational cost reductions that can be achieved by implementing efficient contact detection algorithms are significant. This is a vast research field of its own. It is of the utmost importance to always consider if a specific algorithm is suitable for the specific particle size distribution and particle shape being replicated in the DEM simulation.

Force calculation

Once contacts between particles and boundaries have been identified, the next step is the calculation of contact forces based on the chosen contact model (i.e., force-displacement law). Usually, this involves the estimation of both normal and tangential forces at each contact. Considering contact between two spheres and the simplest contact model (linear elastic), the magnitude of the normal contact force (F_n) is given as a function of the particle overlap, Δ_n as:

$$F_n = k_n \Delta_n$$

where k_n is the normal contact stiffness. For the case of contact between spheres, the contact overlap (Δ_n) is the difference between the sum of the particle radii and the centroidal distance between the two particles. Similarly, the tangential force, F_t, can be calculated as:

$$F_t = k_t \Delta_s$$

where k_t is the tangential/shear stiffness at the contact, and Δ_s is the cumulative tangential/shear displacement at the contacts. The appropriate implementation Δ_s is a key aspect of any DEM software. Additionally, slippage at the contacts needs to be considered. This may be done by

comparing the magnitude of F_t against the product of the coefficient of interparticle friction (μ) and the magnitude of the normal contact force (F_n). If $F_t \geq \mu F_n$, then the contact slips and the magnitude of the tangential force is set to $F_t = \mu F_n$. Contact slippage in DEM simulation is the main form of energy dissipation, and it is aimed to replicate also other forms of dissipation such as heat generation, plastic deformation of contact asperities, etc. The selection of the right value of μ is therefore very important to accurately model geotechnical behavior.

Despite their simplicity, linear elastic models are able to replicate many of the complexities of real soil behavior such as stiffness degradation, stress and strain anisotropy, among others. Having said that, more realistic/complex contact may be used. Nonlinear elastic (i.e., Hertzian) contact models, in which the normal contact stiffness is dependent on the contact area, are also very common. Using rheological principles, hysteretic behavior, viscous effects, and long-range forces can also be modeled. Of particular interest for geotechnical applications, long-range contact models may consider electrostatic interactions (as required for the simulation of clay behavior), tensile strength (needed when simulating bonded/cemented soils), and capillary forces (for unsaturated soil behavior), among others.

Numerical integration procedures

Having calculated the magnitude and direction of forces at each contact, a summation of all contact forces on individual particles should be made. The resulting force (which is normally characterized by its three components on each of the coordinate directions) on each particle will produce an acceleration (a) in the same direction of the force, and it is calculated using Newton's second law

$$a = F/m$$

where F is the resultant force acting at the particle and m is the mass of the particle. Particle rotations are considered in a similar manner using the moment of inertia. An important aspect of any DEM formulation is that any force type may be included in the calculation of F above. Therefore, body forces (i.e., gravity) and external forces in addition to those resulting from the contact model can also be considered.

The final step in the DEM calculation is to use the defined time-step and using a finite-difference integration scheme, to integrate the accelerations, and to obtain particle velocities and updated positions for particles and boundaries. The new geometry is then used to repeat all calculation steps described.

As a result of these calculation steps, particle positions, velocities, accelerations, as well as the details of the interparticle forces for each particle at every-step can be obtained. Getting this information in other ways (i.e., experimentally) can be challenging and/or expensive. Nevertheless, the amount of information that can be gathered from a DEM simulation is significant, and its analysis and understanding are not necessarily simple. In the case of three-dimensional simulations, the interpretation of results is not helped by the fact that a clear visualization of results is a challenging task.

Analysis of DEM data

Fig. 4A illustrates the geometrical configuration of a typical three-dimensional assembly of spheres at a given time-step. Such a plot may be easily modified to visualize (for example) the amount of particle rotation or any other quantity of interest. Visualization of contact force networks is very commonly made. In the case of spherical particles (Fig. 4B), contact vectors connecting particle centroids are illustrated with their thickness proportional to the magnitude of the force. While these visualizations may be attractive and may be used to illustrate specific mechanisms (e.g., arching or shear banding), they are generally just useful in a qualitative manner. Fig. 4B also shows that stress transmission in granular materials is not homogeneous. Interparticle forces are commonly divided into strong and weak force chains/networks according to the average magnitude of the contact forces at a given time-step. Strong and weak force chains have differing and important roles to understand

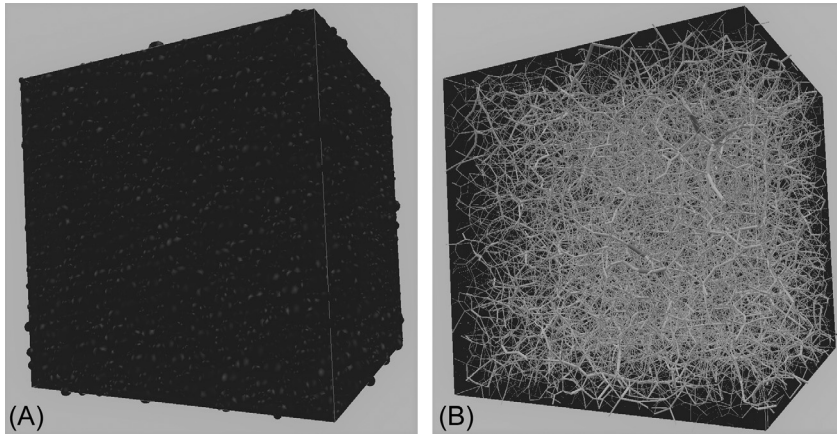

FIG. 4 3D representation of (A) an assembly of spheres and (B) its contact force network.

the geotechnical behavior of soils (e.g., Barreto & O'Sullivan, 2012). The illustrations in Fig. 4 also highlight that 3D visualization is challenging and highlight that quantitative approaches to analyze DEM data may be of more use and practical interest.

Macro-scale variables

Due to the widespread use of continuum approaches in geotechnical modeling, as well as the obvious use of physical experiments to understand soil behavior, the analysis of DEM results should be presented in a similar manner. In other words, particle-scale variables such as contact forces need to be converted into a stress tensor and particle positions, rotations, and velocities may be converted into strains.

The calculation of stresses from interparticle forces is simply a mathematical task, although with exact physical meaning as discussed by Bagi (1996). Homogenization approaches may however differ. A common feature of these approaches is that interparticle forces are averaged over a volume of interest. Due to the heterogeneous nature of stress transmission in granular materials (see Fig. 4B), the choice of such measurement volume is an important decision that depends on the type of simulation performed and what is sought from it. When periodic boundaries are used, the solution is simple because the entire volume can be used for stress calculation, and provided that there is a sufficient number of particles it provides statistically representative data. In contrast, when the problem requires the use of rigid boundaries, the size, shape, and position of the measurement volume need to be considered with care. As discussed before, the stresses near rigid boundaries may be significantly different far from them due to the presence of nonuniformities. Most commercial software uses measurement spheres for quantification of micro- and macroscale variables form DEM simulations. In reality, however, the shape of the volume is not relevant as long as its volume can be calculated accurately. The size of the measurement volume is of significant importance, particularly when a statistically representative sample is required for the calculation of variables. Barreto and O'Sullivan (2012) discussed that for a relatively uniformly graded DEM specimen, they required at least 4000 particles in their simulations using periodic boundaries. A good rule of thumb that may be used when selecting a number of particles in a simulation (or the size) of measurement volume is that at least 5000 particles are required for each significant size fraction (i.e., the fraction that would be retained on a single sieve for a real granulometric analysis).

The calculation of strains is relatively straightforward, particularly for simulations considering laboratory element tests. The reason for this is that strains can be calculated in the same way as in physical experiments

as a function of sample size and boundary displacements. DEM, however, enables to calculate local strains, and these may include variables such as individual particle rotations (e.g., Bagi, 2006; O'Sullivan, Bray, & Li, 2003). Despite this, the most common use of stress/strain calculations in DEM analysis is simply to enable comparison with physical experiments and continuum approaches in which the common stress and strain tensors are used.

Micro-scale variables

The biggest benefit of DEM analysis with respect to other experimental and numerical approaches is that it enables to quantify particle-scale interactions. In that regard, the use of coordination numbers is widespread. In its easiest form, the coordination number (Z) is defined as:

$$Z = (2N_c/N_p)$$

where N_c is the number of contacts and N_p is the number of particles. It represents the average number of interparticle contacts per particle. As such, it is used as a frame of reference characterizing the initial state of particulate assemblies. While its value is dependent on stress level, particle shape, and size distribution, it is normally expected for it to be larger in dense specimens than in loose specimens. Note that alternative definitions of Z may exist. For example, Thornton (2000) defined the mechanical coordination number that considers only the particles with more than one interparticle contact. The rationale behind this definition is that particles with less than two contacts would not contribute significantly to stress transmission within a granular assembly. Of particular interest in geomechanics is that researchers consistently report that coordination numbers are constant at the critical state.

A significant contribution of DEM analyses is the fact that the mechanical behavior of granular materials is intimately linked to their fabric evolution (i.e., the geometry and magnitude of interparticle forces). In fact, various fabric-stress-strain relationships have been proposed (e.g., Kruyt & Rothenburgh, 2019; Li & Yu, 2013). Fabric analysis is complex and varied. Possibly, there are as many definitions of the fabric tensor as there are researchers discussing and using it. However, the shared aim of all the existing approaches is that of quantifying the evolution of interparticle forces to aid the analysis of DEM simulations and to gain further insight into the particle-scale interactions that underlie the observed macro-scale response.

When considering assemblies of spheres, the fabric tensor is normally quantified by separating the individual (Cartesian) components of the branch vectors (i.e., vectors that join the centroids of particles in contact.

Once again, definitions may vary, but commonly a second-order tensor is formulated from which three principal values and their orientation can be calculated. The advantage of this approach is that fabric parameters can be made analogous to stress parameters. In other words, in the same way, that mean effective stress, deviatoric stress, principal stresses, and their orientation can be defined from the stress tensor, then mean fabric, deviatoric fabric, principal values of fabric, and their orientation can also be defined. This approach is particularly helpful to understand the effects of fabric anisotropy (e.g., Barreto & O'Sullivan, 2012) and the response of granular materials under generalized stress conditions.

Another approach that is commonly used is that of fitting Fourier coefficients to the statistical distribution of contact forces in perpendicular planes as proposed by Rothenburgh and Bathurst (1989) and described in detail by Barreto, O'Sullivan, and Zdravkovic (2007). This approach takes advantage of the 2D nature of the corresponding projections of the contact forces on each of the perpendicular planes, and it is particularly useful when analyzing axi-symmetric DEM simulations.

Apart from different definitions for the fabric tensor, different data may be used during fabric analysis. For example, the fabric tensor may be calculated considering all interparticle forces or only those with a magnitude equal or greater to the average contact force magnitude (i.e., strong fabric). It is important to highlight that is also widely accepted that fabric tends toward a critical state, and this has enhanced our current understanding of soil mechanics.

Simulation of realistic soil behavior

It was discussed that using DEM it is possible to replicate particle shapes in an accurate manner. This is a significant step toward realistic numerical simulations. The consideration of particle roughness, particle crushing, mineral dissolution, fluid coupling, and the modeling of clay particle interactions and contact laws are other significant aspects where significant progress has been made in recent years. Some of these advances are briefly discussed in this section.

With the advance of imaging and experimental techniques, it has been possible to characterize the surface characteristics of individual soil particles in a better way. The key parameters considered here are the interparticle friction and surface roughness. Existing experimental research demonstrates that the coefficient of interparticle friction in most common soils varies in a limited range (0.1–0.3 approximately, but this varies among information sources). This is, however, in contrast to the most common value coefficient of interparticle friction used in DEM simulations which is 0.5. In this regard, it is important to highlight that the choice of interparticle friction coefficient has a significant influence on the

response of granular materials. Not just on the initial density, as discussed before and the angle of shearing resistance as demonstrated by multiple researchers. The mechanism of interparticle interaction is also highly dependent on this value. Huang, Hanley, O'Sullivan, and Kwok (2014) highlighted that there is a transition from sliding to rolling behavior at the contact points as friction increases. Surface roughness is a highly debated subject. Here, it is sufficient to state that Otsubo, O'Sullivan, Hanley, and Sim (2016) implemented a DEM contact model that captures the influence of surface roughness while demonstrating that it is fundamental to adequately simulate geotechnical behavior at small strains.

The crushing of individual particles of silica sand at high stresses and/or carbonate sand at moderate stresses is a distinctive feature of the behavior of coarse-grained soils. Several relatively simple approaches have been proposed in the past. Cheng, Bolton, and Nakata (2004) used a statistically flawed sphere clump to accurately replicate crushing effects. Similar approaches have been used recently (e.g., Ciantia, Arroyo, Calvetti, & Gens, 2015; de Bono & McDowell, 2018) with success. A particular consideration is, however, that mass may not be conserved in these simulations even though it does not necessarily affect the observed response. These approaches are specifically used for DEM simulations of spheres and/or sphere clumps. For consideration of both particle shape and crushing effects, the use of more advanced (and computationally expensive) approaches is required. Examples where this is possible include the use of combined DEM-FEM approaches (i.e., Munjiza, 2004). The work by Zhu and Zhao (2019) demonstrates an approach with a significant potential that considers a particulate approach, but not strictly the DEM approach discussed here.

The possibility of dynamically changing the particle size of individual sizes is also a simple way to model complex geotechnical behavior. Using this approach, Bym, Marketos, Burland, and O'Sullivan (2015) successfully modeled ground response due to tunneling using 2D DEM simulations. Such approaches can also be used to simulate the effects of mineral dissolution (e.g., McDougall, Kelly, & Barreto, 2013). Note, however, that these studies are limited to the simulation of circular or spherical particles and do not consider any form of particle-fluid interaction.

Another aspect that is necessary to replicate real soil behavior is solid-fluid interactions. Most commonly, DEM research has focused on saturated and/or dry granular materials. Since stress transmission is via interparticle contacts and governed by the principle of effective stress, simulation of fluid is not strictly necessary for many DEM simulations. In the case of some undrained stress paths, the undrained response can be interpreted by performing simulations of (dry) spheres under constant volume conditions. Similarly, the behavior of unsaturated soil can be modeled with success, particularly if behavior between particles

is governed by the presence of liquid bridges (i.e., the pendular regime). This is possible by introducing long-range particle interactions that depend on the liquid volume or suction value at the contact as discussed in detail by Zhao et al. (2020). Despite these simplified approaches, modeling of solid-fluid interactions in DEM is possible. However, approaches vary and are still very computationally expensive. Some possibilities include the use of CFD-DEM coupling (e.g., Kloss, Goniva, Hager, Amberger, & Pirker, 2012), LBM-DEM coupling approaches (e.g., Han & Cundall, 2012), and SPH-DEM approaches (e.g., Wu, Yang, & Wright, 2016), among others.

An important aspect where some recent advances have been made is on the ability of DEM to simulate clay behavior. Progress in this area has been the result of advances in experimental techniques, the accurate modeling of particle shape, and the wider ability of high-performance computing clusters worldwide. It is however the area that may be considered to still be on its infancy compared to progress in other areas. It is however the focus in many research groups around the world, and the work by Pagano, Magnanimo, Weinhart, and Tarantino (2020) is a good starting point for readers interested in this area.

For the sake of simplicity, most of the discussion above has been limited to DEM simulations of geotechnical laboratory element tests. It is, however, important to highlight that DEM can be used for any boundary-value problem. However, if that is the case, then simplifications are still unavoidable. In fact, even considering element tests, research examples that demonstrate realistic DEM simulation including particle shape, roughness, crushing, and fluid coupling are very limited. There are inherent difficulties that are not only related to computational cost. For example, drag coefficients used in CFD-DEM simulations normally refer to spherical particles. Progress is of course ongoing, but as geotechnical practitioners/researchers, it is always important to be able to focus on the DEM capabilities that are required to analyze/understand the problem at hand.

Simulation advice

The previous sections have attempted to describe the algorithm and the main features and possibilities for DEM simulations, while for simplicity trying to avoid detailed explanations, equations, etc. Such an approach aims to provide a starting point for researchers and/or practitioners who may have the tools and/or background to use this fantastic tool, but that have not done it in the past. As such it is thought appropriate to list some general advice for those readers with limited or no prior DEM experience. The list includes comments from software selection to practical issues, which are important and rarely discussed in the existing literature.

Software selection and its validation

There is a wide selection of software and/or codes available to perform DEM simulations. Listing and describing the capabilities, limitations, and costs of each possibility, is out of scope here. Instead, discussion is focused on important aspects that may influence your selection. Cost is of course the first consideration. Currently, anyone interested in DEM simulation is spoilt for choice in terms of commercial and/or open-source software. Therefore, considerations refer to the programming language used for simulations, documentation quality and support, ease of software modification/update/control, among others.

Existing DEM software may be written using several computer languages that include FORTRAN, C++, MATLAB, among others. Some of them provide control interfaces using other interpreted languages such as Python. Knowledge of the corresponding programming language is of course beneficial if you are likely to require modification for the implementation of new contact laws, boundary conditions, etc. If that is the case, having a detailed documentation is fundamental to have a firm understanding of how the specific implementation works and even to be able to compile and maintain your versions as they are changed and/or updated. To that extent, the support of the software developers might be key. But perhaps the most important consideration when selecting a DEM program is your own ability to validate the results it produces. It will not only test your own ability to operate the program. You need the reliability of knowing that calculations are made appropriately. Some existing codes provide validation examples, whereas others do not. A good starting point is being able to reproduce the behavior of a single particle resting on a horizontal plane under gravity because its behavior can be contrasted against existing analytical solutions for a single degree of freedom system. Similarly, the rolling of a cylinder along an inclined plane enables to test the implementation of the shear/tangential force calculation (e.g., Ke & Bray, 1995). The replication of the stress ratios at failure for Face-Centred-Cubic assemblies of spheres developed by Thornton (1979) can be used to validate simulation results using both rigid and periodic boundaries and are a good opportunity to gain experience developing servo-controls as required for simulations of triaxial compression.

DEM specimen preparation and input parameters

This stage is one of the most time-consuming parts of a DEM study. It takes significant time, and it increases not just with the number of particles included, but also with the contact detection algorithms required, the complexity of the contact models, etc. The first concern is probably an adequate number of particles. As discussed before, this depends on the

particle size distribution and the boundary type. But some simplifications may be used. For example, many researchers ignore the largest and smallest particle sizes of real PSD because, in doing so, a significant reduction in the number of particles can be achieved. Particle size and density scaling are both commonly used approaches to accelerate simulations. Always consider, however, if these simplifications will affect your results. Sensitivity analyses may be required.

Considering particle crushing with sphere assemblies increases the number of particles required, and it may further increase as particles crush. A comminution limit may also be required. While you may vary the coefficient of interparticle friction to achieve different initial densities, the adequate value that is required for the simulation is significantly important. Experimental validation and calibration of other input parameters may be required, particularly with more complex contact laws, for example, those for cemented soils. Engineering judgment and perhaps (more) sensitivity analyses are warranted.

Particle shape, rolling friction? This is a common issue. It is well known that particle shape affects particle rotation. Consequently, some existing research incorporates rolling friction in the DEM contact laws or uses this fact to justify the use of higher values of the coefficient of interparticle friction. This is generally an arbitrary decision that may not adequately replicate soil behavior. Recent research does not recommend the use of rolling friction or high interparticle friction because of the transition between sliding and rolling discussed above.

The most commonly used contact models are linear elastic or Hertzian-based. When using linear elastic models, a ratio of tangential to normal contact stiffness between 0.66 and 1.0 needs to be guaranteed to ensure realistic soil behavior. When using Hertzian models, particle characteristics can be easily measured experimentally (e.g., stiffness modulus and Poisson's ratio). If more advanced contact models are used, calibration may be necessary. In such a case, it is always useful to consider the range of values that are possible for each of the input parameters. This is important because ultimately the same macro-scale response can be obtained with multiple combinations of input parameters. A good approach is to calibrate the response of the material using more than a single stress path (e.g., use triaxial compression and extension tests to calibrate the input parameters).

Finally, it has been discussed that 2D simulations are easy to visualize, unlike 3D simulations. It is, however, well recognized that the material of 2D specimens is not realistic due to the lack of interparticle contacts in the out-of-plane direction. While 2D simulations may be useful to demonstrate implementation details for a new contact model or simulation procedure, their use to analyze real granular material response is definitely not recommended by any experienced DEM researcher.

Simulation control

During specimen preparation, it is necessary to guarantee that the particles have reached a state of equilibrium. Approaches to verify these are generally subjective and include the magnitude of the kinetic energy, the amount of variation of a certain micro-scale parameter (i.e., coordination number), and unbalanced force ratios, among others. Whatever the approach used, it is often convenient to perform (yet another) a parametric study to guarantee that the simulation results are not affected.

In most geotechnical simulations, the quasi-staticity needs to be guaranteed. This is done by performing the simulation using a strain rate, which is suitably low. While empirical criteria such as the inertial numbers (e.g., Lopera Perez, Kwok, O'Sullivan, Huang, & Hanley, 2016) may be used to select the adequate strain rate, these are based (generally) on results of DEM simulations of relatively uniformly sized specimens. Therefore, subsequent parametric studies may be required.

The time-step of every DEM simulation needs to be significantly small to ensure the numerical stability of the finite difference integration scheme. Most codes use an approach based either on the response of a single degree of freedom system or on the speed of transmission of Rayleigh waves through elastic media. Both of these approaches are valid, but it is always recommended to further reduce the value of time-step, particularly when wide particle size distributions are simulated.

For simulations in which a servo-control algorithm is used, the selection of gain parameters may be required, and a trial-and-error process is often required. It is therefore required to always monitor/inspect that the value of stress/required is achieved as expected. This inspection may also require varying the output interval for data to something more frequent before the final choice of gain parameters is made. Note that stress control with servo-control is easier as the simulation progresses, and hence, adequate control needs to be ensured particularly at small strains.

When simulating granular materials using DEM, one of the main assumptions is that particles are allowed to overlap to account for (some) particle deformability. This, however, should be strictly limited and monitored during the simulation. A maximum overlap of between 1% and 5% of the particle radius is often cited.

Damping should be carefully considered. While using a high value of damping might help to reduce the time required for specimen preparation, small values of damping should be used. The reason for this is that the majority of the energy dissipation in granular materials should occur via friction, heat generation, etc. All of these damping mechanisms are generally incorporated by the contact model when using the correct value of interparticle friction. Furthermore, identifying the response of an overdamped DEM specimen may not be straightforward.

Discussion and conclusions

This chapter has briefly discussed the DEM for the simulation of geotechnical behavior. While the coverage of topics is extensive, the depth is limited. The demonstration of equations and specific simulation results and/or analysis examples are purposely avoided with the aim of increasing an understanding of the method's capabilities. Extensive references that do include implementation details and analysis are provided. It is expected that any interested readers have the necessary background to refer to those information sources if so required. The reason for doing so is that in the existing literature, there is extensive detail. Unsurprisingly, DEM is one of the most cited numerical methods in recent scientific literature. There are also several textbook type sources. However, this is the first one to briefly describe DEM for somebody with no experience and perhaps not necessarily interested on coding his/her own code or modifying an existing one and maybe just aiming to understand the basics and go ahead with their attempt to perform a DEM simulation and being aware of the possible pitfalls that are only gained with years of experience and which may not be specifically discussed in the existing literature.

The initial sections of the article were dedicated to describe the DEM algorithm and the most common analyses that are performed. With this basic background, the steps required to simulate realistic soil behavior were discussed. Finally, in the later sections, some practical advice to consider when performing DEM simulations for somebody with limited experience was listed.

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