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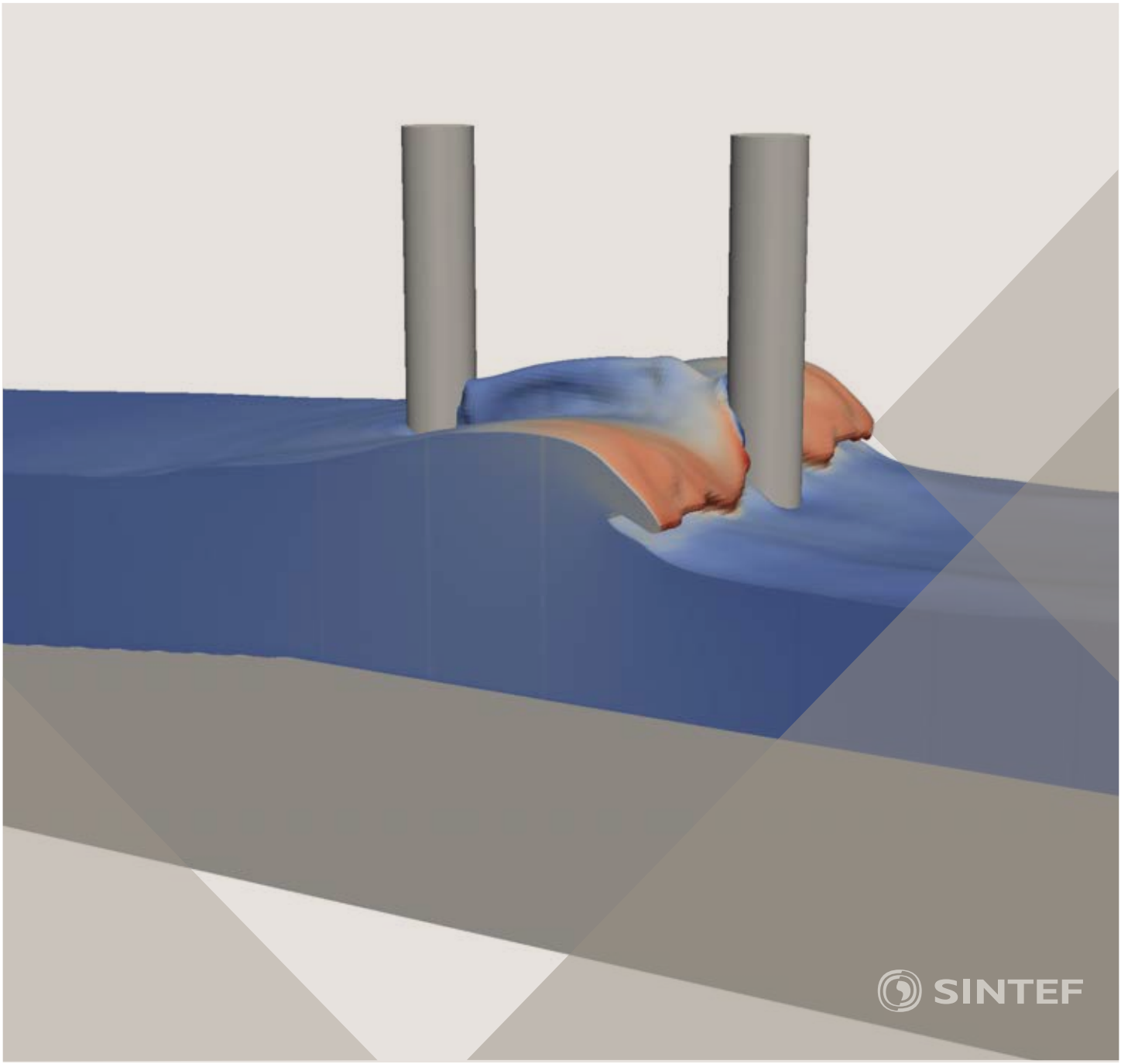
Progress in Applied CFD – CFD2017



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Editors:
Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

NOVEL EFFICIENT HYBRID-DEM COLLISION INTEGRATION SCHEME

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ABSTRACT

A hybrid collision integration scheme is introduced, benefiting from the efficient handling of binary collisions in the hard sphere scheme and the robust time scaling of the soft sphere scheme. In typical dynamic dense granular flow, simulated with the soft sphere scheme, the amount of collisions involving more than two particles are limited, and necessarily so because of loss of energy decay otherwise. Because most collisions are binary, these collisions can be handled within one time step without the necessary numerical integration as needed in a soft sphere method. The remainder of the collisions can still be handled with the classical soft sphere scheme. In this work the hybrid collisions integration scheme is shortly described and tested with a bounding box problem. The hybrid scheme is capable of solving the same problem as a classic soft sphere scheme but is roughly one order of magnitude faster.

Keywords: Discrete Element Method, Collision integration scheme, optimization .

NOMENCLATURE

Greek Symbols

δ	overlap, $[m]$
ω	frequency, $[1/s]$
ζ	damping ratio, $[-]$
η	damping coefficient, $[Ns/m]$
μ	friction coefficient, $[-]$
β	tangential restitution coefficient, $[kg/m^3]$
ρ	density, $[kg/m^3]$
ϕ	solids volume fraction, $[-]$

Latin Symbols

$\bar{F}$	force, $[kgm/s^2]$.
$\bar{J}$	impuls, $[kgm/s]$.
B	collision constant, $[kg^{-1}]$.
R	norm of distance, $[m]$.
N	number of particles, $[-]$.
$\bar{v}$	velocity, $[m/s]$.
t	time, $[s]$.
m	mass, $[kg]$.
k	spring stiffness, $[N/m]$.
$\bar{n}$	normal unit vector, $[-]$.
e	restitution coefficient, $[-]$.
f	frequency, $[1/s]$.
$\bar{x}$	position vector, $[m]$.
$\bar{r}$	distance vector, $[m]$.
p	position, $[m]$.
d	diameter, $[m]$.
c	integration constant, $[-]$.

Sub/superscripts

0	old time step
n	normal
d	dampened
t	tangential
$coll$	collision
a,b	paritcles a,b
$last$	duration of lasting collision
i	index i
max	maximum
s	solids
eff	effective

INTRODUCTION

Since the introduction of the Distinct Element Model (DEM) by Cundall and Strack (1979) for perfect spheres the field of granular flow modelling has expanded dramatically. The model by Cundall and Strack (1979) has since then been extended for various external forces (Xu and Yu, 1997; Pournin *et al.*, 2005; Lu *et al.*, 2015; Marshall, 2009; Mikami *et al.*, 1998; Korevaar *et al.*, 2014; Zastawny *et al.*, 2012). For an overview of the relevant inter-particle and particle-fluid forces see Zhu *et al.* (2007). DEM has been used to model various granular flows as found in industrial applications, 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 more comprehensive overview of these applications can be found in the work of Zhu *et al.* (2008).

The foundation of these models is however the contact model, of which the hard sphere model as discussed by Hoomans *et al.* (1996) and a soft sphere model by Tsuji *et al.* (1993) are the most well known. The hard-sphere approach works on the assumption that all collisions are binary and instantaneous. As such the model only handles particle-pair interactions that follow each other in chronological order. Therefore the hard-sphere model is an event-driven scheme and the simulation time scales with the collision frequency, which scales with the solids fraction and the granular temperature of the system. The hard-sphere scheme is most suited for rather dilute systems, as with increasing solids fraction

and granular temperature the number of collisions increases drastically.

For more dense and highly dynamic systems a soft-sphere method is more often used. The soft-sphere method allows for particle-particle overlap and represents the forces associated with the indentation of the solids with a spring-dashpot system. The spring handles the repulsion and the dashpot handles energy dissipation. The duration of the collision is no longer instantaneous and scales with the ratio of the spring stiffness and the mass of the particle. Because of the finite duration of the collision multiple particles can be in contact at the same time, in this work denoted as Multi-Body Collisions (MBC). Numerical integration of the forces over time allows for proper treatment of the collisions. The soft-sphere method is thus a time-driven scheme.

Both methodologies have their strengths and limitations. The hard-sphere model benefits from the immediate handling of a collision, while the soft-sphere method benefits from the relaxation of the spring-stiffness and thus larger time step. The most time-consuming step in the simulations however is the collision detection, which for the hard-sphere has to be updated with a frequency related to the number of events and for the soft-sphere has to be performed every particle time step; roughly ten times per duration of the collision. Reducing the number of collision detection evaluations thus massively increases the simulation efficiency.

In the soft-sphere method, for dynamical systems, most of the collisions will still be binary. And they have to be mostly binary, because else the energy dissipation rate is no longer maintained, as we will show later. In one of our simulations from earlier work (Buist *et al.* (2015)) we indeed found that most collisions involved only two particles, as can be seen in figure 1.

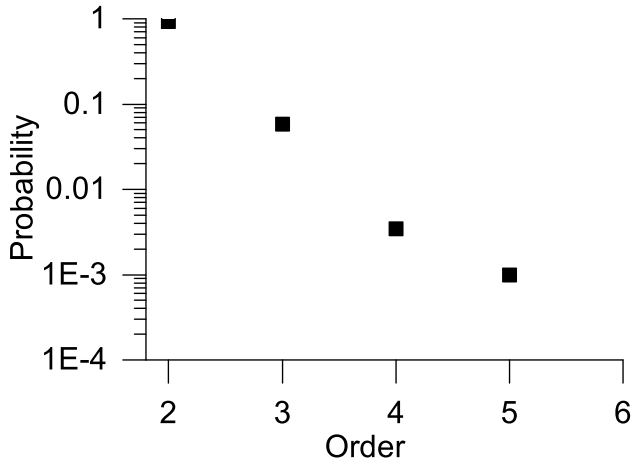


Figure 1: Collision order probability from a simulation of a pseudo 2D fluidized bed, with $\varepsilon = 0-0.6$, $u_{mf} = 3.5$ m/s, $e = 1$, $\beta = 0.33$, $\mu = 0.1$.

All of these binary collisions can of course be handled instantaneously, following the analytical solution of the dampened harmonic oscillator. The binary collision maintains a finite duration and the task that remains is to be able to distinguish between binary collisions and Multi-Body contacts. These MBC's have to be solved with a classical soft-sphere method. The collisions have to be determined only once, and only for the particles colliding in two subsequent time steps additional checks have to be made. The time-step of the simulation is now exactly the duration of a collision, and collision-detection has to be performed only once for most of the particles. This work is a short version of a publication in Chemical Engineering Science, containing the main idea of the hybrid collision integration scheme and the main results. For more details the interested reader is referred to Buist *et al.* (2016).

MODEL DESCRIPTION

The hybrid model is in spirit somewhere in between a hard sphere and a soft sphere methodology. In this work however we will not go into the details of these two methods, for an extensive explanation of both schemes the interested reader is referred to Deen *et al.* (2007).

Hybrid DEM

The new integration scheme can either be viewed as a time-driven hard sphere model with a finite collision duration or as a semi one-step soft sphere model. A time-driven hard sphere approach was first developed by 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). 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 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.

In the hybrid collision integration scheme that is presented here, the chosen time step is exactly the same as the duration of a collision, following the linear spring dashpot model. Because most collisions are assumed to be binary these collisions can be handled at once, following a modified hard sphere approach. And because the time step is the same as the collision duration, only one collision per particle per time step can happen. The only exceptions are the multi-body collisions, that are handled with the classical soft sphere methodology. For the particles involved in a multi-body collision, the time step is divided in ten sub steps. A short schematic overview is given in table 1.

The gain in speed-up is in the use of the collision detection algorithm, which generally has to take place only once every time step, instead of ten times in the classical soft-sphere scheme. Of course the actual choice of the type of collision detection algorithm will have a major impact on the final performance of the codes. In this work the same collision detection algorithm is used for both the classical soft-sphere method and the hybrid method; a kd-tree algorithm from Matlab.

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

Binary collisions

We assume particles are of equal size and mass possessing no tangential component ($\mu = 0$ and $v_{t,0} = 0$). For a binary collision it follows that:

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

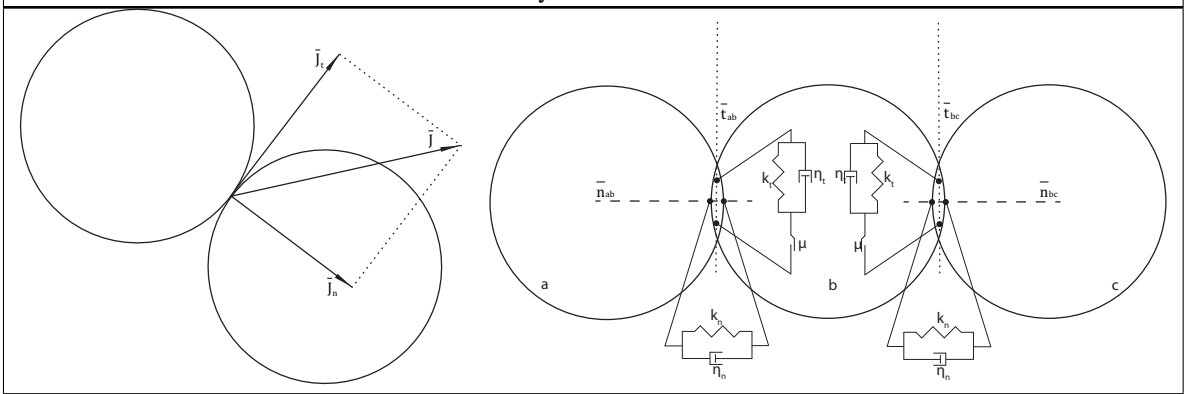
with $\bar{v}_{ab}$ defined as the relative velocity at the point of contact:

$$\bar{v}_{ab} = \bar{v}_a - \bar{v}_b + (\bar{\omega}_a R_a + \bar{\omega}_b R_b) \times \bar{n}_{ab} \tag{2}$$

which consists of a normal and a tangential component:

$$\bar{v}_{ab,n} = (\bar{v}_{ab} \cdot \bar{n}_{ab})\,\bar{n}_{ab} \tag{3}$$

Table 1: Short overview of the hybrid collisions schemes.

Hybrid model	
	
Binary	Multibody
$\bar{v}_{n,a} = \bar{v}_{n,a,0} - \frac{1+e}{2}\bar{v}_{ab,n}$	$\bar{F}_n = -k_n\delta_n\bar{n}_{ab} - \eta_n\bar{v}_{ab,n}$
$\bar{x}_a = \bar{x}_{a,0} + \frac{\bar{v}_a+\bar{v}_b}{2}\Delta t + (\bar{v}_a - \bar{v}_{n,a,0})\,t_{last}$	$\bar{F}_t = -k_t\delta_t\bar{t}_{ab} - \eta_t\bar{v}_{ab,t}$
	or in case of sliding($\bar{F}_t > \mu\lvert\bar{F}_n\rvert$):
$t_{last} = \frac{\left(\bar{r}_{ab}\cdot\bar{v}_{ab} + \sqrt{(\bar{r}_{ab}\cdot\bar{v}_{ab})^2 - (\lvert\bar{r}_{ab}\rvert - (R_a+R_b))^2\lvert\bar{v}_{ab}\rvert}\right)}{\lvert\bar{v}_{ab}\rvert}$	$\bar{F}_t = -\mu\lvert\bar{F}_n\rvert\bar{t}_{ab}$
Time scale collision $t_{coll} = \frac{\pi}{\omega_d}$	Time scale collision $t_{coll} \leq \frac{\pi}{\omega_d}$
Time step $\Delta t = t_{coll}$	Time step dilation in case of multibody $\Delta t = \frac{t_{coll}}{10}$

$$\bar{v}_{ab,t} = \bar{v}_{ab} - \bar{v}_{ab,n} \tag{4}$$

$$\bar{n}_{ab} = \frac{\bar{x}_b - \bar{x}_a}{|\bar{x}_b - \bar{x}_a|} \tag{5}$$

$$\bar{t}_{ab} = \frac{\bar{v}_{ab,t}}{|\bar{v}_{ab,t}|} \tag{6}$$

Finally the position is defined as:

$$\bar{x} = \bar{x}_0 - \bar{v}_0 t_{last} + \frac{\bar{v}_a + \bar{v}_b}{2}\Delta t + \bar{v}t_{last} \tag{7}$$

That is, the new position is the sum of respectively the old position, the displacement until collision based on the old velocity, a shared mean displacement of the two particles during collision and a displacement after the collision till the end of the time step.

Here, $\bar{x}_0$ and $\bar{v}_0$ are the position and velocity at the time step before collision, and $\bar{x}$ and $\bar{v}$ the position and velocity at the time step after the collision. t_{last} is the time between the moment of first contact until the end of the time step. These are given by:

$$\bar{r}_{ab} = \bar{x}_{a,0} - \bar{x}_{b,0}$$

$$\bar{v}_{ab} = \bar{v}_{a,0} - \bar{v}_{b,0}$$

$$t_{last} = \frac{\left(\bar{r}_{ab}\cdot\bar{v}_{ab} + \sqrt{(\bar{r}_{ab}\cdot\bar{v}_{ab})^2 - (|\bar{r}_{ab}| - (R_a+R_b))^2\,|\bar{v}_{ab}|}\right)}{|\bar{v}_{ab}|} \tag{8}$$

Multi-body collisions

The analytical solution to multi-body contacts follows a very similar equation as those for binary collisions:

$$x_i(t) = \sum_{i=1}^{n} e^{-\zeta\omega_n t}\left(d_{1,i}\cos(\omega_{d,i}t) + d_{2,i}\sin(\omega_{d,i}t)\right) \tag{9}$$

where n is the number of contacts. 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. On top of this because of the added amplitudes and frequencies the collision can take both longer and shorter than the original binary collision duration.

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, see also table 1.

Overview of DEM code

Here we will give a brief description of the code. The code is build using MATLAB for simple training purposes. To allow each binary collision to be uniquely described the time step is taken as exactly the duration of a collision following the soft-sphere approach, given by:

$$\Delta t = t_{coll} = \frac{\pi}{\omega_d} = \frac{\pi}{\sqrt{\frac{k_n}{m_{eff}}\left(\sqrt{1-\zeta^2}\right)}} \tag{10}$$

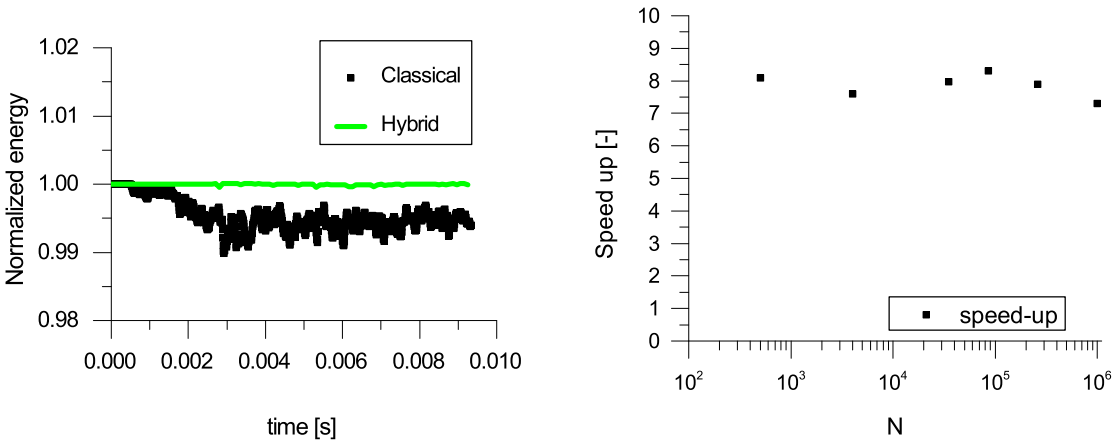


Figure 2: Normalized energy levels per time step for a bounding box problem with e=1. In black the classical soft-sphere method is given, in green the new hybrid model (left). Speed up as a function of the number of particles N (right).

where ω_d is the dampened frequency defined as:

$$\omega_d = \sqrt{\frac{k_n}{m_{eff}}}\left(\sqrt{1-\zeta^2}\right)$$

where ζ is the damping ratio defined as:

$$\frac{-ln(e)}{\sqrt{\pi^2 + ln(e)^2}}$$

A collision detection algorithm; a kd-tree searcher, from MATLAB is used to detect all particles that have overlap. For these particles the duration of the contact is determined using equation 8 and subsequently the collision is processed with the method described earlier. For multi-body collisions the duration of a collision can be slightly longer or shorter as described before. In case the collision takes longer the information has to be appropriately transferred across time steps.
Additionally, checks have to be made for particles that are colliding in two subsequent time steps, because the two collisions might be overlapping, in essence being a multi-body collision. this has extensively been discussed in Buist *et al.* (2016).

RESULTS

Table 2: Parameter values used for the simulations.

parameter	value	
ϕ_s	0.4-0.5	
N_p	$10^3 - 10^6$	
d_p	0.003	m
ρ	2500	kg/m^3
k_n	20000	N/m
e	0.7-1.0	
β	1	
μ	0	
$< v_n >$	0	m/s
v_t	0	m/s
v_{max}	± 0.15	m/s

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 randomly filled with particles, with sizes ranging from 8 to 100 times the particle diameter. 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 simulation data is given in table 2 and are inspired by simulations of a fluidized bed (see figure 1), to match the solids holdup and granular temperature. For the particle-wall contacts we assume the same restitution coefficient as for particle-particle contacts.

Speed up & 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 as well as 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 figure 2. 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 include 10^6 particles. The relative speed up for these systems is shown in figure 2. It can be seen that an average speed up of a factor 7 to 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.

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 sys-

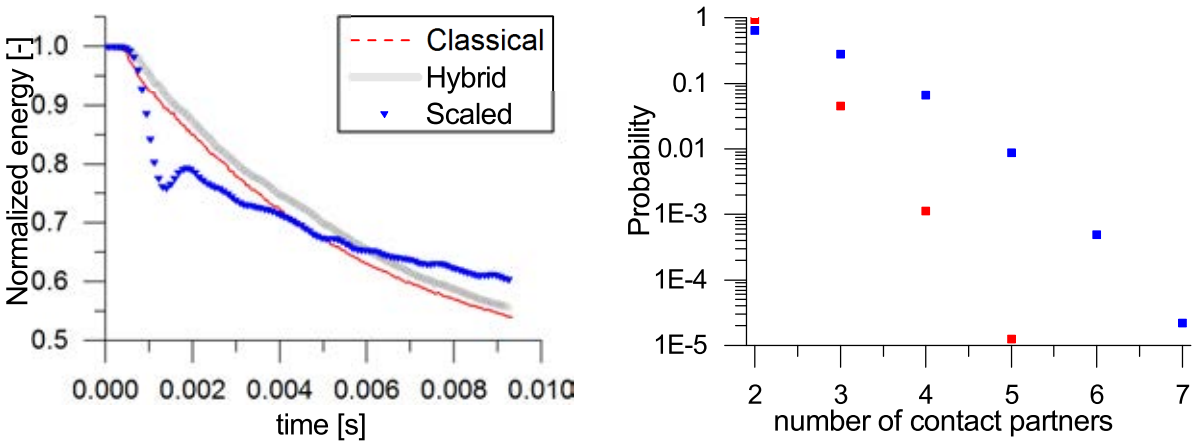


Figure 3: Normalized energy loss over time for the two schemes (left), collision order probability (right), for a bounding box problem with $\varepsilon = 0.5$, $e = 0.9$, $\mu = 0$.

tems 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 figure 3. The left figure shows the normalized 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 figure 3. The hybrid model is thus able to match the density and energy of systems in which typically a soft sphere model is used.

Relaxing the classical scheme

In the classical scheme it is also possible to scale the duration of a collision by scaling the spring stiffness. By reducing the spring stiffness by a factor 100, the duration of a collision is multiplied by a factor ten, i.e. the same as for our hybrid model. This will reduce computation time but will also increase the overlap between colliding particles.

To see if this affects the energy balance of the system, the results of such scaling of the spring stiffness is quantified for the same simulation as before, figure 3 in comparison to the classical and the hybrid schemes. 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 entering collision mode 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 smaller 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. Second, the lower rate of energy dissipation means that the choice of a proper spring stiffness is critical in obtaining meaningful results, especially for dense dynamical systems.

CONCLUSIONS

Most collisions in a soft-sphere granular flow problem are necessarily binary that can be accurately described within one time step. Because of the possible distinction between binary and multi-body contacts a hybrid collision integration scheme was proposed. The binary collisions are solved with a modified hard-sphere approach with a collision duration equal to the classic linear spring dashpot and all multi-body contacts are handled with the classic soft-sphere approach.

The larger time-step of this hybrid integration scheme and the lower amount of collision detection evaluations allows for a factor 7 to 8 computational speed-up. Meanwhile retaining energy and momentum conservation. Because a lower amount of energy is stored in the springs of the spring-dashpot model the energy state of the hybrid scheme more accurately describes the granular behaviour of the system.

The results of this scheme were shown to be scalable with the number of particles up to at least O(10^6) and is capable of handling systems with a solids hold-up and granular temperature resembling the collision dynamics in an actual granular flow system.

Further relaxation of the spring-stiffness in the classical scheme to allow for a similar increase in time-step has proven to be inadequate to quantitatively capture the energy decay of a dense dynamic granular system and was proven to be less computationally efficient as the presented hybrid scheme.

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