CRITICAL TIME STEP FOR DEM SIMULATIONS USING A HERTZIAN CONTACT MODEL AND EULER INTEGRATOR

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Abstract Discrete element method (DEM) simulations usually adopt an explicit, conditionally stable numerical integration scheme. The simulation time step should be maximised to ensure simulation efficiency while ensuring the simulation remains stable at all times. A recent publication [?] has proposed a novel method to determine the critical time step for two contacting Hertzian spheres using a velocity Verlet integrator, based on the fact that the discretised equations of motion can be analysed as a nonlinear map. In this paper, the methodology has been extended to a simpler Euler integrator. An explicit expression for the critical time step is obtained in the absence of damping which is a function of particle shear moduli, radii, densities, Poisson's ratio and the impact velocity of the particles. The expressions derived for critical time step are the same for an Euler integrator as for a velocity Verlet integrator, i.e., the critical time step does not depend on which integrator is selected. Increasing the impact velocity leads to a smaller critical time step.

1 INTRODUCTION

Since its introduction in the 1970s, DEM has become an extremely popular tool for investigating the behaviour of particulate systems at the micro-scale. DEM typically adopts one of a range of explicit, conditionally stable numerical integration schemes [?] to solve the equations of motion as a system of second-order differential equations. The time step chosen for a simulation must be small enough to ensure numerical stability and physically reasonable solutions, but should not be overly conservative as this would lead to unnecessarily long simulation times [?].

For systems with a linear contact model, the critical time step is invariably proportional to $\sqrt{\frac{m}{k}}$ where m is particle mass and k represents stiffness [?]. For nonlinear systems, the Rayleigh time step criterion is often adopted, e.g., [?]. However, this is based on a static analysis and the predicted critical time step does not have any velocity dependence, even though it is known that the time step needs to be reduced to maintain stability when particle velocities are high [?]. Recently, a novel method has been proposed to determine the critical time step for two contacting Hertzian spheres, based on the fact that the discretised equations of motion can be analysed as a nonlinear map [?]. This analysis considered both damped and undamped cases; for the latter case, explicit expressions were found for the critical time step which are a function of the impact velocity of the particles.

This analysis adopted a commonly used velocity Verlet integration scheme. However, it is not known what effect the choice of integration scheme has on the critical time step. Therefore, in this paper, the methodology developed by [?] has been extended to an Euler integrator.

2 MATHEMATICAL DERIVATION

Consider two identical spheres, A and B, of mass m, radius r, shear modulus G, Young's modulus E, Poisson's ratio ν, and moment of inertia $I = \frac{2}{5}mr^2$. These two spheres have a common contact point c. The spheres are oriented such that the branch vector joining the sphere centres, along which the normal force acts, is aligned in the Cartesian z direction. The tangential force acts in the $x - y$ plane. There is no damping in the system.

We define three additional quantities for convenience:

$$E^* = \frac{E}{2(1-\nu^2)} \tag{1}$$

$$G^* = \frac{G}{4(2-\nu)(1+\nu)} \tag{2}$$

$$r^* = \frac{r}{2} \tag{3}$$

Using this notation and frame of reference, we can write the relative acceleration at the contact point of the spheres during the impact phase at some time step $n+1$ as

$$\begin{aligned}
\begin{bmatrix} \ddot{x}_{cx,n+1} \\ \ddot{x}_{cy,n+1} \\ \ddot{x}_{cz,n+1} \end{bmatrix} &= \begin{bmatrix} \frac{2r^2}{I} + \frac{2}{m} & 0 & 0 \\ 0 & \frac{2r^2}{I} + \frac{2}{m} & 0 \\ 0 & 0 & \frac{2}{m} \end{bmatrix} \begin{bmatrix} -8G^* \sqrt{r^* |x_{cz,n+1}|} x_{cx,n+1} \\ -8G^* \sqrt{r^* |x_{cz,n+1}|} x_{cy,n+1} \\ -\frac{4}{3}E^* \sqrt{r^* |x_{cz,n+1}|} x_{cz,n+1} \end{bmatrix} \\
&= \begin{bmatrix} -\frac{14G\sqrt{r/2}}{m(2-\nu)(1+\nu)} & 0 & 0 \\ 0 & -\frac{14G\sqrt{r/2}}{m(2-\nu)(1+\nu)} & 0 \\ 0 & 0 & -\frac{4E\sqrt{r/2}}{3m(1-\nu^2)} \end{bmatrix} \begin{bmatrix} \sqrt{|x_{cz,n+1}|} x_{cx,n+1} \\ \sqrt{|x_{cz,n+1}|} x_{cy,n+1} \\ \sqrt{|x_{cz,n+1}|} x_{cz,n+1} \end{bmatrix}
\end{aligned} \tag{4}$$

for a Hertzian contact model. $\dot{x}_{cx/y/z}$ represents the relative velocity at the contact point while $x_{cx/y/z}$ represents the relative displacement at the contact point, i.e., x_{cz} represents the normal overlap while the particles are in contact. For the Euler integrator, the relative contact velocity and displacement can be expressed vectorially as

$$\dot{\boldsymbol{x}}_{\boldsymbol{c,n+1}} = \dot{\boldsymbol{x}}_{\boldsymbol{c,n}} + \Delta t \ddot{\boldsymbol{x}}_{\boldsymbol{c,n+1}} \tag{5}$$

$$\boldsymbol{x}_{\boldsymbol{c,n+1}} = \boldsymbol{x}_{\boldsymbol{c,n}} + \Delta t \dot{\boldsymbol{x}}_{\boldsymbol{c,n+1}} \tag{6}$$

where Δt is the time step. Eq. **??** may be substituted into Eq. **??** for the relative acceleration. It is noted that the relative displacement/velocity/acceleration at the interparticle contact is easily related to the displacement/velocity/acceleration of A and B:

$$\ddot{\boldsymbol{x}}_{\boldsymbol{c,n}} = \ddot{\boldsymbol{x}}_{\boldsymbol{B,n}} - \ddot{\boldsymbol{x}}_{\boldsymbol{A,n}} \tag{7}$$

$$\dot{\boldsymbol{x}}_{\boldsymbol{c,n}} = \dot{\boldsymbol{x}}_{\boldsymbol{B,n}} - \dot{\boldsymbol{x}}_{\boldsymbol{A,n}} \tag{8}$$

$$\boldsymbol{x}_{\boldsymbol{c,n}} = \boldsymbol{x}_{\boldsymbol{B,n}} - \boldsymbol{x}_{\boldsymbol{A,n}} \tag{9}$$

Here we make the same assumptions as [**?**] in order to determine the critical time step for this system. This requires considering the normal and tangential directions separately.

2.1 Normal direction

The impact is divided into two phases:

Phase 1 The system goes from initial contact to the point of maximum compression. We propose that at least one time step is needed to capture the dynamics of this compression phase.

Phase 2 The system returns from maximum compression to a touching contact. As for Phase 1, at least one time step is needed to capture the dynamics of Phase 2.

The boundary conditions for Phase 1 are $\dot{x}_{cz,n} = v_{z,i}$ (an initial incident velocity), $\dot{x}_{cz,n+1} = 0$ and, from Eq. **??**, $x_{cz,n} \approx x_{cz,n+1} \approx \Delta t v_{z,i}$. Using these boundary conditions in Eq. **??**, we obtain

$$0 = v_{z,i} - \Delta t \frac{4E\sqrt{r/2}}{3m(1-\nu^2)} \left(\Delta t v_{z,i}\right)^{\frac{3}{2}} \tag{10}$$

Solving for Δt,

$$\Delta t = \left(\frac{3m(1-\nu^2)}{4E\sqrt{r v_{z,i}/2}} \right)^{\frac{2}{5}} \tag{11}$$

In the absence of damping, Phase 2 is symmetric to Phase 1 with the boundary conditions $\dot{x}_{cz,n} = 0$, $\dot{x}_{cz,n+1} = v_{z,i}$ as there is no energy dissipation and, from Eq. **??**, $x_{cz,n} \approx x_{cz,n+1} \approx \Delta t v_{z,i}$. Hence, Eq. **??** is also recovered as the critical time step for Phase 2.

2.2 Shear direction

The proposed shear bound follows a similar logic to the normal bounds [?]: the tangential velocity cannot be brought to zero in a single time step, i.e., a velocity reversal cannot take place in the first time step after collision. In the limit of zero tangential velocity at time step $n+1$, the boundary conditions are $\dot{x}_{cx,n+1} = \dot{x}_{cy,n+1} = 0$, $x_{cj,n} \approx x_{cj,n+1} \approx \Delta t v_{j,i}$ for $j = x/y/z$ and $\dot{x}_{cj,n} = v_{j,i}$ by definition. Eq. **??** gives

$$0 = v_{x,i} - \Delta t \frac{14G\sqrt{r/2}}{m(2-\nu)(1+\nu)} \sqrt{\Delta t v_{z,i}} \Delta t v_{x,i} \tag{12}$$

$$0 = v_{y,i} - \Delta t \frac{14G\sqrt{r/2}}{m(2-\nu)(1+\nu)} \sqrt{\Delta t v_{z,i}} \Delta t v_{y,i} \tag{13}$$

Solving for Δt,

$$\Delta t = \left(\frac{m(2-\nu)(1+\nu)}{14G\sqrt{r v_{z,i}/2}} \right)^{\frac{2}{5}} \tag{14}$$

2.3 Critical time step

We now have two equations defining the critical time step for the normal and shear directions: Eq. **??** and Eq. **??**, respectively. Both equations have the same dependence on particle mass, radius and impact velocity. Taking the ratio between the two and substituting $E = 2G(1+\nu)$:

$$\left(\frac{\Delta t_{\text{normal}}}{\Delta t_{\text{shear}}} \right)^{\frac{5}{2}} = \frac{\frac{3m(1-\nu^2)}{4E\sqrt{r v_{z,i}/2}}}{\frac{m(2-\nu)(1+\nu)}{14G\sqrt{r v_{z,i}/2}}} = \frac{21G(1-\nu)}{2E(2-\nu)} = \frac{21(1-\nu)}{4(1+\nu)(2-\nu)} \tag{15}$$

For physically realistic values of $-1 < \nu < 0.5$, Eq. (**??**) decreases as ν increases, attaining a minimum value of $\frac{7}{6}$ when $\nu = 0.5$. Therefore, Δt_{normal} is always larger than Δt_{shear} for $-1 < \nu < 0.5$, meaning that Eq. **??** is the critical time step. This result is the same as [?]. Using a different approach, Tu and Andrade [?] also found that the critical time step for an undamped system is dictated by the shear rather than the normal bounds.

3 COMPARISON WITH VELOCITY VERLET INTEGRATOR

Assume values of $G = 300\,\text{MPa}$, $\nu = 0.25$, $\rho = 1000\,\text{kg}\,\text{m}^{-3}$ and $r = 1.5\,\text{mm}$ which represent an industrial powder [?]. These parameters were also used by [?] in their verification. Fig. **??** compares the critical time step given by Eq. **??** for an Euler integrator with the undamped critical time step obtained by [?] for a velocity Verlet integration scheme. Both show an identical decrease of critical time step as the impact velocity increases.

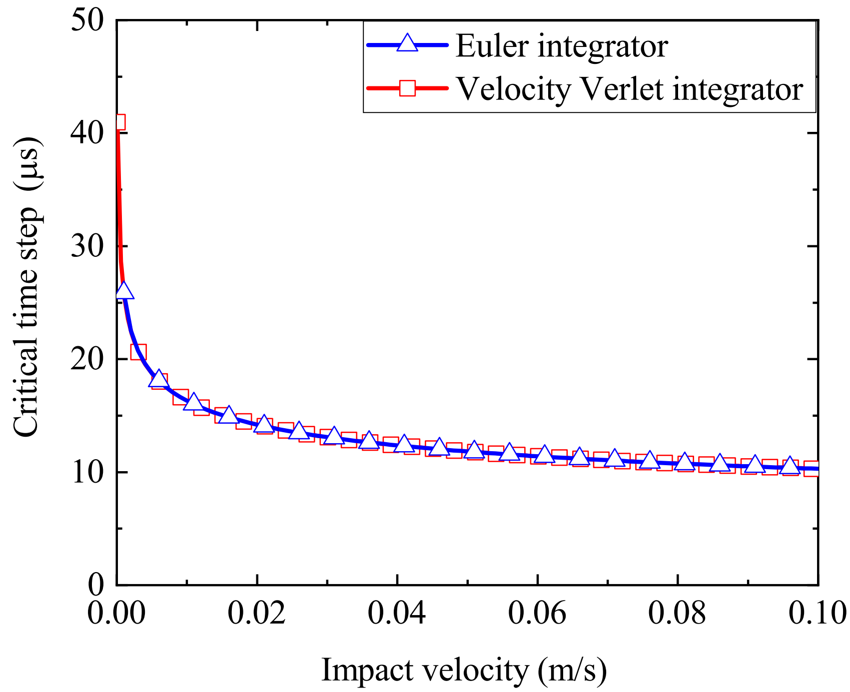

Figure 1: Comparison of critical time steps as the impact velocity varies from zero to $0.1\,\mathrm{m\,s^{-1}}$ for two integration schemes: Euler as investigated in this paper and velocity Verlet from [**?**].

4 DISCUSSION AND CONCLUSION

For the undamped case considered in this paper, the same critical time step is obtained (pertaining to the shear rather than the normal direction) for the Euler integrator as for the velocity Verlet integrator. The critical time step is a function of particle shear moduli, radii, densities, Poisson's ratio and the impact velocity of the particles. Increasing the impact velocity, reducing the particle density ($\propto$ mass) or increasing its stiffness reduce the critical time step. A limitation of this analysis is its restriction to two contacting spherical particles. Otsubo et al [**?**] related the critical time step to the maximum particle coordination number for a specific polydisperse system of spherical particles; it is proposed that the same relationship could be applied to the time step obtained from this two-particle analysis. The authors are currently conducting research to quantify critical time steps for two *non-spherical* particles using an Euler integrator.

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