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Research Paper

Empirical assessment of the critical time increment in explicit particulate discrete element method simulations

Masahide Otsubo, Catherine O'Sullivan *, Tom Shire

Department of Civil and Environmental Engineering, Imperial College London, United Kingdom

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ABSTRACT

This contribution considers the critical time increment (Δt_{crit}) to achieve stable simulations using particulate discrete element method (DEM) codes that adopt a Verlet-type time integration scheme. The Δt_{crit} is determined by considering the maximum vibration frequency of the system. Based on a series of parametric studies, Δt_{crit} is shown to depend on the particle mass (m), the maximum contact stiffness (K_{max}), and the maximum particle coordination number ($C_{N,\max}$). Empirical expressions relating Δt_{crit} to m, K_{max}, and $C_{N,\max}$ are presented; while strictly only valid within the range of simulation scenarios considered here, these can inform DEM analysts selecting appropriate Δt_{crit} values.

1. Introduction

Particulate discrete element modelling (DEM) is well established as a research tool in science in general, and in geomechanics in particular; there has been a consistent increase in the number of DEM-related publications published each year over the past 20–25 years [1,2]. Understandably the emphasis in DEM-related publications has been on application of DEM to simulate physical systems [3], and associated developmental work focussing on implementation of contact models (e.g. [4]), simulating particle crushing, boundary conditions, etc. As is the case with any numerical method, such application orientated research should be supported by studies that examine the method itself, considering issues relating to accuracy (e.g. [5]) and numerical stability (e.g. [6,7]). This contribution specifically considers the issue of numerical stability, and applies eigenmode analyses to a database of DEM simulations to show how the particle characteristics, packing and stress level influence the critical time increment calculated from consideration of the maximum eigenfrequency. The paper includes a background section that discusses the issue of numerical stability in particulate DEM prior to introducing the analysis approach adopted. The results of the eigenmode analysis are then presented and followed by an overall synthesis that considers the effect of packing density, particle size distribution, particle inertia, coordination number and contact stiffness on the critical time increment.

2. Background

As outlined by Hanley and O'Sullivan [5] the second order velocity-Verlet integration scheme has been adopted in a number of DEM codes that are used in geomechanics applications including LAMMPS [8], LIGGHTS [9] and YADE [10] and the commercial codes PFC2D/3D use a related Verlet-based scheme [11]. This numerical method is conditionally stable, i.e. it is only when the time increment used is less than a threshold value (the critical time step, Δt_{crit}) that small perturbations in the initial data will give small changes in the final solution (e.g. [12]). Two approaches are used in the literature to determine Δt_{crit} for DEM simulations; the first is based on the oscillation period of a single degree of freedom system, while the second uses the Rayleigh wave speed.

In their initial description of the discrete element method Cundall and Strack [13] estimated Δt_{crit} by considering a single degree of freedom system of a mass m connected to the ground by a spring K, giving:

$$\Delta t_{crit,SDOF} = 2\sqrt{m/K} \tag{1}$$

Developing this idea, Hart et al. [14] suggest:

$$\Delta t_{crit,Hart} = 2\alpha\sqrt{\frac{m_{min}}{2K_{max}}} \tag{2}$$

where m_{min} is the minimum mass and K_{max} is the largest normal or tangential contact stiffness, α is a user specified parameter that accounts for the presence of multiple contacts for each mass; Hart et al. recommend $\alpha = 0.1$, i.e. $\Delta t_{crit,Hart} = 0.14\sqrt{\frac{m_{min}}{K_{max}}}$. Using these ideas and following a parametric study on monodisperse samples, Tsuji

* Corresponding author at: Dept. Civil and Environmental Engineering, Room 501, Skempton Building, Imperial College London, London SW7 2AZ, United Kingdom.
E-mail address: cath.osullivan@imperial.ac.uk (C. O'Sullivan).

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et al. [15] adopted $\Delta t_{crit,Tsuji} = \frac{\pi}{5}\sqrt{\frac{m}{K}} = 0.63\sqrt{\frac{m}{K}}$. Simple DEM models use linear contact models where a constant spring stiffness is applied to all contacts and K is constant, however many researchers use a Hertzian contact model that uses a non-linear force-deformation relationship at the contacts to account for the variation in contact area with contact force. Referring to Johnson [16], in the contact normal direction the incremental (i.e. tangent) contact spring stiffness ($K_{N,Hertz}$) is then

$$K_{N,Hertz} = \frac{G\sqrt{2\tilde{R}}}{(1-\nu)}\sqrt{\delta} \tag{3}$$

where G is the particle shear stiffness, ν is the particle Poisson's ratio, δ is the contact overlap and $\tilde{R} = \frac{2R_1R_2}{R_1+R_2}$, R_1 and R_2 being the radii of the two contacting particles. The dependency on δ means there will be a range of spring stiffnesses in a DEM model at any given time and $K_{N,\max}$ will vary during a simulation. This complicates application of Eq. (1). Jensen et al. [17] report a modified version of Eq. (1) that is considered in the LS-DYNA DEM code:

$$\Delta t_{crit,Cundall} = 0.2\pi\sqrt{\frac{m_{min}}{\frac{E}{3(1+2\nu)}\beta}} \tag{4}$$

where E is the particle Young's modulus and β is a stiffness penalty parameter that is typically between 0.1 and 0.001. Tu and Andrade [18] argue that Δt_{crit} associated with rotational motion is critical and so

$$\Delta t_{crit,Tu} = 2\sqrt{\frac{2m_{min}}{5K_T}} = 1.2\sqrt{\frac{m_{min}}{K_T}} \tag{5}$$

where K_T is the tangential spring stiffness.

In the PFC codes [19] a critical time step is found for each body by considering both rotational and translational motion to be uncoupled and calculating the ratios $\sqrt{m/k_{tran}}$ and $\sqrt{I/k_{rot}}$ where m and I are the mass and moment of inertia respectively. The translational and rotational stiffnesses (k_{tran} and k_{rot}) are determined by considering the diagonal terms of the contact stiffness matrix at each contact and then summing the contributions from all the contacts assuming the degrees of freedom to be uncoupled. The final critical time step is taken to be the minimum of all the ratios $\sqrt{m/k_{tran}}$ and $\sqrt{I/k_{rot}}$ computed for all degrees of freedom of all bodies. As individual contacts are considered this approach can be applied to Hertzian contacts. Referring to Serra et al. [20], who use a similar approach, this type of implementation is based on Gerschgorin's theorem as outlined by Underwood [21].

Where a Hertzian contact model is used, a number of authors argue that estimates of Δt_{crit} based on Eq. (1) are not valid. For example Boac et al. [22] and Li et al. [23] argue that this approach is inapplicable because the contact model is non-linear. Thornton [24] cited [25] to suggest that the Rayleigh wave speed determines the time step. Li et al. [23] give the following expression for the Rayleigh time step (T_R) (also cited in [17,22,26]):

$$T_R = \frac{\pi R\sqrt{\frac{\rho}{G}}}{0.1631\nu + 0.8766} \tag{6}$$

where ρ is the particle density. Li et al. and Boac et al. [22] specify that R is the average particle radius (R_{ave}); when the same expression is given by Kremmer and Favier [27] and Kafui et al. [28], R is taken to be the minimum particle radius (R_{min}). Li et al. [23] justify this approach for estimating the critical time increment by arguing that it can be assumed that all of the energy in the system is transferred by Rayleigh waves, while Guo et al. [29] explain that this approach considers the time taken for a Rayleigh wave to pass a sphere in a single time increment.

As noted by Burns and Hanley [7] it is clear that application of these different approaches will give different time step values. Whichever approach is used it seems that users view the calculated Δt_{crit} values to be an estimate. As already stated Hart et al. [14] and Tsuji et al. [15] use experience/empirical considerations to apply a factor to Eq. (1). Boac et al. [30] state that in practice some fraction of T_R is used, and suggest this fraction should be 0.2–0.4, with the higher number being more suited to lower coordination numbers. Jensen et al. [17] state that for stability the minimum of the critical time increment calculated using T_R, and Eq. (4) should be multiplied by a factor of 0.2 (they also consider a third approach that takes particle velocity into account). Itasca [19] apply a default factor of 0.8 to their calculated Δt_{crit} and this factor can also be user-specified.

Note that while Thornton [24] also considered artificially increasing the particle density (density scaling) to increase the critical time step, this has consequences for the inertial number and the maximum strain rate that can be applied while maintaining quasi static conditions [31,32] and so density scaling is neither used nor recommended here.

3. Eigenvalue analysis

Stability of explicit time integration approaches applied to multi-degree of freedom systems is also a concern in dynamic finite element analysis. Belytschko et al. [12] state that for a system of constant strain elements

$$\Delta t_{crit,CS} = \frac{2}{\omega_{max}} \leqslant \min_{ele}\frac{2}{\omega_{ele}} = \min_{ele}\frac{l_{ele}}{c_{ele}} \tag{7}$$

where ω_{max} is the maximum frequency of the linearized system, ω_{ele} is the frequency of element *ele*, l_{ele} is a characteristic length of element *ele* and c_{ele} is the current wave speed in element *ele*. Eq. (7) clearly links to the approaches used to determine Δt_{crit}; DEM analysts are implicitly relating the ratio $\sqrt{m/K}$ to ω_{ele}, while consideration of the Rayleigh wave speed relates to the ratio $\frac{l_{ele}}{c_{ele}}$. There is however a basic conceptual difference in the two approaches; the Cundall/Hart SDOF-based approach considers the system to be comprised of rigid bodies connected by springs, while the Rayleigh-wave-based approach considers the particles themselves to be elastic.

O'Sullivan and Bray [6] argued that the particles in a DEM simulation are analogous to the nodes in a finite element model, while the contacts are roughly equivalent to the elements. This conceptual model of a granular material is used in implicit discrete element method formulations such as the particulate form of discontinuous deformation analysis (DDA) as outlined in [11]. O'Sullivan and Bray [6] outlined that if it is assumed that linear stability analysis also holds for non-linear cases, then the maximum stable time increment (Δt_{crit}) is a function of the eigenvalues of the current stiffness matrix (e.g. [36,37]). As acknowledged by Tu and Andrade [18], the maximum frequency, $\omega_{\max}$, is related to the maximum eigenvalue ($\lambda_{\max}$) of the $\mathbf{M^{-1}K}$ matrix as

$$\omega_{\max} = \sqrt{\lambda_{\max}} \tag{8}$$

O'Sullivan and Bray estimated the maximum eigenvalue of the system using the following expression which is an extension of Rayleigh's theorem ([36]):

$$\lambda_{\max} \leqslant \lambda^{ele}_{\max} \tag{9}$$

where $\lambda^{ele}_{\max}$ is the maximum eigenvalue of the $\mathbf{M^{ele-1}K^{ele}}$ matrix for element "*ele*", ($\mathbf{M^{ele}}$ = element mass matrix, $\mathbf{K^{ele}}$ = element stiffness matrix). An estimate for the critical time increment can then be made by applying Eq. (7), once $\lambda^{ele}_{\max}$ is known, and O'Sullivan and