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Time step criterions for nonlinear dense packed granular materials in time-driven method simulations

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ABSTRACT

Discrete-element method (DEM) is a powerful tool for simulations of granular materials. As one branch of DEM, time-driven method (TDM) is suitable for the materials in dense phase. Time step is an important parameter in TDM simulations, which decides the CPU time and the computational accuracy. When a granular system under gravity is deep and nonlinear stress–strain relationship is used to model the particle–particle interaction, some current time step models are not applicable anymore, because the nature frequency of a particle is affected by its boundary conditions. To amend this shortage, a new time step criterion is presented in this paper, which involves the effect from the depth of the system due to gravity. Between this new criterion and that based on Rayleigh time, the smaller one should be the upper limitation of time step in TDM simulations.

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1. Introduction

Granular materials are complex systems with a conglomeration of a large number of solid particles. Research on the motion of granular materials is very active recently because these materials are commonly used in industry and our daily life. Due to the relative velocity between particles, granular materials are classified into three phases, such as gas-like, liquid-like and solid-like[1]. The volume fraction and the coefficients of restitution (COR) are important parameters deciding the phases [2].

With respect to the tasks and accuracy required, various methods may be used in the numerical simulations for granular materials. According to Hogue & Newland [3], the methods can be classified into two approaches: continuum mechanics method (CMM) and discrete element method (DEM). The CMM uses the Eulerian approach for the macroscopic behavior and the DEM uses the Lagrangian approach to simulate the motion of each particle at the microscopic scale (particle level). In addition, DEM can be divided into three main classes [4]: statistical mechanics models, Newtonian dynamics models and hybrid models. Furthermore, the Newtonian dynamics models can be divided into two major groups, event-driven method (EDM) and time-driven method (TDM).

Different to the fixed integration time step in TDM, the time step in EDM is due to the time gap to the next collision (event) [5,6]. Hence, compared with TDM, it is suitable for dilute phases and the number of particles in the system is not too large. Recently, some hybrid algorithms have been developed for a system including both dilute and dense phases [7]. Usually, a fixed time step is used in TDM simulations and therefore the time selection is very important. We found that the depth of a dense packed granular material system affects the selection of the time step. This is because the nature frequency of a particle is changed with the boundary conditions. A similar phenomenon can be observed in beam vibration [8,9]. With different boundary conditions, the beams of same size and same material can be classified as clamp, simple support, free-free and so on. All of them have different nature frequencies. Hence, a new time step criterion for dense packed granular materials and weak perturbation is raised in this paper. Some dynamical simulations of 1-D[10,11] and 2-D particle columns are used to verify this criterion.

The paper is structured as follows: Section 2 reviews the contact and the time step criterions. Section 3 presents the shortage of the existed criterions for dense packed granular materials and raises a new time step criterion for such problems. To show the desirable range of the new time step criterion, a comparison between the new criterion and that based on Rayleigh time is presented in Section 4. Conclusions are drawn in the last section.

2. Contact models

To characterize the normal velocity changes for a binary collision, a COR in normal direction, e is introduced, that is $e = -\mathbf{k}' \cdot \mathbf{u}'^{i,j}/\mathbf{k} \cdot \mathbf{u}^{i,j}$ [12], where the superscripts i and j refer to the two contacting particles, respectively, and $\mathbf{k}$ is defined as $\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}$. $\mathbf{r}_i$ and $\mathbf{r}_j$ are the coordinates of the two particle centers, respectively. Bridges et al. [13] investigated the particles in Saturn's rings from their experiments and claimed that the curve of $\mathbf{u}^{i,j}$ versus e follows the power law, that is

$$e = Bu^{-b}, \tag{1}$$

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where B and b are positive constants, and $u = |\mathbf{u}^{i,j}|$. The shortage of this expression is that when u approaches zero, the value of e becomes infinite. Another expression from Schwager & Pöschel [14] is given as,

$$e = 1-(1-e_0)(u/u_0)^{0.2}, \tag{2}$$

where e_0 and u_0 are two adjustable positive parameters.

The TDM is based on the original method proposed by Cundall & Strack [15] for the contact force imposed on each discrete element. Hence, it is also called force driven model. An integration method is employed to calculate the change of velocities and position for each particle after a certain time by considering all the forces on the particle, such as Euler methods [16], Verlet integration methods [17,18] and predictor–corrector [19,20]. Velocity Verlet algorithm is the most commonly used one. These integration methods offer different accuracies and require different time step as well. In this paper, Velocity Verlet algorithm is employed in the simulation part. Some of the forces acting between particles originate from the deformation of the particles when they are in contact with their neighbors. The simplest and most robust normal force model perhaps is called linear spring dashpot model (LSD) which involves a linear elastic term (sprint), F^e, and a linear viscous term (dashpot), F^d, as [21–23],

$$\begin{aligned} F &= F^e + F^d \\ &= K_l\delta + \eta_l\dot{\delta}, \end{aligned} \tag{3}$$

where δ is the overlap, $\delta = R^i + R^j - d^{i,j}$, $(\delta > 0)$, K_l is the linear effective stiffness and η_l is the linear damping coefficient, $R^{i,j}$ is the radius of each particle and $d^{i,j}$ is the distance between the centers of the particles, that is $d^{i,j} = |\mathbf{r}^i - \mathbf{r}^j|$. The contact time, t_c, equals half of the oscillation period, given by [12],

$$t_c = \frac{\pi}{\sqrt{4K_l - \eta_l/4m_r}}, \tag{4}$$

where m_r is called relative mass, that is $m_r = m^i m^j/(m^i + m^j)$. If the COR, e, is chosen as a constant, the viscous coefficient η_l is given as,

$$\eta_l = 2\kappa\sqrt{m_r K_n}, \tag{5}$$

where $\kappa = \frac{\ln(e)}{\sqrt{\ln^2 e + \pi^2}}$.

The maximum dimensionless desirable range of overlap, $\delta^+ = 2\delta/d^{i,j}$, is 0.1–1.0% for this model when K_l is in order of 10^{6-7} N/m. Experimental results showed that the COR,e, is affected by many parameters, such as particle size, relative velocity between colliding particles and material properties [13].

Sinkovits and Sen [24] extended the elastic term to nonlinear form of power-law type, $s = K_n\delta^\zeta$. Later, Ramírez et al. [25] and Luding [12] extended the viscous term, given as,

$$F = \begin{cases} K_n\delta^\zeta + \eta_n\delta^\xi\dot{\delta} & (\delta > 0) \\ 0 & (\delta \le 0) \end{cases}. \tag{6}$$

This model is also named nonlinear spring dashpot model (NSD). By means of dimensionless analysis on Hertz's theory [26], it can be shown that the exponent $\zeta = 3/2$ and the nonlinear elastic coefficient [6,27],

$$K_n = \frac{4}{3}Y_r\sqrt{R_r}, \tag{7}$$

for spherical particles, where R_r and Y_r are relative radius and relative Young's modulus, respectively. They are defined as $R_r = R/2$, and $Y_r = Y/2(1-\nu^2)$ for the two contacting particles with the same radius R, Young's modulus, Y and Poisson's ratio ν. For different materials, the values of ξ perhaps are not same [28]. The range of ξ is from 0.25 [29,30] to 0.5 [31]. For a given constant COR,e, Huang et al. [32] summarized an expression for the viscous coefficient with $\xi = 1/4$ based on Ref. [33], that is:

$$\eta_n = -\kappa\sqrt{5K_n m_r}. \tag{8}$$

where m_r is the relative mass. For the two particles with the same mass m, $m_r = m/2$. Except the models based on expression in Eq. (6), there are some other advanced models [34,35].When granular materials approach the highest packing density, the granular temperature approaches zero [36], which means that the relative velocity between particles approaches zero. Hence, the elastic part plays the main role in the equations for contact force(Eqs. (3) and (6)). For elastic process, the contact time is given as [27],

$$t_c = 2.87\left(\frac{m_r^2}{R_r Y_r^2 u}\right)^{\frac{1}{5}}. \tag{9}$$

If the contact is a linear viscoelastic process with a constant $e$in Eq. (3), the contact time equals half of the period of the oscillation [12,21,22], given as,

$$t_c = \frac{\pi}{\sqrt{(2K_l/m_r)(1-\kappa^2)}}. \tag{10}$$

According to Babîc [21], the time step, dt_{TDM}, used in TDM, is 10% of contact time, t_c, while Ji & Shen [28] suggested that $dt_{TDM} < 0.02t_c$. It is clear that this time step based on LSD model cannot be used for NSD. They [28] also gave another criterion for time step that dt_{TDM} cannot exceed the minimum Rayleigh time in the system of viscoelastic contact. Here, Rayleigh time is the time required for a Rayleigh wave to travel the diameter of an elastic particle, given as

$$t_R = \frac{\pi R_{min}}{c_R}, \tag{11}$$

where R_{min} is radius of the smallest particle in the system and c_R is the phase velocity of Rayleigh wave. An approximation of c_R for free surface of an elastic half-space is given by Achenbach [37], that is,

$$c_R = \frac{0.862 + 0.114\upsilon}{1+\upsilon}c_T, \tag{12}$$

where $c_T = \sqrt{G/\rho}$ and G is the shear modulus. As ν varies from 0 to 0.5, c_R increases monotonically from $0.652c_T$ to $0.955c_T$. It is found that the speed of sound propagation in a granular column scales with depth by Hertz's contact theory [38,39]. With the increments of sound speed, whether the second criterion based on Rayleigh time is still valid or not for dense packed granular materials, namely in depth with high external pressure, is questionable.

3. Time step for nonlinear contact model

Firstly, to simplify the question, one column of N tiny viscoelastic spherical particles as shown in Fig. 1(a) is discussed. The roughness between the wall and the particles is zero. Gravitation, g, is considered in the system. The total force acted on the j-th particle is balanced at $t = t_0$, that is,

$$\sum F_0^j = F_0^{k,j} + F_0^{i,j} + m^j g - m^j y_0^j = 0, \tag{13}$$

where y is the position, subscript 0 indicates the time step of $t = t_0$, and $F_0^{i,j}$ and $F_0^{k,j}$ are the contact forces with the upper i-th particle and lower k-th particle, respectively, which are

$$F_0^{i,j} = \sum_{K=1}^{j-1} m^K g, \tag{14}$$

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