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On an efficient hybrid soft and hard sphere collision integration scheme for DEM

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HIGHLIGHTS

- Novel hybrid collision integration scheme for discrete element methods.
- Using hard sphere methodology for binary collisions and soft sphere for multibody collisions.
- Comparison of classical and hybrid methods by monitoring the energy budget of a bounding box problem.

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ABSTRACT

This paper introduces a novel hybrid collision integration scheme that combines the benefits of the hard-sphere and the soft-sphere methodology. It assumes that the larger part of the collisions are binary and can be solved in one step. The remainder of the collisions involving more than two particles are handled with a classical soft-sphere scheme. Results for a bounding box problem, employing the classical soft-sphere scheme and the hybrid scheme are compared in terms of energy budget conservation. The hybrid scheme is more accurate and more importantly it is roughly one order of magnitude faster.

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1. Introduction

Since the introduction of the distinct element model by Cundall and Strack (1979) for perfect spheres the field of granular flow modeling has expanded dramatically. The model by Cundall and Strack (1979) has since then been extended for solid-fluid interactions, CFD-DEM (Xu and Yu, 1997), non-spherical particles (Pourlin et al., 2005; Lu et al., 2015) and other external forces as van der Waals forces (Marshall, 2009), capillary forces (Mikami et al., 1998), electrostatics (Korevaar et al., 2014) and lift forces (Zastawny et al., 2012). For an overview of the relevant inter-particle and particle-fluid forces see Zhu et al. (2007).

Applications of these models in granular flow are widespread, ranging from fluidized beds (Van Buijtenen et al., 2011), rotating drums (Gonzalez Briones et al., 2015; Yang et al., 2008) and tumbling mills, chute flow (Shirsath et al., 2014) to sedimentation and hoppers (Cleary and Sawley, 2002). A comprehensive overview of the many applications of discrete particle modeling can be found in the work of Zhu et al. (2008). The foundation of these models is however the contact model, which can be split into a hard sphere model as discussed by Hoomans et al. (1996) and a soft sphere model by Tsuji et al. (1993). Regarding the soft sphere models, we can also make a distinction between different force models, most of which are based on variations of the spring-dashpot model.

In the hard-sphere approach, collisions are binary and instantaneous. The model can only handle particle–pair interactions and collisions involving multiple particles that are not considered. In simulations the collisions are handled in chronological order. Meaning the simulation time scales with the collision frequency; it is an event-driven technique. As such the hard-sphere model is much more efficient in dilute systems.

For higher density or highly dissipative systems a soft-sphere method is to be preferred. In a soft-sphere method, Newton’s equations of motion are integrated and a contact force model is introduced to account for particle–particle interaction, based on the deformation or overlap of contacting particles. Because particle overlap is allowed, overlapping of particles with multiple
partners is also allowed. The time step for a soft-sphere method depends on the chosen number of steps during a contact, which scales with the chosen spring stiffness of the system; therefore it is a time-driven simulation.

The strength of the hard-sphere model lies in the fact that each collision can be handled instantaneously instead of in a number of steps. The strength however of the soft-sphere method lies in the relaxation of the spring stiffness, which allows taking a larger time step. The most time-consuming step for these simulations is always the determination and updating of the collision partners. Upon analysis of CFD-DEM simulations of dense gas-particle flows, we found that the number of collision partners in a typical soft-sphere simulation is limited. An example of this is given in Fig. 1, from a simulation of a pseudo-2D fluidized bed, which was validated with two experimental techniques in Buist et al. (2015). It can be seen that over 90% of the contacts involve two particles. This means that most collisions are binary, just as in a hard sphere model. The rest of the particles have predominantly two other collision partners and on occasion three or more.

To benefit from the efficiency of the hard sphere model and the robustness of the soft sphere model in this work a hybrid collision integration scheme is introduced. This scheme combines elements of a soft-sphere and a hard-sphere method: all binary contacts will have a collision duration but are handled only once. All Multi-Body Contacts (MBC) are handled with a classical soft-sphere methodology. As such this scheme is still time-driven but with a 10 times larger time step compared to the classical soft-sphere method. This work is organized as follows: first a short overview is given of the classical contact schemes, second the hybrid scheme is discussed in more detail, followed by results of several tests comparing the classical soft-sphere and the hybrid scheme.

2. Classical collision schemes

The two most used collision integration schemes for Discrete Particle Models are the so-called soft-sphere and hard sphere models. Both schemes will be shortly discussed here. A comprehensive overview is given in Table 1. A more extensive explanation of both schemes can be found in Deen et al. (2007).

![Fig. 1. Collision order probability from a simulation of a pseudo 2D fluidized bed, with $\varepsilon = 0.6$, $u_{\text{ref}} = 3.5 \text{ m/s}$, $\varepsilon = 1$, $\beta = 0.33$, $\mu = 0.1$.](image)

### 2.1. Hard sphere scheme

The hard sphere collision integration scheme assumes that each collision is instantaneous and binary. The collisions are solved in order of occurrence, as such the hard sphere method is an event-driven model. An efficient method to keep track of the sequence of collisions is needed, and for very dense systems with a high collision frequency, the hard sphere scheme is less efficient than the soft sphere scheme. In this work the hard sphere model is not used but rather shortly discussed as a reference, because we mostly discuss a relatively dense system and because the hybrid model has the most resemblance to a soft-sphere method.

### 2.2. Soft sphere scheme

The soft sphere model is often based on the linear spring-dashpot model with a frictional slider. The force of the collision scales with the overlap of the particles and is used to update the translational and rotational velocities as follows:
Time is discretized with a time step which typically amounts to \( \sim 10 \) times smaller than the duration of a collision. The duration of the collision is associated with the ratio of the spring stiffness with the mass of the particle as well as the damping ratio \((\zeta)\) as follows:

\[
t_{\text{coll}} = \frac{\pi}{\omega_d} = \frac{\pi}{\sqrt{k_r/m_{\text{eff}} \left( \sqrt{1 - \zeta^2} \right)}} \tag{3}
\]

where \(\omega_d\) is the dampered frequency defined as:

\[
\omega_d = \sqrt{\frac{k_r}{m_{\text{eff}} \left( \sqrt{1 - \zeta^2} \right)}}
\]

where \(\zeta\) is the damping ratio defined as:

\[
\zeta = \frac{-\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}}
\]

For a full derivation of these properties the interested reader is referred to Appendix A. Here \(t_{\text{coll}}\) is independent of the impact velocity \(v_{ab}\) only for the linear spring dashpot model. For nonlinear models the duration of a collision is dependent on the impact velocity (Antypov and Elliott, 2011).

The spring stiffness is based on particle material properties and usually quite high, leading to small time steps. For the soft sphere integration scheme the spring stiffness is chosen such that the maximum overlap \(\delta_{\text{max}}\) is \(\sim 1\)% of the particle radius: It is possible to show that \(k_o\) follows from:

\[
\delta_{\text{max}} = \frac{2 \ln(\rho)}{\sqrt{\pi^2 + \ln(\rho)^2}} \cos^{-1} \left( \frac{-\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}} \right)
\]

\[
k_0 = \frac{v_{ab} m_{\text{eff}}}{\delta_{\text{max}}} \left( \frac{2 \ln(\rho)}{\sqrt{\pi^2 + \ln(\rho)^2}} \cos^{-1} \left( \frac{-\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}} \right) \right)^2 \tag{4}
\]

Fig. 2 shows the dependence of the spring stiffness on the ratio of the chosen maximum overlap \((\delta_{\text{max}})\) and the impact velocity. Also the damping on the spring stiffness as a function of the restitution coefficient is shown, which is near linear. In Appendix B a full derivation is given. The tangential spring stiffness is given as:

\[
k_t = k_0 \frac{2 \ln(\rho)}{\pi^2 + \ln(\rho)^2} \tag{5}
\]

With respect to reality the spring stiffness is thus relaxed. Because overlap is allowed, collisions involving more than two particles is possible: Multi-Body Contacts (MBC). In Fig. 1 it is shown that for a typical DPM simulation the number of MBCs is limited to a few percent of the total number of collisions. Because the main part is binary, we suggest a hybrid collision scheme that can handle the binary collisions instantaneously, whereas the MBCs are treated with a classical soft sphere scheme.

### 3. Hybrid collision integration scheme

The first researchers using a time-driven hard sphere approach are Helland et al. (2002). In their work however, each collision is still quasi-instantaneous. The first to couple a hard sphere and a soft sphere approach was Gui et al. (2016). An extended version of the hard particle model for square particles in 2D was proposed, coupled to a soft sphere methodology. In their work however the time step used is still considerably smaller than the duration of a collision. The use of a hard sphere methodology however allows

---

**Table 1**

<table>
<thead>
<tr>
<th>Soft sphere</th>
<th>Hard sphere</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear spring dashpot</td>
<td>Impulse vector</td>
</tr>
<tr>
<td>(\vec{F}<em>0 = -k_o \vec{v}</em>{ab} - q_0 \vec{v}_{ab,0})</td>
<td>(m(\vec{v} - \vec{v}_0) = \vec{f})</td>
</tr>
<tr>
<td>(\vec{F}<em>0 = -k_r \vec{v}</em>{ab} - q_r \vec{v}_{ab,0})</td>
<td>(\vec{f}<em>n = -(1 + \epsilon) \frac{\vec{v}</em>{ab}}{\vec{v}<em>{ab} \cdot \vec{v}</em>{ab}})</td>
</tr>
<tr>
<td>or in case of sliding ((\vec{F}_r &gt; \mu \vec{F}_n)):</td>
<td>(\vec{f}<em>t = -(1 + \mu) \frac{\vec{v}</em>{ab}}{\vec{v}<em>{ab} \cdot \vec{v}</em>{ab}})</td>
</tr>
<tr>
<td>(\vec{F}_r = -\mu \vec{F}_n)</td>
<td>Collisions instantaneous</td>
</tr>
<tr>
<td>Time scale of collision</td>
<td>(t_{\text{coll}} = 0)</td>
</tr>
<tr>
<td>(t_{\text{coll}} = \frac{\pi}{\omega_d})</td>
<td>Time step</td>
</tr>
<tr>
<td>(\Delta t = \frac{t_{\text{coll}}}{10})</td>
<td>(\Delta t = \frac{1}{f_{\text{coll}}})</td>
</tr>
</tbody>
</table>

---

\(\vec{v}_0 = \vec{v}_0 + \left( \vec{F}_0 + \vec{F}_r \right) \frac{\Delta t}{m}\) \hspace{1cm} (1)

\(\omega = \omega_d + \frac{\pi}{T} \Delta t\) \hspace{1cm} (2)
for an accurate description of collisions, while maintaining a \( \sim 10 \) times larger time step with respect to a classical visco-elastic methodology for non-spherical particles.

The hybrid collision integration scheme, that is presented here, assumes that most collisions are binary and have a fixed well-defined duration, based on the linear spring dashpot model. The binary collisions are solved using a modified hard sphere methodology. All collisions involving more than two collision partners are solved using a classical soft sphere methodology. A short schematic overview is given in Table 2.

The chosen time step is exactly the duration of a collision, generally 10 times larger than for a classical soft sphere model. As such only one full collision can be solved per particle per time step. The collision detection has to be done once every time step. For reference, the classic soft sphere methodology would need the collision detection 10 times per collision duration. With the collision detection being the most time consuming step in a simulation, the simulation time is expected to be roughly and at best ten times lower.

In the next few sections we will discuss in a bit more detail binary collisions and multibody collisions. Finally an overview of the model is given that shows the main extra steps that need to be taken into account.

### 3.1. Binary collisions

For the new model, we first assumed particles are of equal size and mass possessing no tangential component (\( \mu = 0 \) and \( v_{0,t} = 0 \)). For a binary collision it follows that:

\[
\bar{v}_n = \bar{v}_{n,0} - \frac{1 + e}{2} \bar{v}_{ab,n}
\]

with \( \bar{v}_{ab} \) defined as the relative velocity at the point of contact:

\[
\bar{v}_{ab} = \bar{v}_a - \bar{v}_b + r (\bar{n}_a + \bar{n}_b) \times \bar{r}_{ab}
\]

which consists of a normal and a tangential component:

### Table 2

<table>
<thead>
<tr>
<th>Hybrid model</th>
<th>Binary</th>
<th>Multibody</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{v}<em>{n,0} = \bar{v}</em>{n,0,0} + \frac{1 + e}{2} \bar{v}_{ab,0} )</td>
<td>( \bar{v}<em>{n,0} = \bar{v}</em>{n,0,0} + \frac{1 + e}{2} \bar{v}_{ab,0} )</td>
<td>( \bar{v}<em>{n,0} = \bar{v}</em>{n,0,0} + \frac{1 + e}{2} \bar{v}_{ab,0} )</td>
</tr>
<tr>
<td>( x_n = x_{n,0} + \frac{1 + e}{2} x_{ab} \Delta t + \left( v_n - v_{n,0,0} \right) t_{last} )</td>
<td>( x_n = x_{n,0} + \frac{1 + e}{2} x_{ab} \Delta t + \left( v_n - v_{n,0,0} \right) t_{last} )</td>
<td>( x_n = x_{n,0} + \frac{1 + e}{2} x_{ab} \Delta t + \left( v_n - v_{n,0,0} \right) t_{last} )</td>
</tr>
<tr>
<td>( \Delta t = eab \left( 1 + e \right) [\bar{v}<em>{ab} \cdot \bar{v}</em>{ab} - (\bar{v}<em>{ab} - \bar{n}</em>{ab} \bar{r}_{ab})^2] )</td>
<td>( \Delta t = eab \left( 1 + e \right) [\bar{v}<em>{ab} \cdot \bar{v}</em>{ab} - (\bar{v}<em>{ab} - \bar{n}</em>{ab} \bar{r}_{ab})^2] )</td>
<td>( \Delta t = eab \left( 1 + e \right) [\bar{v}<em>{ab} \cdot \bar{v}</em>{ab} - (\bar{v}<em>{ab} - \bar{n}</em>{ab} \bar{r}_{ab})^2] )</td>
</tr>
<tr>
<td>Time scale collision</td>
<td>( t_{coll} \leq \frac{\pi}{\omega} )</td>
<td>( t_{coll} \leq \frac{\pi}{\omega} )</td>
</tr>
<tr>
<td>Time step</td>
<td>( \Delta t = \frac{t_{coll}}{\frac{1}{10}} )</td>
<td>( \Delta t = \frac{t_{coll}}{\frac{1}{10}} )</td>
</tr>
</tbody>
</table>

**Fig. 2.** The spring stiffness as a function of the ratio of the maximum overlap and the impact velocity for the two bounds \( e = 0 \) and \( e = 1 \) (left), and the damping (exponential part of Eq. (4)) on the spring stiffness as a function of the restitution coefficient (right).
\[ v_{ab,n} = v_{ab} - n_{ab} \]  
\[ v_{ab,t} = v_{ab} - v_{ab,n} \]  
\[ n_{ab} = \frac{x_b - x_a}{|x_b - x_a|} \]  
\[ \ell_{ab} = \frac{v_{ab,t}}{|v_{ab,t}|} \]  
Finally the position is defined as:
\[ x = x_0 - \frac{v_0}{2} \Delta t + v_0 \Delta t \]  
That is, the new position is the sum of respectively the old position, the displacement until collision based on the old velocity, a center of mass displacement during collision and a displacement after the collision till the end of the time step.

Here, \( x_0 \) and \( v_0 \) are the position and the velocity at the time step before collision, respectively, and \( x \) and \( v \) the position and the velocity at the time step after the collision, respectively. \( \ell_{fast} \) is the time between the moment of first contact until the end of the time step. These are given by:
\[ \ell_{ab} = x_a - x_b \]  
\[ v_{ab} = v_a - v_b \]  
\[ \ell_{last} = \frac{t_{ab} v_{ab} + \sqrt{(t_{ab} v_{ab})^2 - (v_{ab}^2 - (R_a + R_b))^2 |v_{ab}|}}{|v_{ab}|} \]  
if the tangential component is added, an extension on the normal and tangential velocity is needed. Also a frictional limit has to be defined, for a full derivation see also Appendix C.

### 3.2. Multibody collisions

Multibody contacts cannot be treated analytically. Of course the position and the velocity can be easily determined and follow a very similar equation as those for binary collisions. However, the time of collision cannot easily be determined. The typical solution of a multibody contact involves:
\[ x_i(t) = \sum_{j=1}^{n} e^{-\omega_i t} \left( d_{ij} \cos(\omega_{ij} t) + d_{ij} \sin(\omega_{ij} t) \right) \]  
where \( n \) is the number of contacts. It is possible to solve this for a number (>1) of simultaneous contacts, but each (>2) possible simultaneous contact situation would have a unique solution. Even though it is possible to determine trajectory and the change of velocity of the MBC, it is not possible to determine the duration of the collision analytically, as the sum of sinusoids with differing frequencies and amplitudes cannot be easily simplified. As such it is not possible to determine the outcome of a MBC in this particular way.

Keeping the above in mind it is simpler to use the classical soft sphere treatment, and divide the contact time into a number of steps only for the particles in an MBC.

### 3.3. Overview

To give a more clear overview of the hybrid integrations scheme, we go through the several phases of a time step, see also Fig. 3. In the classical soft sphere scheme, first a collision detection scheme is used, in this work a kd-tree searcher is used that searches for all collision partners. Once all possible collision pairs are found the forces associated with the collisions are calculated. The last step is to sum all the forces of a particular particle and update the velocity and position of the particles. This process is then repeated.

The hybrid scheme follows a reversed order, we have to start the explanation with the collision detection however. The collision detection is done at the end of the collision, to determine the particles that are in collision mode, but because the time step is the same as the duration of a collision, the collision will finish in the next time step. In a new time step first all particle positions and velocities are updated. Part of this update is the update of all collision partners that have been determined during the last time step, because their collisions end in this time step. After these updates, collision detection is performed for all particles. In the final step we have to check if collision partners, from the collision detection, contain particles that in the previous time step already had been in collision mode. These collisions might overlap and have to be solved separately, which is discussed later.

An overview of all possible types of collision is given in Fig. 4. In this figure the numbers relate to a particle and the black lines to the different time steps. The colored lines signify the duration of the collision. In the first time step we notice through collision detection that particles 1 and 2 are undergoing a binary collision, they however keep their respective artificial position and velocities. We solve for the collision in the second time step because
the collision should be finished by then.

Particles 3, 4 and 5 are found to be in contact in the third time step. Because this is a multibody collision, the time step, for these particles only, is split in ten sub steps, and the collision is solved following the classical soft sphere methodology.

After the collision detection is performed, all particles in contact are referenced against the particles in collision in the previous time step. The particles that are in contact in both time frames are special cases and have to be solved separately and have three possible outcomes. For instance in Fig. 4, particles 6 and 7 are found to be in contact in the first time step and are solved in the second, but there find particles 7 and 8 to be in contact. Thus particle 7 is found to be in a collision both in time steps 1 and 2. Now the two collisions can be completely separate or adjoining, and when adjoining could last till the second or the third time step. These three situations are depicted in Table 3.

In the first case the two collisions are non-overlapping and completely separate, meaning nothing is wrong and the collision between particles 7 and 8 can commence in the next time step as usual. The second and third cases are when the two collisions are overlapping, with one lasting until the second time step and one lasting past the second time step. These have to be solved using a soft-sphere method i.e. as a MBC. For the second case the collision has to be solved in the third time step using a soft-sphere method as well, but now taking information from the second time step instead of two time steps back as usual. In that case, particles 7 and 8 get a special tag, signifying the need for special treatment.

To distinguish between these situations the $t_{last}$ (Eq. (13)) of both the collisions has to be determined. The sum of the $t_{last}$ of the new collision and $\Delta t - t_{last}$ of the old collision makes the distinction between the first and the last two cases. $\Delta t - t_{last}$ is the amount of time the collision between particles 6 and 7 is taking place in the time step from $\Delta t$ to $2\Delta t$, if the sum of this with the collision duration from particles 7 and 8 is smaller than $\Delta t$ the two collisions are separate. If the sum is larger than $\Delta t$ the two collisions are overlapping. All particles in the last two situations have to be checked for new collision partners or remaining overlap. In the case of new collision partners, the collisions have to be solved again. In the case of remaining overlap they get a special tag, and in the case of no remaining collision partners nothing has to be done in the next time step.

4. Results

In this section the first results of the new integration scheme will be shown. First tests are done for a bounding box problem. This problem consists of a cubic box, with sizes ranging from 8 to 100 times the particle diameter, randomly filled with particles. The particles have zero mean velocity and are given a velocity drawn from a Gaussian distribution. The maximum velocity, solids fraction and the box size can be varied to scale the problem. The properties of the simulation are given in Table 4 and are inspired by simulations of a fluidized bed (see Fig. 1), to match the solids holdup and the granular temperature. For the particle-wall contacts we assume the same restitution coefficient as for particle-particle contacts.

4.1. Speed up and scalability

The first test involves a bounding box containing 4000 particles with a solids volume fraction of 40%. The particles are allowed to freely bounce in the box for 0.1 s of real time. Simulations were conducted using both the new collision integration scheme and the classical soft sphere scheme. This resulted in on average 50 collisions per particle and 0.4 multibody collisions per particle. In this test the particles have ideal collision properties. This implies that the total energy in the system should remain constant. The normalized total kinetic energy of the particles is shown in Fig. 5. The total energy is normalized to the energy given at $t=0$.

The classical soft sphere method shows regular dips in the energy-level, associated with energy being stored in the springs as a consequence of the collisions. The hybrid model has a largely static energy profile as most collisions are binary. Both models are capable of maintaining proper energy conservation, as expected. The difference is however that the hybrid model is about eight times faster.

To test for the scalability of the hybrid model and the robustness of the gained speed up, the size of the bounding box is gradually increased to $10^6$ particles. The relative speed up for these systems is shown in Fig. 6. It can be seen that an average speed up of a factor 8 is possible with the new hybrid collision integration scheme. This speed up can be attributed to the lower number of collision detection evaluations that are necessary. The maximum possible speed-up factor 10 is not reached because of the overhead associated with the check for overlapping collisions, as discussed in the previous section and Table 3.

4.2. Varying restitution coefficient

To check if the two models work for a varying restitution coefficient the simulations were run with $e=0.7$, 0.8, 0.9 and 0.97 and a solids volume fraction of 50%. The time duration was about 0.05 s real time, allowing for 75% of the total energy to dissipate. The result is presented in Fig. 7. It can be seen that in the first few time steps no energy is lost, because the particles are initialized on
a lattice and no collisions take place. With lowering the restitution coefficient the energy drops faster, as can be expected. The agreement between the two schemes is very good.

4.3. Number of contact partners

For the new hybrid model to be competitive with the classical soft sphere model, it has to be capable of dealing with systems with similar solids fractions and granular temperatures. It is the combination of these two parameters that determines the amount of multibody collisions. For this reason a simulation was run with a solids fraction of 50% and a maximum velocity of 0.15 m/s. The results are shown in Fig. 8. The left figure shows the normalized energy levels per time step for a bounding box problem with ε = 1. In black the classical soft-sphere method is given, in green the new hybrid model.

<table>
<thead>
<tr>
<th>Case</th>
<th>Schematic</th>
<th>t_{last} + (Δt - t_{last})</th>
<th>Solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><img src="image1.png" alt="Diagram 1" /></td>
<td>&lt;Δt</td>
<td>Next time step N=2</td>
</tr>
<tr>
<td>2</td>
<td><img src="image2.png" alt="Diagram 2" /></td>
<td>&gt;Δt</td>
<td>MBC this time step</td>
</tr>
<tr>
<td>3</td>
<td><img src="image3.png" alt="Diagram 3" /></td>
<td>&gt;Δt</td>
<td>MBC this time step</td>
</tr>
</tbody>
</table>

### Table 3
Overview of the three different situations in case of possible overlapping collisions with $t_{last}$ the duration of the collision of particles 7 and 8 at $2\Delta t$ defined by Eq. (13) and $t_{last}$ the duration of the contact between 6 and 7 at $1\Delta t$.

<table>
<thead>
<tr>
<th>Case</th>
<th>Schematic</th>
<th>$t_{last} + (\Delta t - t_{last})$</th>
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<td>Next time step N=2</td>
</tr>
<tr>
<td>2</td>
<td><img src="image2.png" alt="Diagram 2" /></td>
<td>&gt;Δt</td>
<td>MBC this time step</td>
</tr>
<tr>
<td>3</td>
<td><img src="image3.png" alt="Diagram 3" /></td>
<td>&gt;Δt</td>
<td>MBC this time step</td>
</tr>
</tbody>
</table>

### Table 4
Parameter values used for the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_s$</td>
<td>0.4-0.5</td>
</tr>
<tr>
<td>$N_p$</td>
<td>$10^3$-$10^6$</td>
</tr>
<tr>
<td>$d_p$</td>
<td>0.003 m</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2500 kg/m$^3$</td>
</tr>
<tr>
<td>$k_n$</td>
<td>20,000 N/m</td>
</tr>
<tr>
<td>$e$</td>
<td>0.7-1.0</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1</td>
</tr>
<tr>
<td>$\mu$</td>
<td>0</td>
</tr>
<tr>
<td>$\langle v_n \rangle$</td>
<td>0 m/s</td>
</tr>
<tr>
<td>$v_{t_1}$</td>
<td>0 m/s</td>
</tr>
<tr>
<td>$v_{max}$</td>
<td>$\pm 0.025$-$0.15$ m/s</td>
</tr>
</tbody>
</table>

### Fig. 5
Normalized energy levels per time step for a bounding box problem with $\varepsilon=1$. In black the classical soft-sphere method is given, in green the new hybrid model.
energy of the system for the two schemes, the figure on the right shows the probability of the number of contact partners, with 2 being binary and every higher number signifying extra particles participating in the collision. It can be seen that the two models show the same trend, now with more energy stored in the springs for the classic model. The amount of multibody collisions add up to about 5% of all collisions which matches the result of Fig. 1. The number of contact partners is also shown for the scaled model. The first thing that can be seen is that the scaled scheme has a very sudden and large drop in energy, associated with a lot of particles going into collision at the same time, often with multiple collision partners. Binary collisions only make up for 65% of all collisions. The rate of energy loss is also much slower than for the classical and the hybrid schemes. This underestimation of the dissipation rate is entirely attributable to the number of multibody contacts and was also found for pure multibody contacts in Pournin et al. (2001). The relative speed up of the scaled model is only in the order of 2.5. The poor performance of this scaled classic model, in terms of both the energy conservation and the speed up of the model, shows the power and need of a hybrid model all the more.

5. Conclusions

A novel hybrid collision integration scheme based on the classical soft-sphere and hard-sphere schemes is presented. Most of the prevailing collisions for a typical dense gas-particle flow problem were shown to be binary, which can be accurately handled in a single time step. All Multi-Body Contacts are handled using a classical soft-sphere methodology. The time step of this new scheme was taken to be exactly the duration of a collision, based on the linear spring-dashpot force model.

This novel scheme benefits from a reduction in the number of time steps, by skipping the numerical integration for all binary collisions, and the reduction in the number of collision detection steps. As such, a typical speed-up factor 8 was found for this new scheme, while retaining energy and momentum conservation. Even more so, because for the larger part of the system no energy is stored in the springs of the contact model, the instantaneous velocities of the particles represent the true velocity of the energy state of the system.
The results from this scheme were scalable for the number of particles within the system and showed very good comparison for varying restitution coefficients. The novel scheme is capable of simulating reasonably dense systems, with sufficient energy to resemble an actual granular flow problem.

It was also found that relaxing the spring stiffness of the classical scheme, to match the time step of the hybrid scheme, resulted in an energy dissipation rate that differs distinctly from the classical and novel scheme. Moreover, because of the number of collision partners for each particle, the simulation was only 2.5 times faster with a 10 times larger time step. As such there is a trade off between not over-relaxing the spring stiffness, and not using a too small time step to be able to handle a sufficient amount of particles. With the novel scheme, simulations can either be faster and/or bigger.

The work discussed here serves as a base of principle for a novel hybrid collision integration scheme. For future work we expect to extend the model to include rotation, solid-fluid coupling, non-spherical particles and applications within granular flow problems.

Acknowledgments

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Appendix A

This appendix serves as a precursor to Appendices B and C. This appendix gives the full derivation for the linear ordinary homogeneous second order differential equation related to the linear spring-dashpot model:

\[ m_{\text{eff}}\ddot{x} + \nu \dot{x} + kx = 0 \]  \hspace{1cm} (15)

This expression signifies the relation between the acceleration, the velocity and the position. Now we will define a few new parameters, the natural frequency:

\[ \omega_n = \sqrt{\frac{k}{m_{\text{eff}}}} \]  \hspace{1cm} (16)

the damping ratio:

\[ \zeta = \frac{\nu}{2m_{\text{eff}}\omega_n} \]  \hspace{1cm} (17)

and the damped frequency:

\[ \omega_d = \omega_n \sqrt{1 - \zeta^2} \]  \hspace{1cm} (18)

With these parameters Eq. (15) can be rewritten as:

\[ \frac{1}{2} \ddot{x} + \zeta \omega_n \dot{x} + \frac{1}{2} \omega_n^2 x = 0 \]  \hspace{1cm} (19)

This ODE has a solution of the form of \( x = e^{st} \). Upon substitution of \( x = e^{st} \) into Eq. (19) and division by \( e^{st} \) we obtain the characteristic polynomial in terms of parameter \( s \):

\[ \frac{1}{2}s^2 + \zeta \omega_n s + \frac{1}{2} \omega_n^2 = 0 \]  \hspace{1cm} (20)

with roots of the characteristic equation given by:

\[ -\zeta \omega_n \pm \sqrt{\zeta^2 \omega_n^2 - \omega_n^2} = \left( -\zeta \pm \sqrt{\zeta^2 - 1} \right) \omega_n \]  \hspace{1cm} (21)

If \( \zeta < 1 \) than we have an under damped system and a general solution of the form:

\[ x(t) = c_1 e^{(-\zeta + \sqrt{\zeta^2 - 1}) \omega_n t} + c_2 e^{(-\zeta - \sqrt{\zeta^2 - 1}) \omega_n t} \]  \hspace{1cm} (22)

which can be rewritten with the use of Euler’s formula as:

\[ x(t) = e^{-\zeta \omega_n t} \left( d_1 \cos(\omega_d t) + d_2 \sin(\omega_d t) \right) \]  \hspace{1cm} (23)

Now we need to define the initial conditions to solve for the two integration conditions \( d_1 \) and \( d_2 \). At \( t=0 \) we have:

\[ x(t = 0) = x_0 \]

\[ v(t = 0) = v_0 \]

Combination with Eq. (22) gives:

\[ x(0) = e^{-\zeta \omega_n 0} \left( d_1 \cos(\omega_d 0) + d_2 \sin(\omega_d 0) \right) \]  \hspace{1cm} (24)

\[ x(0) = e^{-\zeta \omega_n 0} \left( d_1 \cos(\omega_d 0) + d_2 \sin(\omega_d 0) \right) \]  \hspace{1cm} (25)

\[ x(0) = d_1 \]

\[ x(t) = e^{-\zeta \omega_n t} \left( x_0 \cos(\omega_d t) + d_2 \sin(\omega_d t) \right) \]  \hspace{1cm} (26)

Differentiation of this function leads to:
\( x(t) = e^{-\omega dt} \left[ x_{0u} \sin (\omega dt) + d_{2u} \cos (\omega dt) - \zeta_{0u} \left[ x_{0} \cos (\omega dt) + d_{2} \sin (\omega dt) \right] \right] \)

\( x(0) = v_{0} = (d_{20u} + \zeta_{0u} x_{0}) \cos (\omega dt) + (x_{0u} + \zeta_{0u} d_{2}) \sin (\omega dt) \)

\[
\begin{align*}
\frac{d_{2}}{\omega_{u}} &= \frac{v_{0} + \zeta_{0u} x_{0}}{\omega_{u}} \\
\end{align*}
\]

(27)

and:

\( x(t) = e^{-\omega dt} \left[ x_{0} \cos (\omega dt) + \frac{v_{0} + \zeta_{0u} x_{0}}{\omega_{u}} \sin (\omega dt) \right] \)

(28)

To continue our derivation we will first assume \( x_{0} = 0 \). For two colliding spheres this is correct, since we will always solve for the full collision:

\( x(t) = v_{0} e^{-\omega dt} \left[ \frac{1}{\omega_{u}} \sin (\omega_{u} dt) \right] \)

(29)

\( x(t) = v_{0} e^{-\omega dt} \left[ \cos (\omega_{u} dt) + \frac{\zeta_{0u}}{\omega_{u}} \sin (\omega_{u} dt) \right] \)

(30)

From Eq. (29) it is easy to see that the duration of a collision is given by \( \frac{\pi}{\omega_{u}} \).

**Appendix B**

The maximum overlap is given when the relative velocity is zero:

\( \dot{x}(t) = v_{0} e^{-\omega dt} \left[ \cos (\omega_{u} dt) - \frac{\zeta_{0u}}{\omega_{u}} \sin (\omega_{u} dt) \right] = 0 \)

(31)

\[
A \cos (bx) + B \sin (bx) = \sqrt{A^2 + B^2} \cos \left( bx - \tan^{-1} \frac{B}{A} \right)
\]

(i)

Using identity (i) we can simplify Eq. (31) to:

\[
\cos (\omega_{u} dt) - \frac{\zeta_{0u}}{\omega_{u}} \sin (\omega_{u} dt) = \sqrt{1 - \left( \frac{\zeta_{0u}}{\omega_{u}} \right)^2} \cos (\omega_{u} dt) - \tan^{-1} \frac{\zeta_{0u}}{\omega_{u}} = 0
\]

(32)

Taking only the time dependent part:

\[
\cos \left( \omega_{u} dt - \tan^{-1} \frac{\zeta_{0u}}{\omega_{u}} \right) = 0
\]

Upon rearranging we get:

\[
\omega_{u} dt - \tan^{-1} \frac{\zeta_{0u}}{\omega_{u}} = \frac{\pi}{2}
\]

Solving for \( t \) and using several trigonometric identities we obtain:

\[
\frac{\pi}{2} - \tan^{-1} (x) = \cos^{-1} \left( \frac{x}{\sqrt{1 + x^2}} \right)
\]

(ii)

\[
\cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u} \sqrt{1 + \frac{\zeta_{0u}^2}{\omega_{u}^2}}} \right) = \frac{\pi}{2} - \tan^{-1} \frac{\zeta_{0u}}{\omega_{u}}
\]

\[
\frac{\pi}{2} - \tan^{-1} \left( \frac{\zeta_{0u}}{\omega_{u}} \right) = \cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u} \sqrt{1 + \frac{\zeta_{0u}^2}{\omega_{u}^2}}} \right)
\]

(33)

\[
\cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u} \sqrt{1 + \frac{\zeta_{0u}^2}{\omega_{u}^2}}} \right) = \frac{\pi}{2} - \tan^{-1} \left( \frac{\zeta_{0u}}{\omega_{u}} \right)
\]

(34)

If we substitute this into the equation for the relative distance (overlap) we obtain:

\[
x_{\text{max}} = v_{0} e^{-\omega dt} \left( \frac{1}{\omega_{u}} \sin \left( \omega_{u} dt \omega_{u} dt \right) \cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u}} \right) \right)
\]

(35)

\[
\sin \left( \cos^{-1} (x) \right) = \sqrt{1 - x^2}
\]

(iii)

Using identity (iii) and the definitions of \( \omega_{d} \) and \( \omega_{n} \) to simplify Eq. (35):

\[
x_{\text{max}} = v_{0} e^{-\omega dt} \cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u}} \right)
\]

(36)

\[
x_{\text{max}} = \frac{v_{0}}{k_{n}} \sqrt{\frac{m_{\text{eff}}}{m}} \cos^{-1} \left( \frac{\zeta_{0u}}{\omega_{u}} \right)
\]

(37)

We could thus determine the spring stiffness by solving the above equation for \( k_{n} \) to obtain:

\[
k_{n} = \frac{v_{0}^{2} m_{\text{eff}} \sqrt{1 - \zeta_{0u}^2}}{x_{\text{max}}^2}
\]

(38)

The damping factor \( \zeta \) might be thought to depend on \( k \) via both the damping coefficient \( \eta \) and the natural frequency \( \omega_{n} \). However the spring stiffness factors out:

\[
\zeta = \sqrt{2 \ln(e) \frac{k_{n} m_{\text{eff}}}{2 m_{\text{eff}} \frac{k_{n}}{m}}} = \frac{-\ln(e)}{\sqrt{\ln(e) + \ln(e)^2}}
\]

which gives:

\[
k_{n} = \frac{v_{0}^{2} m_{\text{eff}} \sqrt{1 - \zeta_{0u}^2}}{x_{\text{max}}^2} \left( \frac{2 \ln(e) \frac{k_{n} m_{\text{eff}}}{2 m_{\text{eff}} \frac{k_{n}}{m}}} \right) \cos^{-1} \left( \frac{-\ln(e)}{\sqrt{\ln(e) + \ln(e)^2}} \right)
\]

(39)

This expression indicates that the spring stiffness depends on the maximum overlap the maximum relative velocity and the effective mass of the collision pair. This is then corrected for damping with the exponential part of the function. The nice thing is that when restitution is 1 the exponential part is equal to 1, giving:

\[
k_{n} = \frac{v_{0}^{2} m_{\text{eff}}}{x_{\text{max}}^2}
\]

(40)

**Appendix C**

Derivation of the update of the tangential velocity and the friction limit following the hard sphere approach is as follows:

\[
m_{\text{eff}}(v_{0} - \bar{v}_{0}) = f
\]

(41)
\[ l_a(\omega_a - \omega_{a,0}) = -\left( R_a n_{ab} \right) \times f \]  
with \( f \) given as:  
\[ f = f_n + f_t \]  
\[ f_n = -(1 + \varepsilon) \frac{\dot{q}_{ab,0} \cdot n_{ab}}{B_2} \]  
\[ f_t = -(1 + \beta) \frac{\dot{q}_{ab,0} \cdot l_{ab}}{B_1} \]  
or for the sliding limit if:  
\[ \mu < \frac{(1 + \beta) \dot{q}_{ab,0} \cdot l_{ab}}{|l_{ab}| B_1} \]  
with \( B_1 \) and \( B_2 \) defined as:  
\[ B_2 = \frac{1}{m_a} + \frac{1}{m_b} \]  
\[ B_1 = \frac{7}{2} \left( \frac{1}{m_a} + \frac{1}{m_b} \right) \]  
still assuming spheres of equal mass we now have for the normal velocity:  
\[ m(\dot{q}_n - \dot{q}_{a,0}) = -(1 + \varepsilon) \frac{\dot{q}_{ab,0} \cdot n_{a,0}}{B_2} - (1 + \beta) \frac{\dot{q}_{ab,0} \cdot l_{a,0}}{B_1} \]  
rearranging and discarding the mass leaves:  
\[ \dot{q}_n = \dot{q}_{a,0} - (1 + \varepsilon) \frac{\dot{q}_{ab,0} \cdot n_{a,0}}{2} - (1 + \beta) \frac{\dot{q}_{ab,0} \cdot l_{a,0}}{7} \]  
To obtain the normal and tangential component we can now simply project it onto the normal and tangent:  
\[ \dot{q}_{n,R} = \dot{q}_{a,0,n} - (1 + \varepsilon) \frac{\dot{q}_{ab,0} \cdot n_{a,0}}{2} \]  
\[ \dot{q}_{n,T} = \dot{q}_{a,0,t} - (1 + \beta) \frac{\dot{q}_{ab,0} \cdot l_{a,0}}{7} \]  
The sliding limit can be rewritten in terms of the initial ratio of the projection of the relative velocity in the normal and tangential directions, or also the impact angle:  
\[ \mu < \frac{(1 + \beta) \left| \frac{\dot{q}_{ab,t} \cdot l_{ab}}{\dot{q}_{ab,0} \cdot l_{ab}} \right|}{(1 + \varepsilon) \left| \frac{\dot{q}_{ab,t} \cdot n_{ab}}{\dot{q}_{ab,0} \cdot n_{ab}} \right| B_1} \]  
\[ \mu < \frac{(1 + \beta) \left| \frac{\dot{q}_{ab,t} \cdot l_{ab}}{\dot{q}_{ab,0} \cdot l_{ab}} \right| B_2}{(1 + \varepsilon) \left| \frac{\dot{q}_{ab,t} \cdot n_{ab}}{\dot{q}_{ab,0} \cdot n_{ab}} \right| B_1} \]  
\[ \mu < \frac{(1 + \beta) \left| \frac{\dot{q}_{ab,t} \cdot l_{ab}}{\dot{q}_{ab,0} \cdot l_{ab}} \right| 7}{(1 + \varepsilon) \left| \frac{\dot{q}_{ab,t} \cdot n_{ab}}{\dot{q}_{ab,0} \cdot n_{ab}} \right| 2} \]  

In which case:  
\[ \dot{q}_{a,t} = \dot{q}_{a,0,t} + \mu (1 + \varepsilon) \left( \frac{\dot{q}_{ab,0} \cdot \dot{q}_{ab,t}}{2} \right) \]  

## References


