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Research Paper

Dimensionless input parameters in discrete element modeling and assessment of scaling techniques

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ABSTRACT

A set of dimensionless input parameters were defined for DEM using a characteristic time which is a function of density and elastic modulus of particles and an arbitrary characteristic length. Dimensionless strain rate and mass damping ratio are inversely proportional to the characteristic time, and stress is normalized by elastic modulus to give dimensionless stress. It was demonstrated that the response of a model in the dimensionless scale is invariant with the choice of density, elastic modulus and the characteristic length if dimensionless strain rate and mass damping ratio are kept constant. Small time step is a prohibitive aspect of DEM. Scaling techniques are widely employed to enlarge the time step. Using the dimensionless scheme, it was learned that density scaling is equivalent to the use of a higher strain rate, and stiffness scaling results in a higher strain rate and an elevated stress state in the dimensionless scale.

1. Introduction

It is necessary to select appropriate input parameters to perform a realistic simulation using Discrete Element Method (DEM) There are various parameters in discrete element modeling, e.g. density of particles, elastic modulus (or contact stiffness), particle size distribution (PSD), deformation rate, damping, and inter-particle friction coefficient. Some of the parameters are artificial and have no physical meanings such as damping and strain rate for the quasi-static analyses, while others have physical origins such as density of particles and contact stiffness. However, even the parameters with physical meanings are usually manipulated to obtain responses close to experimental results within a reasonable runtime. Limited number of guidelines for selection of the input parameters can be found in literature (e.g. [14]). To comprehend the effect of each individual parameter on the behavior of particulate models, we aimed to identify the parameters that influence the response independently. This article shows that density, contact stiffness, characteristic size of particles, applied strain rate, and damping are not independent from each other. These parameters can be related through the characteristic time and length. A set of dimensionless parameters is introduced that facilitate the study of the effect of each individual input parameter independently. The periodic boundaries, a simplified Hertz-Mindlin contact model [9], and mass damping model are adopted.

1.1. Damping

In DEM, it is inevitable to apply an artificial damping to attain the equilibrium and especially for modeling a quasi-static loading conditions. Damping has been implemented into DEM through different methods, such as viscous damping [3], local contact damping [4] and global mass damping.

Cundall and Strack [5] proposed a system of global damping in the form of mass proportional damping, which can be envisioned as the effect of dashpots connecting each particle to the ground. The amount of this damping for each particle is proportional to its mass, so called global mass damping.

Munjiza et al. [13] introduced a new class of mass proportional damping in the following form.

$$\alpha = (k/m)^n \xi \tag{1}$$

where k and m are stiffness and mass of a single (or a multi) degree of freedom system respectively, and α and ξ are damping coefficient and damping ratio, respectively. In this method n can be tuned to target a specific frequency range of vibrations.

1.2. Applied deformation rate

Static loading is of great interest in the field of geotechnical engineering. For many applications of DEM in geomechanics the objective is to simulate a static response particularly in the drained

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conditions which need greater strains to arrive the critical state. For a DEM model to approximate a response sufficiently close to the static conditions, the deformations have to be applied very slowly using a small strain rate to prevent large dynamic effects and to minimize the error. This type of loading is called quasi-static. In the quasi-static conditions, the system is not flowing and is in, or is close to, a state of static equilibrium, and it is assumed that the velocities of particles and the inertia-induced forces and moments are very small compared to the inter-particle contact forces and moments. The inertia force is represented by the out-of-balance force of each particle, which is the resultant of contact forces of a particle, and is in charge of moving the particles to the equilibrium position. By monitoring the equilibrium state of the particles, one can ensure that the unbalanced forces are relatively small, thus that the quasi-static conditions are fulfilled [8]. Hence, care must be taken in selection of the speed at which a sample is compressed or sheared.

Quantitative measures exist to assess whether the system is in equilibrium. Various dimensionless indices have been created in DEM to evaluate and monitor the equilibrium state of granular assemblies. Ng [14] defined the Unbalanced Force Ratio (UFR). This index shows magnitude of the average out-of-balance forces relative to the contact forces. A small UFR value, for example less than 1%, indicates that the quasi-static conditions are fulfilled.

1.3. Scaling techniques

There are various reasons that require DEM users to adopt small time increments such as to avoid the numerical instability encountered in explicit solutions, to capture the moments of contact formation and separation, to capture the nonlinearity of the contact model (if a nonlinear model is used), to limit the influence of the particles to the immediate neighboring particles [17], and to minimize the truncation error [3]. On the other hand, the strain rate needs to be small in quasi-static simulations to prevent from developing dynamic effects (propagation of wave through the assembly) and to maintain equilibrium conditions. The choice of a small time increment along with a small strain rate leads to excessive runtime. This encourages DEM users to artificially increase the time step to reduce the computational cost [16]. Three approaches have been used to increase the allowable time step, Density Scaling (also called mass scaling, [19]), Stiffness Scaling (e.g. [12]), and Size Scaling or Coarse Graining (e.g. [7]).

In density scaling, a higher mass value is assigned with the sole purpose of achieving quasi-static state with larger time step. For example, Thornton and Antony [20] scaled the particle density up to 10^{12} times. It is believed that a heavier mass results in less significant dynamic effects. The parametric study of Tu and Andrade [21] indicates that the density scaling method is not ideally effective in helping a discrete element model to obtain quasi-static solutions. They showed that setting the mass scale to an arbitrary large number tends to yield unrealistic results distant from the quasi-static state.

Numerous authors have used the DEM to simulate granular materials at a larger size scale (e.g. [6]). This approach is similar to the density scaling in the sense that by the increase of the characteristic length the particles' mass increase.

In contrast to particle mass and size, the critical time increment is inversely proportional to the square root of the contact stiffness. According to Malone and Xu [10], reducing the contact stiffness is another approach to increase the time step in DEM to reduce the runtime. Milburn et al. [11] mentioned that the properly selected stiffness value resulted in very small inter-particle overlaps, and the dynamics of the system did not change appreciably when they increased the stiffness.

2. Dimensionless formulation of DEM

In a mechanical model, all of the variables can be expressed by means of three fundamental dimensions, namely, **M**, mass, **L**, length, and **T**, time. Therefore, based on the Buckingham π theorem, three independent variables can be used to express all of the variables. In DEM, we select E, the elastic modulus of the particles as we use a Hetzian contact model, ρ, the density of the material of particles, and L_0, an arbitrary characteristic length such as diameter of the smallest particle in the assembly.

In a discrete element model, the equation of translational motion of a particle i is generally expressed in the following form:

$$m_i\ddot{x}_i + F_i^d = F_i^p \tag{2}$$

where m_i is the mass of particle i, F_i^p is the resultant of the contact forces acting on the particle, x_i is the displacement vector, and F_i^d is the damping force defined in the following form where a viscous damping model is adopted.

$$F_i^d = C_i\dot{x}_i \tag{3}$$

C_i is the damping constant, and "$\cdot$" denotes the derivative with respect to the time variable, t. In a mass damping model, as in the present study, C_i is calculated as follows:

$$C_i = \alpha m_i \tag{4}$$

where α is the damping coefficient. According to the classical dynamics, we have:

$$C_i = 2m_i\omega_i\xi \tag{5}$$

ω_i is the natural frequency and ξ is the damping ratio.

Eqs. (4) and (5) result in $\alpha_i = 2\omega_i\xi$. In practice, an equal mass-damping coefficient is applied to all of the particles in an assembly. By targeting the highest natural frequency, ω_{max}, we assume:

$$\alpha = 2\omega_{max}\xi \tag{6}$$

As in DEM, where the differential equations of motion are solved by an explicit scheme, the time steps should be limited to a critical value, Δt_c, to avoid numerical instability. According to Belytschko [1]:

$$\Delta t_c = 2/\omega_{max} \tag{7}$$

On the other hand, an approximate Δt_c can be obtained through:

$$\Delta t_c = l_{min}\sqrt{\rho/E} \tag{8}$$

referring to Šmilauer and Chareyre [18] who suggest:

$$l_{min} = 2R_{min} \tag{9}$$

for periodic boundaries, as in this study or $l_{min} = R_{min}$ for the rigid wall conditions.

Using Eqs. (7)–(9), the highest natural frequency is inferred approximately as follows:

$$\omega_{max} = R_{min}^{-1}\sqrt{E/\rho} \tag{10}$$

An arbitrary length is selected as characteristic length, L_0; for example we select:

$$L_0 = 2R_{min} \tag{11}$$

$2R_{min}$ is the size of the smallest particle in the assembly. A nominal length can be taken for L_0 where non-spherical particles are used, such as the diameter of a sphere with an equal volume to that of the particle.

The characteristic time, T_0, is defined as:

$$T_0 = L_0\sqrt{\rho/E} \tag{12}$$