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A Review on the Discrete Element Modeling of Dynamic Laboratory Tests for Liquefaction Assessment

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ABSTRACT

The purpose of this review paper is to present different techniques used in geotechnics for numerical modeling, recent advances and laboratory testing and gap areas in numerical modeling of dynamic laboratory tests. Numerical modeling of laboratory tests is essential for understanding the basic processes occurring in soil during dynamic loading. The review begins by explaining the discrete nature of soil and difficulties when attempting to model their inherent characteristics, different continuum and discontinuum methods available with detailed review on discrete element method. The significance of laboratory testing, drawbacks and the essence of numerical modeling of laboratory testing are discussed. The different types of dynamic laboratory tests for high strain conditions each (cyclic triaxial, torsional shear and cyclic shear test) are outlined, together with a discussion on how to obtain the necessary parameters for the models. The states-of-the-art associated with 2D and 3D numerical modeling of these tests is presented in detail. Finally, the outstanding issues in the subject are listed and the research gaps in the topic were highlighted.

KEYWORDS: liquefaction, discrete element method, cyclic triaxial, cyclic shear, torsional shear etc.

INTRODUCTION

Granular materials such as soils are highly non-linear and their response is to be recorded at multiple scales (temporal and spatial) to understand the inherent behaviour and their interactions. Usual state of granular systems is metastable state which is far from equilibrium. They can be activated with vibrations, shear, external volume forces (such as gravity, electric and magnetic fields), and motion of the interstitial fluid or gas (e.g. water or air). Such driving forces can induce transitions between solid and fluid. By nature, the length scales involved in these contact interactions are much smaller than the particle size. External loading leads to particle deformations as well as particle rearrangements.

In geomechanics, soils such as gravel, sand or non-plastic silts that have zero cohesive strength are granular in nature and are called as ‘granular soils’. The overall behaviour of the soil composite is significantly influenced by the material parameters such as stiffness of the particle, nature of fluid filling the voids, grain geometry etc. For example, in dry sand only repulsive forces exist between the particles whereas, in wet sand, both adhesive and cohesive forces act. Granular soils can wither flow or maintain an inclined surface and form a pile in a specific state. When this state is disturbed by any external force, it may lead to disaster situations such as avalanches/landslides, cyclic mobility, flow liquefaction etc. Liquefaction damage during earthquakes can be prevented if the performance of liquefiable soils and its interaction with structure can be predicted beforehand. Even though there was significant development in the field of testing (Centrifuge and 1-g testing) phenomena such as liquefaction are dictated by micro-level mechanisms.

The scale at which uncertainties and deformations occur in granular materials is significant to model them. Analytical methods consist of assumptions such as elasticity, isotropy, homogeneity, time independency etc which are not true in reality, especially when considering granular materials. Analytical methods are useful in geomechanics to provide results with limited effort and identify the variables the affect the problem solution. Numerical simulations facilitate the study of phenomena which cannot be predicted by analytical methods, and inaccessible to experiments. To understand the micromechanical interactions that cause the failure in granular materials like soils, one needs to take the aid of numerical simulations.

DISCRETE ELEMENT MODELING

Most of the numerical methods can be divided into macro-scale continuum framework and micro-scale discontinuum. These can be further categorized as mesh or gird-based and meshless methods (Figure 1). Mesh based continuum methods are Finite Element Method (FEM), Finite Difference Method (FDM) and Boundary Element Method (BEM). Recently, meshless /mesh-free/element-free continuum methods were also developed (ex: smooth particle hydrodynamics (Monaghna, 1988; Randles and Libersky, 1996), Diffuse element method (Nayroles et al. (1992), Element-free Galerkin method(EFG) (Belytschko et al., 1994), Finite point method (Oňate et al., 1996; Sulsky and Schreyer, 1996), Natural element method (NEM) (Sukumar et al.,1998) etc . Apart from the above methods, hybrid continuum/discontinuum methods are available: hybrid FEM/BEM, hybrid DEM/DEM, hybrid FEM/DEM, Applied Element Method (AEM) etc. The drawbacks of continuum based methods are that, they are incapable of simulating large deformation problems mostly encountered in geotechnical engineering. The instability is termed as ‘element locking’ caused due to distortion of the mesh. The interpolation functions used in these methods predict the accurate solution when the meshes are of regular shapes. However, this limitation can be overcome by using adaptive re-meshing (Khoei and Lewis, 1999). Also, fragmentation and flow of material cannot be modelled during large fractures in 3D.

Discrete Element Method (DEM) and Discrete Fracture Network (DFN) method, Discontinuous Deformation Analysis (DDA) are the popular discontinuum methods being employed. In all the numerical methods the difficulty arises from the conceptualization of the physical process. Selection and application of each method depends on the type and importance of the problem. The relevance of a method to specific problem depends on the size, scale and discontinuities involved. A suitable simulation method considers all the factors related to both the force and geometry. In the case of granular soils, it is straight forward to treat them as discrete models due to their discontinuous nature.

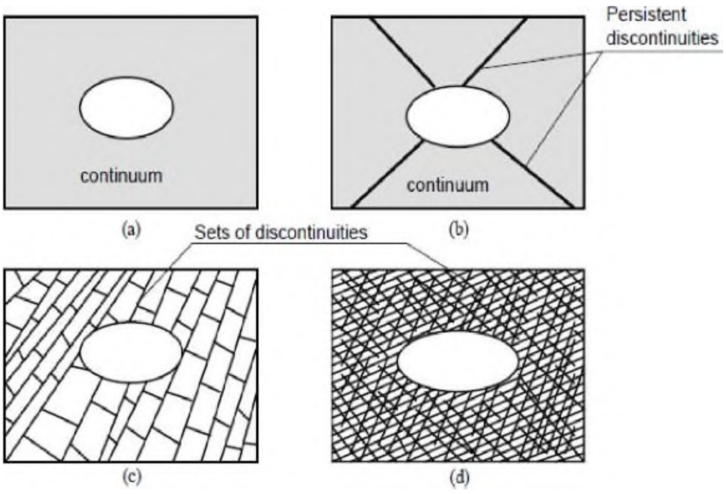


Figure 1: Selection of different numerical methods (a) continuum method, (b) continuum with fracture element or discrete method, (c) discrete model and (d) continuum method with equivalent properties (Jing, 2003)

The most notable method of all the discontinuum methods is the Discrete Element Method (DEM) proposed by Cundall and Strack (1979) first formulated by Cundall (1971) for application in Rock Mechanics. In the discrete element method, deformation between the contacts between the components of a considered system evolve continuously rather than being constant like in the case of continuum methods (Figure 2). Instead of grids, DEM tracks a set of particles modelled, at regular intervals of critical time (calculated from the material properties). The application of DEM is diverse and phenomenal in the fields of geotechnics, powder technology(Moakher et al.,2000; Cleary, 2004,2008; Cleary and Sawley, 1999; Rajamani et al., 2000; Bertrand et al., 2003; Stewart et al., 2001; Szépvölgyi and Endoh, 2001), mining, metallurgy, pharmacy, agriculture, space research (moon and Marxian regolith), structural analysis, rock mechanics, fluid mechanics, energy production, computer animation, materials (concrete engineering, rock mechanics, soil dynamics), multi-body systems, robot simulation, social simulation, plant sciences and zoology. Such varied applications of DEM are due to the modeling capabilities provided by the method. The real material properties such as particle morphology (shape, size, surface), joints, cementation, orientation and state can be exactly represented while using this method. Based on the particle shape considered, DEM can be categorized as particulate DEM and block DEM.

Cundall (1988) defined DEM as the method that:

- Allows finite displacements and rotations of discrete bodies, including detachment between bodies
- Which automatically recognizes the new contacts between particles including the contacts

Also a DEM must address three main issues (Cundall and Hart, 1992) i.e, Contact representation, solid material representation and detection and revision of contacts during execution.

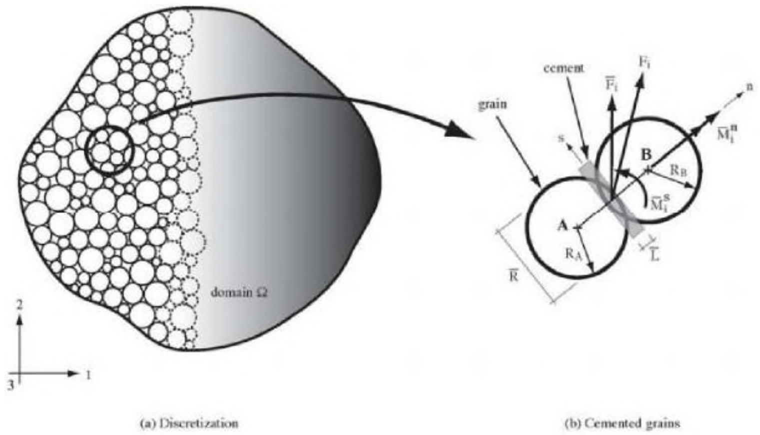


Figure 2 : Particulate DEM model (Bobet, 2009)

In Discrete Element Method the behaviour of the system is simulated using particles which are rigid. It is an assemblage of particles that interact with each other at the specified contact point. The DEM methods used in geotechnics can be classified as smooth contact approach or non-smooth contact/hard contact approach. Different time integrators are used for these methods namely: event driven method (EDM)/contact dynamics (CD) (Luding et al., 1996), molecular dynamics method (MD) (Moreau, 1994; Jean, 1995). EDM considers only one particle at a time while the collision occurs and post-collision velocities and acceleration are identified using a collision operator (Walton and Braun, 1986). Unlike EDM, molecular dynamics considers multiple contacts and is more suitable for systems like geomaterials. In molecular dynamics the interaction force is dependent on the overlapping area.

In the classical discrete element method, the computations are governed by two laws: Newton's second law of motion and force displacement law. The contacts of each particle are detected and using the relative position of each particle, from the force displacement law, the contact forces acting on each particle are evaluated. Solving the set of equations takes very small computer time and also the information to be stored occupied a very less space. Nevertheless, the time taken for detection of contact type (edge-edge, face-face and edge-face) and type of bond is significant of the algorithm during execution. Various approaches are proposed to identify the contacts such as global search algorithm, contact or field zone, binary tree structures, buffer zone definition, space decomposition, altering digital tree etc (Dowding et al., 1983; Cundall, 1988; Ghaboussi and Barbosa, 1990; O'Conner and Dowding, 1992; Hocking, 1992). Later, the law of motion is used to calculate the acceleration and moment acting on the particle and is integrated to obtain particle velocity. The execution of both the equations constitutes a calculation cycle. The particle velocities and positions are updated by using different integration methods such as leap-frog integration, Verlet integration, Beeman's algorithm etc.

The force-displacement law is based on the contact model adopted and it can vary from linear to non-linear (Hertz-Mindlin). Even if a linear model is adopted the results are productive compared to the continuum methods, as the equations are solved at particle level (Figure 3). The contact laws of a constitutive model can vary from the most simple linear contact law to a non-linear law. To attain a more realistic behaviour of material, selections of a suitable model is necessary. Before applying the actual simulation to complex models, the parameters in the contact models are obtained by running model tests.

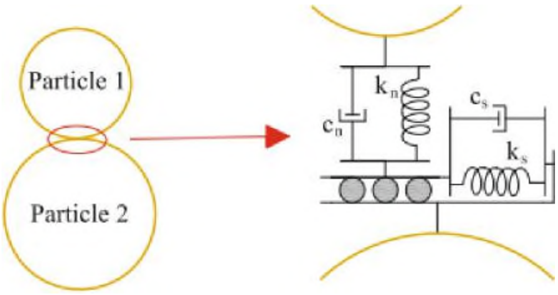


Figure 3: Schematic of the constitutive law of normal and shear contact forces between two particles (Zamani and El Shamy, 2011)

The realism of DEM simulations is fully dependent on the underlying model of the interactions. So in addition to the basic laws previously described, several authors have introduced more complex interaction laws to model hysteretic damping (Walton and Braun, 1986), adhesion (Thornton and Yin,1991), cementation (Potyondy and Cundall, 2004), rolling resistance (Iwashita and Oda, 1998; Jiang et al., 2005), time dependent response (Burger's model).

Even though the equations of motion are standard and their integration is well documented, we present these developments here for completeness of presentation. The force-displacement law gives the relation between the force acting on a particle (F_i), particle stiffness $_{(k_i)}$ and displacement (δ_i). The suffix 'i' indicates the contact point number. The formulation is also termed as 'smooth contact method'. When two particles (A and B) are in contact at a point x_i, the force acting on a particle acts along a plane perpendicular to the contact represented by a unit normal n_i. The normal is directed along the line segment joining the centre of A and B. Also, the contact point lies within the infinitesimal overlapping volume of the particles. Translations and rotations can be converted into resultant forces by multiplying with the corresponding stiffness. Resultant moments (M_i) caused by the normal and shear forces can be calculated using Eq.1. The summation of all the forces and moments on each contact point of the particle gives the resultant force on a particle.

The moments due to the eccentricity of the normal and shear contact force is exerted on the centroid of particle and is calculated by . From the resultant force and moments acting on each particle, the acceleration and velocity of each particle can be calculated using Newton's law. The time integration of these velocities gives the resultant displacement of the particle i.e., the new position by using the mid interval values.

The time step for each cycle is calculated from the critical time step for numerical stability. The critical time step given by Hart et al., (1988) is given in Eq.1

$$\Delta t_{crit} = k\sqrt{\frac{m_{min}}{2K_{max}}} \tag{1}$$

where, $_{mmin}$ is the smallest mass of the element/sphere, $_{Kmax}$ is the largest normal/shear stiffness and k is the factor that takes into account that the element may be in contact with more than one element. A value of 0.1 is suggested by Hart et al. (1988).

DYNAMIC LABORATORY TESTS

The nature of dynamic loads on the granular material influences its response. The response is controlled by the mechanical properties of the material, in this case granular soils. Soil consists of skeleton of soil grains which are in frictional contact with each other and form an open/closely packed structure. The soil skeleton forms an interstitial system connecting spaces or pores. These pores consist of some water and the flow of water in the pores can be restricted by the size of the pores and degree of saturation. The time dependent flow of water in the soil under applied load is termed as 'consolidation' –when the water flows out of loaded zone and 'swelling'-when the water flows into unloaded zone. By this means, the total stress is transferred from pore pressure to structural loading of the soil skeleton measured by effective stress. The effective stress controls the deformation of soils and results in short term (undrained strength) or long term stability (drained strength) in soils. The maximum capacity of a soil skeleton is termed as 'shear strength' because soil fails in shear.

The deformability of the soil skeleton is measured by moduli of deformation: Young's modulus (E), Poisson's ratio (υ) and shear modulus (G). Engineering behaviour and key properties of soil strength and stiffness are governed by the size and size distribution of particle and their densities of packing. It is therefore, the structure of geo-materials that controls the engineering behaviour of the ground during dynamic loading. Low strain phenomena and wave propagation in soil are influenced by parameters such as stiffness, damping, Poisson's ratio and density of soil. Stiffness and damping are the major parameters that not only influence the cyclic characteristics of soil at low strains but also at intermediate and high strains due to the nonlinearity of soil. At high strains, influence of the number of cycles of loading on shear strength and volume changes are also important. Phenomena such as liquefaction are caused by the reduction in void space during dynamic shaking that leads to the build-up in pore water pressure. It is also associated with stiffness degradation and loss of inter particle contacts. The level of shaking-induced shear strains and associated volumetric strains play a major role in the onset of liquefaction and the rate of pore-pressure build up.

The measurement of these important soil properties can be done by either field or laboratory testing. Field tests can be performed in-situ, in the existing state of the soil rather they do not allow the effect of conditions other than in situ to be investigated easily. Also, the pore water drainage to be controlled. In many field tests, the soil property required is not measured directly but from theoretical analysis or from empirical relationships (Kramer, 1996). In contrast to the field tests that are performed in infinite space, laboratory tests are performed on small specimens that are tested as elements. Elements as per Kramer (1996) are defined as those subjected to uniform initial stresses and uniform changes in stress or strain conditions.

To evaluate these mechanical properties of soil under dynamic loading, various laboratory tests are conducted based on the strain range required. High strain behaviour ($>10^{-3}$) is studied using cyclic triaxial tests, cyclic direct shear cyclic torsional shear etc. Cyclic shear apparatus measures the maximum shear modulus whereas torsional shear is used for element tests and can apply rotation of principal stresses. The properties of soil are inherent and independent of the tests type whereas soil parameters are dependent on test type (e.g. undrained strength). Accuracy of a laboratory tests depends on its ability to simulate the initial conditions and loading conditions of the problem that is to be evaluated. As the rotation of principal axes, ranges of stress and strain paths cannot be represented by a single test, we require to perform different tests based on the requirement.

The drawbacks of element tests is that the results differ between tests due to the difference in soil fabric between natural and re-constituted soil specimens even when the densities and applied stresses are similar. Sample disturbance which causes the change in fabric may result in the erroneous results especially, in the case of low strain tests ($\leq 10^{-3}$). While void ratio and stress conditions can be recreated in these tests, but factors such as fabric, age, strain history etc cannot be. Sampling for the element tests is also difficult, for example, even when thin walled sampling is considered for clean sands, significant disturbance is caused (densification of loose sands and dilation of dense sands) (Marcuson et al.,1977). Laboratory tests are accompanied by the problem with system compliance (volume changes due to testing apparatus/ effect of the stiffness of drive head and apparatus base) which leads to error in pore pressure measurement and volume change. System compliance is also caused by membrane penetration in case of coarse grained soils.

In summary, though laboratory tests are very useful in simulating conditions like void ratio and stress histories, the factors (fabric, ageing, cementation etc) that are to be investigated or effect the micro structural (particle level) cannot be recorded, observed temporally in case of mechanical testing. In order to cater to these limitations, the numerical modeling of the dynamic laboratory tests needs to be employed. In this paper, the numerical modeling of three different laboratory tests are discussed which are important for high strain measurements of cyclic behaviour of soils in the laboratory namely: cyclic shear, cyclic triaxial and torsional shear test.

LIQUEFACTION MODELING

Soil is an aggregation of discrete particles and it requires to be modelled as discrete elements. Discrete element methods have the capacity to capture the mechanical interaction of discrete particles which cannot be solved by continuum based methods. From the discrete particle model of an idealized granular assembly, the motion of individual particles can be estimated. Using this method, quantification of required properties is from microscopic to macroscopic behaviour of the considered assembly. Particle interactions and overall behaviour of the system apart from internal and external physical conditions are predominantly influenced by material parameters such as the stiffness of the particles, nature of fluid filling the space between them, grain geometry (size, shape, and surface roughness). The state of the granular particles ascertains the forces acting on them. A constitutive model that considers such factors is to be postulated and used for the study. When modeling a laboratory test, it is necessary to simulate the exact boundary conditions, particle shape, particle deformation, fabric (pores and particles) etc which majorly affect the micro scale interactions.

Modeling Parameters

In any DEM simulations, we can use either rigid boundary, periodic boundary, membrane boundary and mixed boundary conditions. In the case of the dynamic laboratory tests considered in this paper, the rigid platens can be aptly simulated by using rigid boundary type. When considering a rigid boundary it can planar or curved and has not inertia force. These are similar to displacement boundary conditions in FEM. Contacts cannot develop between the rigid walls and particles when they interact. A planar rigid wall is defined by a single co-ordinate and normal vector which gives the orientation of the wall. A spherical or cylindrical wall is defined by specifying the center of symmetry and radius. The contact forces that are obtained at the particle-wall boundary is used to update the particle co-ordinates only.

Sample boundary

A periodic boundary consists of periodic cells, which are identical copies of itself. These boundaries are useful when simulation of very large assemblies of particles is required or when the granular material is infinite in extent. An advantage of periodic boundary in case of laboratory simulations is that the number of particles required for the simulation can be drastically decreased. In the case of membrane boundary, membrane the membrane that encloses the soil specimen in the case of cyclic triaxial and torsional shear test can be modeled by using either marking the boundary particles present in the specimen as a single entity or by creating a mesh around the specimen that has the membrane properties which is discussed in the latter paragraphs.

The best possible way to simulate a cyclic triaxial test and torsional shear test is to consider the platens as rigid boundary and the latex membrane as membrane boundary. The membrane is required to be simulated such that it does not impose any constraint on the lateral deformation. Instead of a membrane boundary, if a rigid boundary is used for the lateral confinement it hinders the natural development of localization and significant non-uniformity in stress applied along the boundary is evident. A membrane boundary ensure the uniform distribution of confining pressure on the two lateral sides of the specimen throughout the simulation. To model the flexible latex membrane enclosing the specimen in triaxial tests, Cui et al., (2007) (Figure 4) used Voronoi diagram. A force was applied to each of the spheres on the outside of the specimen to maintain the required confining pressure. To calculate the forces required a Voronoi diagram was constructed considering the centroids of these outer spheres. The force applied to each sphere was then equal to the product of the Voronoi cell surrounding that sphere and the required cell pressure. Wang and Yan (2011b) adopted a flexible membrane formed by a single layer of frictionless uniform spherical particles linked by strong but flexible contact bonds in a hexagonal packing geometry (Figure 5a and b). Knuth et al., (2012) simulated lattice membrane made of triangular elements scaled an order of magnitude smaller than the grains to be studied (Figure 5c). It is able to conform to the grains, but be elastic enough to move with them.

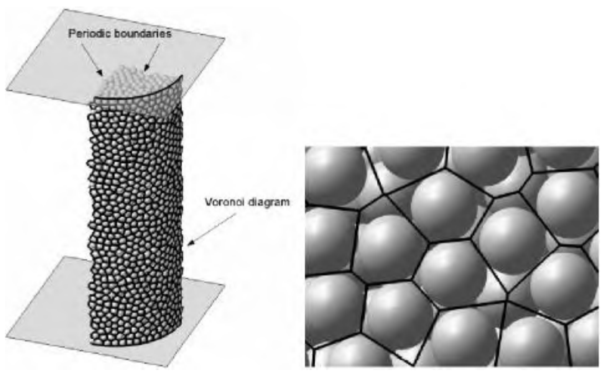
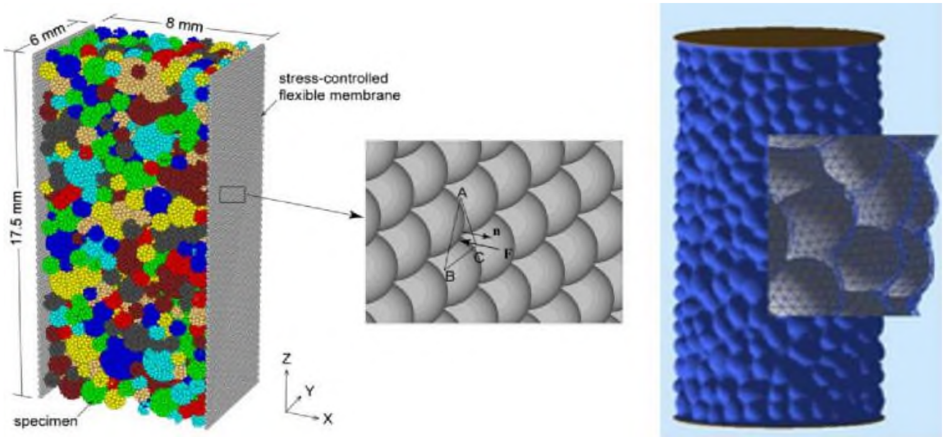


Figure 4 : DEM specimen in the simulation and subplot of Voronoi diagram (Cui et al.,2007)



(a) (b) (c)

Figure 5: Flexible boundary adopted by Wang and Yan (2011b) (a) typical specimen comprising of crushable agglomerates; (b) equivalent force applied on a unit particle triangle (c) DEM GTSC simulation the triangular lattice membrane (Knuth et al., 2012)

Particle shape

The particle deformation when two particles come into contact is represented by the particle overlap in DEM. The approach is also termed as soft sphere approach due to this. Soft spheres are sensitive to calculated overlap and hence geometry is to be accurately determined. Contact forces are very sensitive to the calculated overlap, therefore, geometry of the contact must be very accurately determined and this motivates the restriction of particle geometries to shapes that can be easily described analytically. Therefore, the accuracy of any numerical experimentation of soils is based on the representative shape selected for the analysis. Size and shape of grains represent the history of formation of soil and the macro scale behaviour is reflected by the micro scale interactions of the soil. Choice of the particle shape has to be done after assessment of the benefits and challenges involved in obtaining the specific shape. Cho et al., (2006) showed that the shaped influences the critical state friction angles, critical state line.

Based on the soil origin, different shapes can be selected, for example, for particles of fluvial origin; ellipsoidal grains can be selected while for crushed rock aggregates polyhedrons maybe used (Figure 6). Polyhedrons are mostly used in block DEM simulations to represents deformable blocks of rocks. Disks and spheres are the most common particle types considered in DEM simulations. The limitation of using such particles is the slippage factor; whereas in reality particle interlock and are crushed decreasing the shear strength. Shear strength and liquefaction characteristics of granular soil also depend on particle size, grain size distributions, shape and surface texture of the individual grains. When irregular particle shapes (such as ellipsoids, polyhedrons, ovaloids) are considered, they provide the interlocking that prevents the resistance to rotation; i.e., the normal component of contact force imparts a moment to the particles and can resists the rotation. Another drawback with using spheres or disks is that these shapes is that the rotations the particles experience is more than that in the real soil conditions under equivalent loading. This increases the angle of internal shearing resistance of spherical particles compared to angular ones.

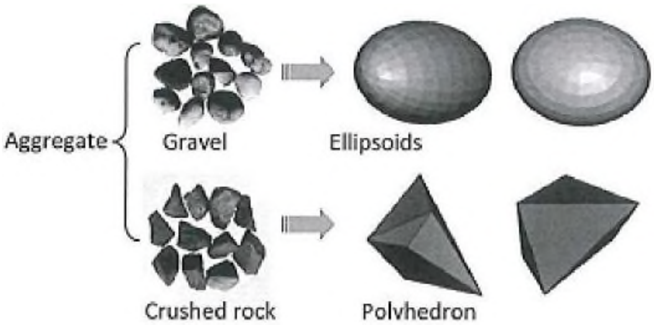


Figure 6 : Representation of gravel and crushed rock by ellipsoids and polyhedrons (He et al., 2012)

In a DEM simulation, the number of contacts is more than the number of particles and the contact resolution is more computationally expensive part of the DEM algorithm. Spheres or Disks are the most popularly used as it is easy to identify the contact and geometry of contacting point. Majority of the studies in particle shape modelling were concentrated in two dimensions. Many researchers used DEM for modelling of the particles but considering the particles as circular/spherical, elliptical, polygon, oval etc. Many programs that use spheres or discs are TRUBAL (Cundall and Strack, 1979), CONBAL (Ng, 1989; Ng and Dobry, 1991), GLUE (Bathurst and Rothenburg, 1989), DISC (Ting et al., 1989), DMC (Taylor and Preece, 1989) etc.

Crushing of particles

In general, natural material such as sand is compressible, deformable and behave plastically when expose to high strains. When, rigid incompressible rounded particles are considered, they cannot capture the plastic state behaviour, dilatancy and critical state (Robertson and Bolton, 2001). Crushing is a major contributor of strain accumulation in cyclic loading (Harireche and McDowell, 2003). So, particle crushing cannot be omitted from any DEM simulation of sand under high strains. Crushing is influenced by the particle strength, angularity, porosity, gradation, moisture content etc. the change of grain size distribution due to particle crushing may create more drastic change in internal structure than that can be achieved by particle rearrangement alone (Bolton et al., 2008). Particle breakage/crushing leads to reduction of volumetric dilation, peak stress ratio and plastic deformation mechanisms (Wang and Yan, 2011b). Particle breakage dissipates negligible amount of input energy by inter-particle friction and fabric change. At small strains particle breakage disrupts strain energy build up and at large strains when the particle breakage is stabilized, mechanical damping and steady energy dissipation are caused (Wang and Yan, 2012). Grain crushing is influenced by mineralogy type, confining pressure, mean effective stress, relative density and stress path.

Voo (2000) and McDowell (2002) showed that the Weibull statistical distribution captures the experimental variation of tensile strength of ‘silica sand’. The survival probability P_s (d) is given by the following equation (Weibull, 1951).

$$P_s(d) = \exp\left[-\left(\frac{\sigma}{\sigma_0}\right)^m\right]$$

(2)

where σ is the tensile strength of particle given by dividing the compressive force at failure with square of initial diameter of particle. σ_0 is the characteristic tensile stress corresponding to 37% survival probability. m is the Weibull modulus

Particle crushing can be performed by modeling agglomerates of micro particles and allowing for individual particles to disintegrate (Jensen et al., 2001; McDowell and Harireche, 2002; Cheng et al., 2003). The method is computationally intensive and an alternative approach can be adopted (Astrom and Herrmann, 1998; Tsoungui et al., 1999; Lang, 2002; Lobo-Guerrero and Vallejo, 2005; Lobo-Guerrero et al., 2006) in which pre-crushed particles are substituted by post fracture fragments once the crushing criterion is met. The latter method requires crushing criterion and splitting mode (to determine number of fragments). The advantage of considering the latter method is its simplicity and ease of implementation. However, it is difficult to choose the adequate number and size distribution of the fragments. The space between the fragments also represents an important loss of mass (Cantor et al., 2015). The first method represents more realistic complex shapes of crushed fragments, large quantity of grains are required and thereby involves large computational time. Also, the size of smaller grains induces the artificial scale parameter in the system.

The method proposed by Lobo-Guerrero and Vallejo (2005) may be applicable only for granular sample that is composed of uniform particles (Figure 7). As, the granular sample that consists of different sizes of particles contains larger particles that surround the small grains and so they do not allow the grains to break by providing confinement to larger ones (they produce a hydrostatic state of stress). Wang et al., (2015) introduced a particle breakage criterion for heterogeneous granular sample. For this, a parameter (B_f) that reflects the anisotropy of the normal contact force is suggested.

$$P_s(d) = \exp\left[-\left(\frac{\sigma}{\sigma_0}\right)^m\right] \tag{3}$$

where F(ϴ) is the algebraic sum of the contact forces oriented at the angular interval between ϴ and ϴ+ Aϴ

∑ F(ϴ) is the algebraic sum of all the contact forces.

In the authors paper, Aϴ was predefines to be 20°

Different correlations with soil parameters such as mean effective vertical stress and void ratios at failure were previously adopted to quantify the breakage. But a better correlation was found using the total energy input in the test for all types of soils. To develop micro-mechanics based constitutive laws in case of sands it is required to understand the energy dissipation under particle breakage.

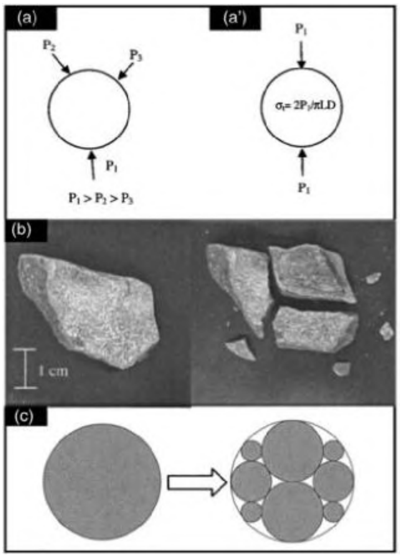


Figure 7 : Idealization of induced tensile stress, and fragments produced after tensile failure of real aggregate and idealized material (Lobo-Guerrero and Vallejo, 2005)

Fluid-Particle interaction

Response of a granular material/soil to dynamic loading is usually measured in terms of effective stresses. In DEM, effective stresses are studied by modeling the system in dry condition. In the case of liquefaction or slope stability problems, the fluid associated with the pores flow and the pressure change due to this flow results in decrease of effective stress. To understand the criteria that trigger liquefaction during earthquakes can be done by simulating the undrained laboratory tests where the change in deviatoric stress with the number of cycles is observed. Therefore, an independent solution of the response of the system in a single phase is insufficient to model such problems. Therefore, simultaneous equations of other phases of the particle void assembly are to be coupled to obtain a solution. In particulate DEM, Biot theory and Zienkiewicz and Taylor (2000) approach are used for such modeling.

When the particles are submerged in a fluid, their interactions with the fluid results in various types of forces on the particles classified as hydrostatic and hydrodynamic forces. Hydrostatic force is the buoyancy force due to the pressure gradient around the particle. Hydrodynamic forces consist of the drag force, virtual mass force and the lift force. Virtual mass force is the force required to move the liquid surrounding the particle. Lift force is caused due to particle rotation. This force is usually smaller than the drag force. Pressure gradient and drag force are the most important interaction forces that have measureable impact on the particle motion and fluid flow (O’Sullivan, 2011). Using, DEM, the particle velocities and porosity of the granular material can be known, a fluid coupling approach is required to estimate the velocity of fluid surrounding the particles. The influence of fluid on the particle motion can then be evaluated by adding a drag force to the resultant force acting on each particle.

The most popular approaches available for fluid coupling in the increasing order of the complexity of their application and computational demand are i) Constant volume assumption during undrained loading ii) Application of Darcy’s law and iii) Numerical solution of Navier-Stoke’s equation on coarse grid. These methods are applicable only for the fully saturated flow. Additional forces are required to be imparted if the soil is unsaturated or partially saturated.

Constant volume assumption is the simplest method to model the response of the particle-fluid system. The bulk modulus of the pore fluid in saturated soil subjected to undrained loading is sufficiently larger than that of the soil and this results in a constant volume deformation. This facilitates the simulation of the response of the particle-fluid system without explicit consideration of the fluid phase. This approach is limited to completely undrained condition and mostly applicable to simulate ideal situations considered in laboratory experiments.

Undrained simulations of laboratory test can be performed by employing constant volume method. The assumption of constant volume is the most suitable for laboratory testing as it aptly represents the laboratory conditions and the simulation is computationally straight forward. Undrained tests are useful to supplement the drained simulations when we accurately need to find the position of critical state line. Ng and Dobry (1994) initially used this approach for the simulation of cyclic simple shear tests. Sitharam et al., (2003, 2009) conducted undrained simulations of cyclic triaxial testing on polydisperse and monodisperse spheres in 3D. Zhou et al. (2007) applied strain controlled boundary to simulate the undrained condition in biaxial compression test. Undrained biaxial tests were conducted by Shafipour and Soroush (2008) by adopting this approach. Yimsiri and Soga (2010) conducted undrained triaxial compression tests. Yang et al. (2011) used the constant volume approach to simulate undrained triaxial shear tests.

The constant volume can be performed by using strain controlled boundary. The first step is to estimate the assembly dimensions after the consolidation i.e, after applying the initial confining pressure. If the dimensions are r_s and h_s corresponding to radius and height, the velocity for upper and lower platens are v_h , the velocity to be applied in the radial direction of the specimen is equal to:

$$v_r = -\frac{r_s}{h_s} v_h$$

(4)

The excess pore water pressure, u_g in this case can be calculated by using the following equation:

(5)

where σ’$_{3o}$ and σ’$_3$ are initial effective stress and lateral effective stress of side wall.

The drawbacks of assuming constant volume is that extremely high deviatoric stresses and pore water pressures can be generated for dense samples (these are visible in lab tests) and the results can be highly sensitive to strain rate selected. As per Hanley et al. (2013), the assumption of constant volume becomes invalid when the stresses reach the MPa range. Also, the study by these researchers suggest that for dense specimens, the DEM simulation showed that there is 30% overlap by the end of the test and a max. of 40% overlap whereas, the assumed largest overlap in the DEM which forms the basis is about 5% at the point of contact of two particles. So, while applying constant volume method, care has to be taken such that the stresses are below MPa range and the saturation is maintained at 100%.

Cyclic Triaxial Test

In cyclic triaxial testing the specimen can be exposed to high strains and tested up to failure. To numerically model the triaxial test, the major micro-mechanical parameters required are contact modulus of elasticity, contact Poisson's ratio, contact stiffness, inter-particle friction angle. Friction angle and dilatancy angle for a material level and particle level are not similar.

Global friction and dilatancy angle decrease with increase in confining pressure. To account for sand grain roughness, the spheres in numerical simulations can be modelled using contact moments. The following paragraphs consist of detailed review on the experimental and numerical cyclic laboratory testing conducted worldwide.

Sitharam (2003) to understand the effect of cyclic loading on the granular soils, conducted cyclic biaxial tests on cubic assembly in both drained and undrained conditions. The tests were conducted both on polydisperse and monodisperse particles. Micromechanical explanations of the behaviour of the disk assemblage was presented in terms of co-ordination number, force and fabric anisotropy co-efficient. The boundary type employed in this study was periodic. O'Sullivan et al., (2008) conducted strain controlled cyclic triaxial tests on a steel spheres (ideal granular material) to validate the capability of axis-symmetric DEM model using mixed boundary conditions. The experiments were conducted by considering cylindrical periodic boundary and three dimensional stress controlled membrane. This parametric study identified that under small amplitude cyclic loading (~0.1%) the fabric continues to evolve and steady state is not achieved even after 200 cycles of loading. Also, the deviator fabric is more related to the stress strain response at macro scale than with the co-ordination number.

Sitharam and Vinod (2010) simulated strain controlled cyclic triaxial tests on spherical particles to determine the influence of number of cycles, confining pressure, void ratio, gradation, initial anisotropy and stress path on the dynamic properties (G and D).

Figure **8** shows the biaxial and triaxial specimens generated by different researchers. Anitha and Sitharam (2010) conducted undrained cyclic triaxial test under axisymmetric loading conditions. The simulations considered spherical and elongated particles to understand their influence on liquefaction resistance.

Nguyen et al., (2014) conducted stress controlled cyclic triaxial test at different excitation amplitudes and frequencies is performed on these samples at different static stress states. These simulations were conducted at low strain amplitude to understand the strain accumulation using cubical sample.

When performing undrained cyclic triaxial test, liquefaction resistance of the soil can be observed and Chen and Chuang, (2001) observed that sample preparation (moist tamping, dry tamping and multiple sieving pluviation techniques) has an effect on fabric which in turn influences liquefaction resistance. From the study it was identified that moist tamped samples had the highest liquefaction resistance. Jefferies and Been (2006) also suggested the influence of fabric on cyclic soil behaviour is more pronounced than that on static behaviour.

Most of the DEM simulations done by the researchers discussed above had considered cubical/parallelopiped specimen and were either 2D simulations. Very few numerical simulations were done in 3D. Only, O'Sullivan (2008) considered cylindrical specimen which is modelled using periodic boundary. Crushing of the sand specimen at high strains has not been considered by any of them. As crushing influences the formation of shear band and deviatoric strength of the specimen, it forms a major consideration in understanding the liquefaction resistance of soil. Almost all the studies have considered spherical particles and this does not provide an accurate measure of the real soil condition.

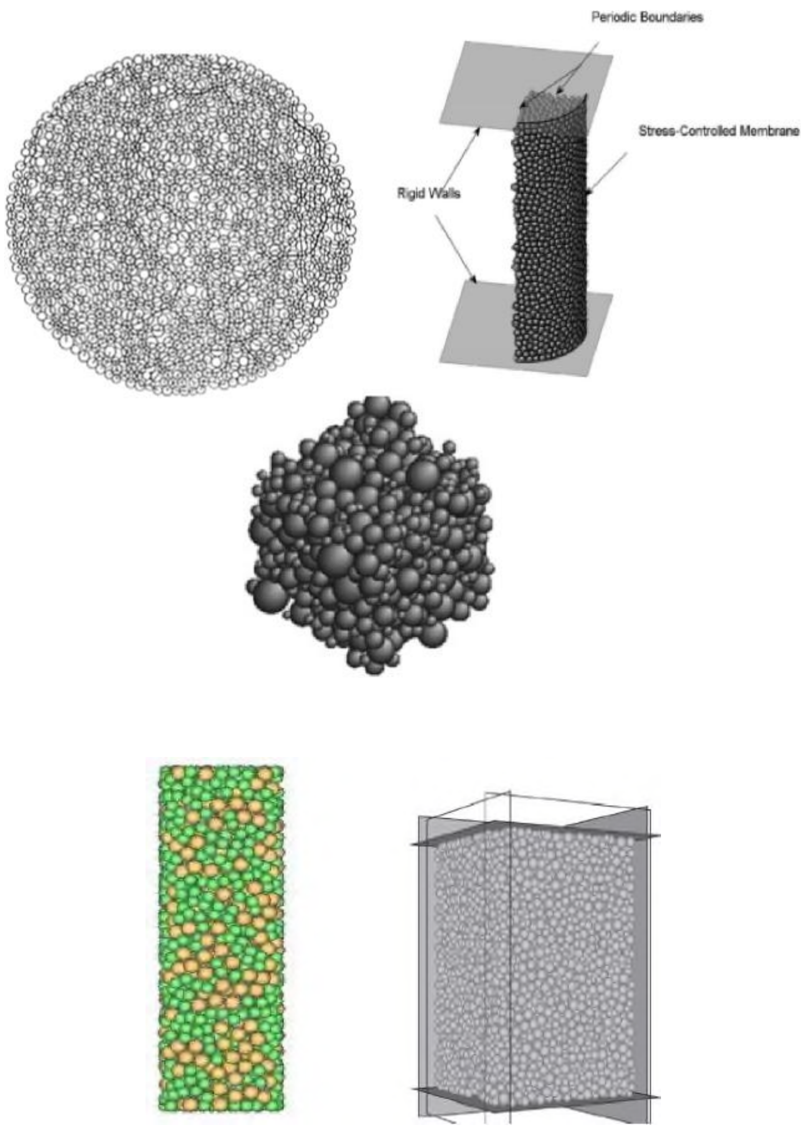


Figure 8: Biaxial and Triaxial samples generated by Sitharam (2003), O'Sullivan et al .,(2008), Sitharam and Vinod (2010), Anitha and Sitharam (2010) and Nguyen et al., (2014).

Torsional Shear Test

Torsional shear testing is used to study the monotonic and cyclic behaviour of soils. It can be employed to measure response of fine to medium geomaterials (clay, silt, sand) when subjected to strains of the range 0.01% -10%. It was initially used in 1930's (Cooling and Smith, 1936 as cited by Frost and Drnevich, 1994) and later developed in 1960s and 70s by many researchers (Drnevich, 1985; Alarcon-Guzman et al., 1986). The difference in results from different Torsional shear testing may crop up from the specimen type, specimen diameter, length-to-diameter ratio, wall thickness; applied boundary stresses method of loading and means of measuring the specimen response. In the Torsional shear tests, monotonic or cyclic loading is applied to one end of a hollow cylindrical specimen while the other end is fixed. The major advantages of torsional shear test over other test methods is that unlike ring shear and direct shear test, the specimen has no restricted deformation and can measure for large to small shear strains (unlike resonant column and cyclic triaxial which are restricted to specific strain levels). The limitation of this test is its complexity and higher cost.

A solid or hollow cylindrical specimen can be tested in a torsional shear test. When a solid specimen is used, the strain distribution is not uniform in the radial direction in the horizontal plane of the sample and this effect can be minimized by using a hollow sample. A hollow cylindrical apparatus helps to identify the extent of anisotropy as the principal stress axis rotation can be controlled. The selection of geometry for hollow cylindrical specimen for torsional shear testing influences the reduction in stress non-uniformity in stress distribution (Saada, 1988; Hight et al., 1983). The level of non-uniformity for a fixed wall thickness reduces with the increase in diameter of specimen (Porovic, 1995) as shown in Figure 9.

The frequency range tested in a torsional shear test is usually below 10Hz. Nevertheless, some apparatus are available which can be used to perform both torsional shear and resonant column tests. In case of torsional shear test, instead of determining the resonant frequency, the stress-strain hysteresis loop is determined from measuring the torque-twist response of the specimen. Shear modulus and material damping are then calculated from the stress-strain loop. Shear modulus is obtained from the slope of hysteresis loop whereas damping is measured from the area of the loop similar to a cyclic triaxial test.

The effect of initial static shear on liquefaction depends on the testing method employed (Chiaro et al., 2012). Yang and Wang (2012) dynamic torsional shear test in PFC^{3D} to investigate the effect of shear strain, loading frequency and friction on damping ratio. It was observed that damping ratio decreased as the particle friction increased.

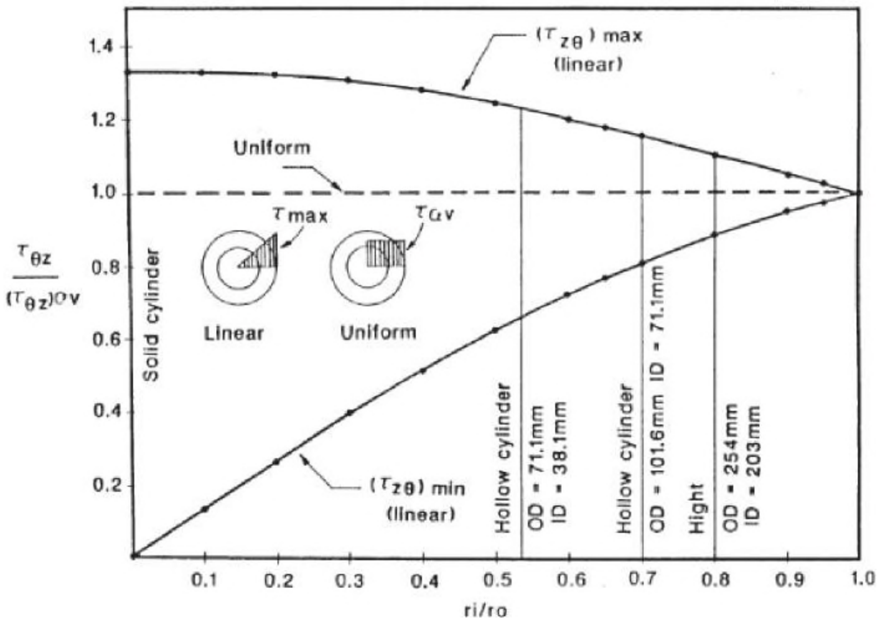


Figure 9 : Shear stress distribution in a hollow Torsional shear specimen (Porovic, 1995)

Cyclic Shear Test

Direct shear tests are famous for their simplicity and the progressive failure of the sample.
In a simple shear device, the specimen is a cylindrical sample enclosed in a wired membrane (Norwegian Geotechnical Institute) or a parallelepiped specimen enclosed between rigid platens (Cambridge Device). A simple shear device was introduced to overcome the limitation of a direct shear test which produces non uniform shear stress distribution. Cyclic simple shear device is convenient to measure the damping ratio and shear modulus of soils. The advantage of a simple shear device is that it is more representative of the field conditions as the specimens are consolidated at the K_0 state. These can be conducted over a wide range of strain which is about 10^{-2} % to 5% . The pore water pressure can be measured at the boundaries whereas this is not possible in resonant column tests. Another type of test known as simple shear is available, in which the difference is that the direction of principal stress and principle stress rotation.

The liquefaction resistance of sands was evaluated by Vaid & Sivathayalan (1996) and Riemer & Seed (1997) by comparing the dimensions and lateral boundary conditions in both cyclic triaxial and simple shear tests. They studied cylindrical specimens which have height larger than diameter with flexible boundary in triaxial tests, and flat disk-shaped specimens with rigid boundary in simple shear tests either NGI type or Cambridge type devices. It was observed that the differences of shape, dimensions and boundary conditions of specimens may affect the test results which made the exact comparison difficult and complex. Also it was observed that application of precise undrained and constant volume conditions are difficult in these simple shear apparatus because of the shorter height of the specimen and the rigid boundary confinement (Hoshono and Yoshimini, 2004). So, the numerical simulation of simple shear tests facilitates the comparison of macroscopic parameters from different tests and also prevents the constraints imposed by laboratory tests such as specimen size, sample preparation, system compliance etc.

Ng and Dobry (1994) conducted constant volume cyclic simple shear tests to simulate liquefaction in quartz spheres. The effect of inter particle friction and particle rotation on the results was also studied on both 2D and 3D specimens. Ashmawy et al. (2003) performed undrained cyclic shear simulations to assess the liquefaction susceptibility with particle of varying degree of angularity. It was observed that at maximum void ratio liquefaction susceptibility is independent of particle shape whereas it is significant for sands prepared at same void ratio (Figure 10).

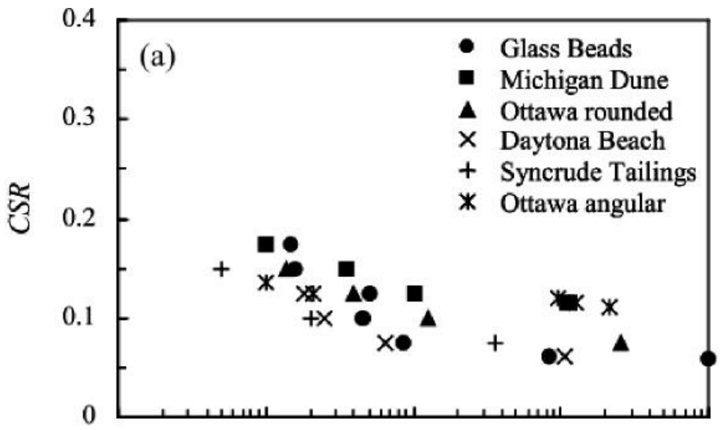


Figure 10 : Liquefaction susceptibility for different simulated soil samples (Ashmawy et al., 2003)

VALIDATION

Validation of a numerical model is necessary to prevent any hardware sensitivity errors in the simulation and to check the correct implementation of the algorithm. It can be performed analytically or experimentally. By analytically validating the code on can get the information on the performance of the model whereas experimental validation or verification confirms whether the physical material response is captured or not. Most of the previous studies (Cundall and Strack, 1979) were performed using photo elastic particles. Comparison of images of particle motion during DEM simulation and during experimental testing can be done. These methods necessitates high spatial and temporal resolution images. Also, they validate the DEM code at particle/micro scale.

When simulating the laboratory tests, the initial stage involved is the consolidation of the specimen. This is usually achieved by employing the servo control algorithm. To assess the success of the servo control algorithm, the target stress and actual stress are to be plotted as output and comparison can be made. This is suitable for the DEM simulation with rigid walls. To ensure if the forces applied along the boundaries are in equilibrium, in case of a triaxial simulation, the total force on the bottom boundary must be equal to the total force on the top boundary throughout the simulation.

The results obtained in DEM simulations are very sensitive to the initial geometry of the specimen or system to be analysed. To be as realistic as possible, the number of particles in the simulation are limited. It is also computationally intensive to exactly replicate the shape and size of the laboratory specimens in DEM. A sample in the size of mm even contains millions of particles. The response of smaller samples is more sensitive to small variations in the distribution rather than larger samples. From theoretical knowledge, it is understood that as long as the specimen slenderness ratio is maintained at 2.0 (typical geometric ratio used in the experiments), the results of the discrete model do not depend on the characteristic size of the discrete elements. Local parameters take this into account (Belheine et al.,2009).

For the validation of undrained simulations, the key characteristics of any undrained simulations that are evident during laboratory tests are to be checked for. For example, for undrained tests on sand, the denser samples dilate with a reduction in excess pore water pressure giving an increase in the mean effective stress. In case of the looser samples, a phase transformation point marking a transition from dilative to compressive behaviour is to be observed. In simple terms, the loose samples get compressed and generate positive excess pore water pressure and dense samples generate negative excess pore water pressure.

When performing tests on soils, the model can be validated for confining pressure dependent behaviour, density dependent behaviour. Deviatoric stress and volumetric strain increases with the increase in confining pressure. Dense assemblies undergo large dilation when compared to loose specimens. So, the plots for deviatoric, stress and volumetric strain are required (Figure 11). The co-ordination number change with the strains can also be tracked for differently packed samples (dense and loose).

To validate the undrained cyclic laboratory tests (for liquefaction), the build-up in excess pore water pressure and decrease in stress as the number of load cycles are progressed can be recorded. In case of the cyclic laboratory testing, evaluation of shear modulus and damping ratio at different strain ranges can be validated with the laboratory results (Figure 12).

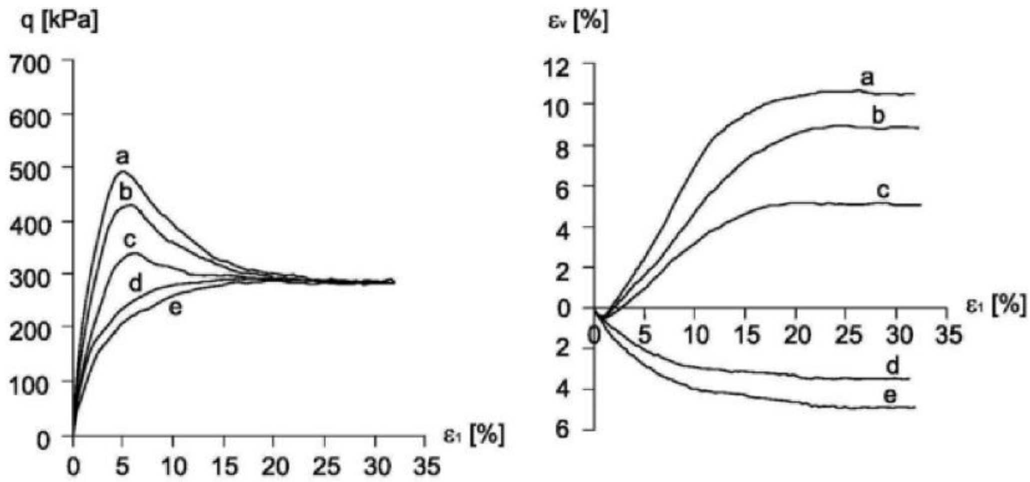


Figure 11: Discrete simulations of triaxial test for granular specimen: global deviatoric stress and volumetric strain versus axial strain for different initial void ratio e0: a) e0 = 0.50, b) e0 = 0.60, c) e0 = 0.70, d) e0 = 0.80, e) e0 = 0.90 (Ec = 30 GPa, νc = 0.3, μ = 30o, β = 0.15, η = 1.0, p = 100 kPa, d50 = 5 mm) (Widulinski et al.,2009)

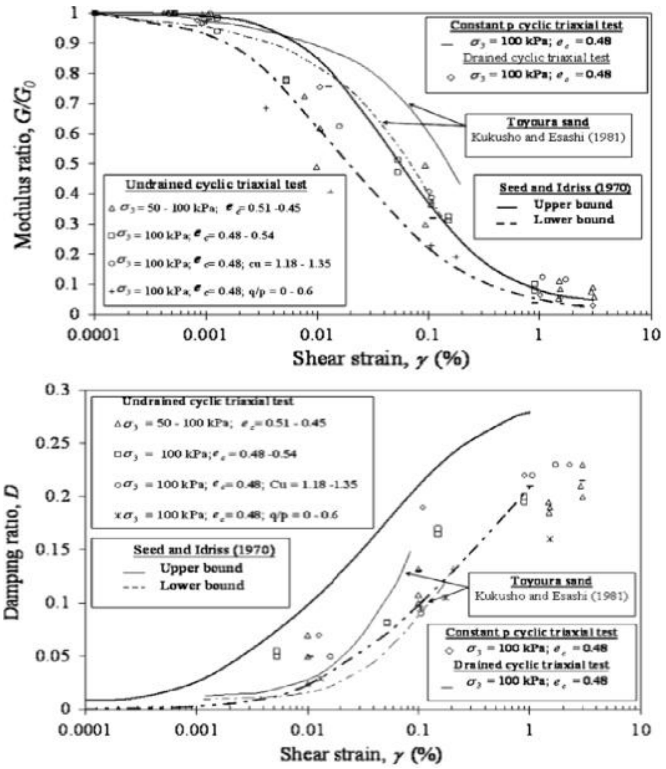


Figure 12: Comparison of shear modulus and damping ratio obtained and numerical tests with standard curves (Sitharam and Vinod, 2010)

DISCUSSION

This review began with the overview of the methods available for numerical modeling of granular materials, categorizing them into continuum, discrete-continuum and discrete methods available. The discrete element method was described in detail with the equations employed and different approaches such as soft contact and hard contact approach. The dynamic laboratory tests and their importance was discussed and the need for numerical modeling of these tests was highlighted. To understand the micro mechanical mechanisms underlying the macroscopic response of granular materials such as sands resulting in phenomena such as liquefaction, exact modeling of the boundary conditions, particle shapes, pore water pressures need to be achieved. So, different boundaries such as rigid, periodic and mixed boundaries that can be modelled in the laboratory simulations were discussed in detail. For the exact representation of the platen loading in laboratory tests, it was identified that rigid boundaries are suitable to be adopted. Though different approaches are available for the simulation of the pore pressure in the granular material testing, constant volume approach aptly represents the ideal conditions prevailing in the laboratory tests and hence, this method can be aptly applied for any such simulations. Different studies conducted on the exact representation of particle shapes were discussed. The consideration of the method of simulation of particle shapes depends on the computational cost and the scope of the study. The research studies conducted on the laboratory testing and numerical modeling of dynamic triaxial, cyclic shear and torsional shear tests were discussed in detail and the gap areas in numerical modeling of dynamic laboratory tests for liquefaction modeling can be summarized as follows.

- The simulations of 3D cyclic triaxial experiments on sand specimens are still being explored. Research gaps were observed in the consideration of the effect of particle shape and grain size distribution on the micro-mechanical response and liquefaction resistance. Particle crushing also needs to be incorporated in the future simulations to exactly capture the liquefaction phenomenon. Most of the 3D simulations were performed by simulating the rigid confinement instead of a membrane boundary. Membrane boundaries are required to be incorporated. To understand the liquefaction resistance of sand, the simulations would be performed under undrained conditions using Darcy's law and Navier-Stokes equations. Few available studies were conducted mostly using constant volume approach. Evolution of the micromechanical characteristics such as co-ordination number, contact density, contact normal, contact force etc during different stages of the respective simulations can be recorded. The dynamic soil properties i.e., Young's modulus, Shear modulus and damping ratio of specimens with different particle shapes, sizes and distribution, effect of crushing under different boundary condition can also be evaluated.
- It was identified that torsional shear and cyclic direct shear testing are still a novel technique and there is a lack of detailed numerical modeling results on torsional shear tests in either 2D or 3D. From, the numerically modelling of torsional shear and simple shear test, shear modulus and damping properties from the tests at different strain rates, confining pressure and void ratio can be estimated. The influence of cyclic strain history and fabric on the small strain modulus of sand using the micro-mechanical parameters such as co-ordination number, contact normals, contact forces etc can be assessed. To the effect of grain size distribution and particle shapes on the dynamic soil properties at different test conditions can also be studied.

The following gap areas can be considered by the reader while attempting to simulate the dynamic laboratory tests mentioned. Also, the validation for different parameters during the simulation discussed in the paper could be followed.

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