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Event-driven DEM of Soft Spheres

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Abstract. In this paper an algorithm is described which combines the efficiency of event-driven Molecular-Dynamics (eMD) and the physical correctness of force-based Molecular-Dynamics (MD) for dilute granular systems of frictionless spheres.

Keywords: Molecular-Dynamics, event-driven Molecular-Dynamics, granular Gases, hard-sphere model
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INTRODUCTION

It is commonly assumed that granular systems of spherical particles may be modeled by hard spheres (HS) whenever the frequency of many-body collisions may be neglected compared to the frequency of pair collisions. Consequently, the highly efficient eMD-algorithm (e.g. [1]), being nothing but a direct implementation of the HS-model, was also assumed to deliver correct results in these cases. Recently it was shown, that, even under the above precondition of exclusively binary interaction, the eMD-algorithm (relying on the HS-model) may fail if compared to the more physical MD (see e.g. [2]) where the system dynamics are obtained by solving Newton's equations of motion [3, 4].

Fig. 1 illustrates the problem by showing the trajectories of two excentrically colliding spheres obtained by MD and eMD respectively. To model the interaction force needed within the MD-simulation, the linear-dashpot model

$$F = k(l - r) - \gamma \dot{r} \tag{1}$$

was used, where k denotes the elastic and γ the dissipative constant. $l = R_1 + R_2$ represents the sum of the colliding particles radii and r their center to center distance. The coefficient of restitution ε needed for the eMD-simulation was chosen correspondingly (see [5]). Using the soft-sphere model or MD respectively as a benchmark, the trajectories obtained by the eMD-algorithm clearly deviate from the MD reference regarding their spacial and, indicated by the symbols in Fig. 1, temporal properties.

To visualize the mismatch between the particle trajectories obtained by eMD and the reference trajectories obtained by MD, the parameters used for the plot in Fig. 1 correspond to very soft particles. A careful analysis [3, 4] shows that the differences may be large also for more realistic material and system properties. The fundamental problems detailed in the introduction are *always*

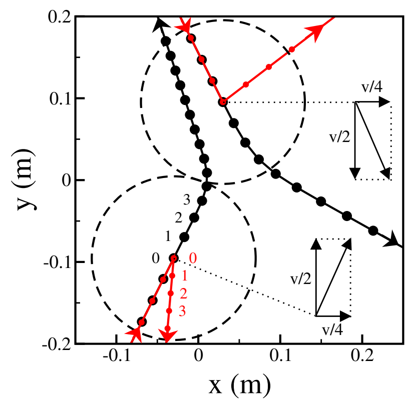

FIGURE 1. (color online) Traces of two colliding spheres. Black lines show the numerical integration of Newton's equation (MD), red lines show the trajectories as obtained from eMD. Symbols and numbers (of the respective color) indicate the particle positions at equidistant points in time. The number 0 stands for the moment when the particles touch and 7 corresponds to the end of the collision (stepsize $dt = \tau/7$). The dashed circles show the spheres at the moment of impact. Parameters: $k = 2$ kN/m, $R_{1,2} = 0.1$ m, mass density $\rho = 1140$ kg/m^3, $v = 5$ m/s, $\gamma = 0$, $\varepsilon_n = 1$.

present when collisions of physical particles are modeled by eMD assuming instantaneous collisions.

Consequently, on one hand we have the stunning efficiency of eMD based on the hard-sphere model. On the other hand there is the universality and physical correctness of the soft-sphere model leading to MD. Combining the advantages of both approaches is a highly desired aim.

In this work we derive an algorithm for the event-driven simulation of *soft* smooth spheres. For dilute systems of frictionless particles the presented method allows for a correct computation of the trajectories (as MD) while preserving the efficiency of event-driven simulations.

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COLLISION OF SPHERES

Separating the center of mass motion, the collision of two smooth spheres takes place in a plane. The system is hence completely described by the center to center distance $r = |\vec{r}(t)|$ of the two particles and the rotation angle $\varphi(t)$ of inter-center unit vector $\vec{e}_r = \vec{r}(t)/|\vec{r}|$. The collision-plane is perpendicular to the (conserved) orbital angular momentum $\vec{L} = m_{\mathrm{eff}}\,\vec{r}\times\dot{\vec{r}} \equiv L\vec{e}_L$ whit the effective mass $m_{\mathrm{eff}} = \frac{m_1 m_2}{m_1+m_2}$ of two particles with the masses m_1 and m_2. Thus, with the coordinate system Σ spanned by

$$\vec{e}_x \equiv \vec{e}_r^{\,0}\,, \quad \vec{e}_z \equiv \vec{e}_L\,, \quad \vec{e}_y \equiv \vec{e}_z \times \vec{e}_x\,, \tag{2}$$

and with its origin in the center of mass $\vec{R}$, the collision takes place in the $\vec{e}_x$-$\vec{e}_y$–plane [1]. Upper index 0 denotes values just before the collision.

Measuring time in units of T, length in units of X and angles in units of Φ, and using the dimensionless quantities

$$\tilde{r} = \frac{r}{X}\,, \quad \tilde{t} = \frac{t}{T} \quad \text{and } \tilde{\varphi} = \frac{\varphi}{\Phi}\,, \tag{3}$$

the collision dynamics are fully governed by

$$\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}} = \frac{c_\varphi}{\tilde{r}^2} \quad \text{and} \quad \frac{\mathrm{d}^2\tilde{r}}{\mathrm{d}\tilde{t}^2} = \tilde{r}\left(\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}}\right)^2 \Phi^2 + \frac{F}{m_{\mathrm{eff}}}\frac{T^2}{X}\,, \tag{4}$$

where X and T are length and time scales typical for the given normal force F, Φ is an arbitrary scale for measuring angles and c_φ reads

$$c_\varphi = \frac{T}{\Phi X^2}\frac{L}{m_{\mathrm{eff}}}. \tag{5}$$

The corresponding dimensionless initial conditions read

$$\tilde{\varphi}(0) = 0, \quad \tilde{r}(0) = \frac{r(0)}{X} \quad \text{and} \quad \frac{\mathrm{d}\tilde{r}}{\mathrm{d}\tilde{t}}(0) = \dot{r}(0)\frac{T}{X}. \tag{6}$$

The collision terminates at time $t = \tau$ where [5]

$$\dot{r}(\tau) > 0 \quad \text{and} \quad F = 0. \tag{7}$$

According to Eq. (7) the scaled contact duration reads $\tilde{\tau} \equiv \tau/T$.

COLLISION MAPPING

Hard spheres interact with δ-shaped forces. Their collision is hence characterized by an instantaneous exchange of momentum:

$$\dot{\vec{r}}\,' \cdot \vec{e}_r^{\,\prime} = -\varepsilon\,\dot{\vec{r}}^{\,0} \cdot \vec{e}_r^{\,0}\,, \tag{8}$$

[1] For central collisions we have $\vec{L} = \vec{0}$. In this case $\vec{e}_z$ may be any unit vector perpendicular to $\vec{e}_x$, ($\vec{e}_x \cdot \vec{e}_z = 0$).

where primes indicate post-collisional quantities and ε the coefficient of normal restitution. Because the particle positions do not change during the collision $\vec{e}_r^{\,\prime} \equiv \vec{e}_r^{\,0}$ is implied and Eq. (8) degenerates to

$$\dot{\vec{r}}\,' \cdot \vec{e}_r^{\,0} = -\varepsilon\,\dot{\vec{r}}^{\,0} \cdot \vec{e}_r^{\,0}\,. \tag{9}$$

Eq. (8), relating the pre- and post-collisional velocities, is the governing equation of eMD. Because only the particles velocities change during the collision, it completely maps the pre-collisional system state to post-collisional one.

Contrary, the collision of soft (physical) spheres is governed by *finite* interaction forces leading to a finite contact duration. During their contact, the spheres compose a deforming dumbbell-shaped object which moves through space with the center of mass (COM) velocity of both spheres, and additionally rotates around the COM in case of non-central impact. Rotation, translation and deformation of the dumbbell are neglected within HS approximation as well as the actually finite contact duration. Fig. 1 illustrates the results.

To capture the above described motion of colliding soft spheres, the coefficient of restitution ε (Eq. 9) is not sufficient obviously. Hence, further quantities are needed, to map the pre-collisional system state to the post-collisional values $\tilde{r}(\tilde{\tau})$, $\dot{\tilde{r}}(\tilde{\tau})$, $\tilde{\varphi}(\tilde{\tau})$ and $\dot{\tilde{\varphi}}(\tilde{\tau})$, which are obtained by solving the scaled equation of motion Eq. (4) for the initial conditions Eq. (6) from the beginning of the collision at time $\tilde{t} = 0$ until its end at $\tilde{t} = \tilde{\tau}$ (see Eq. (7)). Note that $\dot{\tilde{\varphi}}(\tilde{\tau})$ may be computed from $\tilde{r}(\tilde{\tau})$ and conservation of angular momentum L. Hence, the four dimensionless quantities

$$\varepsilon_r \equiv \frac{\tilde{r}(\tilde{\tau})}{\tilde{r}(0)}\,, \quad \varepsilon_\varphi \equiv \tilde{\varphi}(\tilde{\tau})\,, \quad \varepsilon_{\dot{r}} \equiv \frac{\dot{\tilde{r}}(\tilde{\tau})}{\dot{\tilde{r}}(0)}\,, \quad \varepsilon_t \equiv \tilde{\tau} \tag{10}$$

entirely relate the pre- and post-collisional system state. ε_t is obviously needed to update the COM position and to explicitly consider the *finite* contact duration.

IMPROVED COLLISION RULE

To apply the collision mapping Eq. 10 to the event-driven simulation of *soft* spheres, the post-collisional particle coordinates $\vec{r}_1^{\,\prime}$, $\vec{r}_2^{\,\prime}$, $\vec{v}_1^{\,\prime}$, $\vec{v}_2^{\,\prime}$ need to be computed from the pre-collisional coordinates $\vec{r}_1^{\,0}$, $\vec{r}_2^{\,0}$, $\vec{v}_1^{\,0}$, $\vec{v}_2^{\,0}$ for a given set of material parameters, particle masses and a given collision mapping ε_r, ε_φ, $\varepsilon_{\dot{r}}$ and ε_t. For convenience, we use two (fixed) reference frames: The laboratory system Σ^{L} (spanned by $\vec{e}_x^{\,\mathrm{L}}$, $\vec{e}_y^{\,\mathrm{L}}$, $\vec{e}_z^{\,\mathrm{L}}$) and Σ as defined in Eq. (2). $\hat{X}$ indicates, that the vector X is expressed in the reference frame Σ. Vectors without a hat are expressed in Σ^{L}, respectively.

Position Update. The base vectors $\hat{\vec{e}}_i^{\mathrm{L}}$ of the laboratory frame Σ^{L} expressed in Σ, the direction of the relative coordinate $\vec{e}_r^{\,\prime}$ after the collision expressed in Σ^{L} and Σ ($\hat{\vec{e}}_r^{\,\prime}$) read

$$\hat{\vec{e}}_i^{\mathrm{L}} = \begin{pmatrix} \vec{e}_i^{\mathrm{L}} \cdot \vec{e}_x \\ \vec{e}_i^{\mathrm{L}} \cdot \vec{e}_y \\ \vec{e}_i^{\mathrm{L}} \cdot \vec{e}_z \end{pmatrix}, \hat{\vec{e}}_r^{\,\prime} = \begin{pmatrix} \cos(\varepsilon_\varphi \Phi) \\ \sin(\varepsilon_\varphi \Phi) \\ 0 \end{pmatrix}, \vec{e}_r^{\,\prime} = \begin{pmatrix} \hat{\vec{e}}_r^{\,\prime} \cdot \hat{\vec{e}}_x^{\mathrm{L}} \\ \hat{\vec{e}}_r^{\,\prime} \cdot \hat{\vec{e}}_y^{\mathrm{L}} \\ \hat{\vec{e}}_r^{\,\prime} \cdot \hat{\vec{e}}_z^{\mathrm{L}} \end{pmatrix}. \tag{11}$$

The distance r' between the two spheres after the collision is given by $r' = r^0 \varepsilon_r$, where r^0 is its precollisional value. With this, the vectors pointing from the origin of Σ to particle 1 and 2 after the collision read

$$\begin{pmatrix} \Delta \vec{r}_1^{\,\prime} \\ \Delta \vec{r}_2^{\,\prime} \end{pmatrix} = \begin{pmatrix} -m_2 \\ m_1 \end{pmatrix} \frac{1}{m_1 + m_2} \left(r' \vec{e}_r^{\,\prime} \right). \tag{12}$$

expressed in the laboratory frame Σ^{L}. The center of mass coordinate after the collision reads $\vec{R}' = \vec{R}^0 + \dot{\vec{R}}^0 \varepsilon_t T$ expressed in the laboratory frame and, with this, the post-collisional particle positions expressed in the laboratory frame read

$$\vec{r}_i^{\,\prime} = \vec{R}' + \Delta \vec{r}_i^{\,\prime} \tag{13}$$

Velocity Update. The angular velocity at the instant of collision and the corresponding postcollisional value read

$$\dot{\varphi}^0 = \frac{L}{m_{\mathrm{eff}} \left(r^0 \right)^2} \quad \text{and} \quad \dot{\varphi}' = \frac{\dot{\varphi}(0)}{\varepsilon_r^2}. \tag{14}$$

The derivative of the unit vector of the postcollisional relative coordinate expressed in the reference frame Σ and Σ^{L} read

$$\hat{\vec{e}}_{\dot{r}}^{\,\prime} = \begin{pmatrix} -\dot{\varphi}' \sin(\varepsilon_\varphi \Phi) \\ \dot{\varphi}' \cos(\varepsilon_\varphi \Phi) \\ 0 \end{pmatrix} \text{ and } \vec{e}_{\dot{r}}^{\,\prime} = \begin{pmatrix} \hat{\vec{e}}_{\dot{r}}^{\,\prime} \cdot \hat{\vec{e}}_x^{\mathrm{L}} \\ \hat{\vec{e}}_{\dot{r}}^{\,\prime} \cdot \hat{\vec{e}}_y^{\mathrm{L}} \\ \hat{\vec{e}}_{\dot{r}}^{\,\prime} \cdot \hat{\vec{e}}_z^{\mathrm{L}} \end{pmatrix}. \tag{15}$$

The normal component $\dot{r}'$ of the relative velocity between the two spheres after the collision is given by $\dot{r}' = \dot{r}^0 \varepsilon_{\dot{r}}$, where $\dot{r}^0$ is its pre-collisional value. With this, the post-collisional velocity of the particles measured from the origin of Σ, expressed in the laboratory frame Σ^{L} read

$$\begin{pmatrix} \Delta \vec{v}_1^{\,\prime} \\ \Delta \vec{v}_2^{\,\prime} \end{pmatrix} = \begin{pmatrix} -m_2 \\ m_1 \end{pmatrix} \frac{1}{m_1 + m_2} \left(\dot{r}' \vec{e}_r^{\,\prime} + r' \vec{e}_{\dot{r}}^{\,\prime} \right). \tag{16}$$

With this, the post-collisional velocities expressed and measured in the laboratory frame read

$$\vec{v}_i^{\,\prime} = \dot{\vec{R}}' + \Delta \vec{v}_i^{\,\prime}, \tag{17}$$

In absence of external fields we have $\dot{\vec{R}}' = \dot{\vec{R}}^0$.

Together with the collision mapping, Eq. (10), Equations (13) and (17) establish a complete set of equations for the computation of the post-collisional positions and velocities from the pre-collisional values.

LINEAR-DASHPOT MODEL

Although physically questionable, the linear-dashpot model Eq. 1 is widely used in the literature for the simulation of granular systems. Since its consequence, the constant coefficient of restitution, simplifies the analytical analysis largely, except for very few examples, e.g. [6], virtually the entire Kinetic Theory of granular gases relies on this assumption.

Applying the scaling (see Eq. 3)

$$\Phi \equiv 1, \quad T \equiv \frac{1}{\omega}, \quad X \equiv \frac{\dot{r}(0)}{\omega}, \quad \omega \equiv \sqrt{\frac{k}{m_{\mathrm{eff}}}}, \tag{18}$$

the interaction force F in Eq. 4 reads

$$\frac{F}{m_{\mathrm{eff}}} \frac{T^2}{X} = \left(\tilde{l} - \tilde{r} \right) - c_{\mathrm{dis}} \frac{\mathrm{d}\tilde{r}}{\mathrm{d}\tilde{t}}, \quad \tilde{l} \equiv \frac{l}{X}, \quad c_{\mathrm{dis}} \equiv \frac{\gamma T}{m_{\mathrm{eff}}}. \tag{19}$$

The collision mapping, Eq. (10), is then obtained by solving Eq. (4) with the initial conditions (see Eq. (6))

$$\tilde{\varphi}(0) = 0, \quad \tilde{r}(0) = \tilde{l} \quad \text{and} \quad \frac{\mathrm{d}\tilde{r}}{\mathrm{d}\tilde{t}}(0) = -1 \tag{20}$$

for a given set of $\{\tilde{l}, c_\varphi, c_{\mathrm{dis}}\}$ in the interval $0 \le \tilde{t} \le \tilde{\tau}$, where $\tilde{\tau}$ is the time where the collision ceases given by the condition Eq. (7).

The reduced set of parameters, $\{\tilde{l}, c_\varphi, c_{\mathrm{dis}}\}$, follows from both, material parameters (k, γ, mass density ρ), particle sizes (R_1, R_2) and impact parameters (impact velocity v and eccentricity $e \equiv d/l$, see Fig. 2). For practical application, the collision mapping, Eq. (10), is needed for a wide range of the (physical) system parameters, corresponding to a certain area in the $\{\tilde{l}, c_\varphi, c_{\mathrm{dis}}\}$-space of complicated shape. [7] describes a way of building efficient lookup-tables for the desired values.

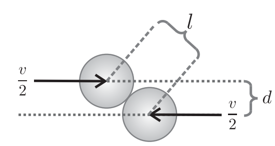

FIGURE 2. Eccentric collision of spheres.

IMPROVED EVENT-DRIVEN MOLECULAR DYNAMICS

In this section an algorithm is outlined, which uses the precomputed collision mapping Eq. 10 and the collision rule described in Sec. "*Improved Collision Rule*" to compute the physically correct soft-sphere trajectories by executing three *instantaneous* events. At least for dilute systems of frictionless spheres it allows for *event driven*

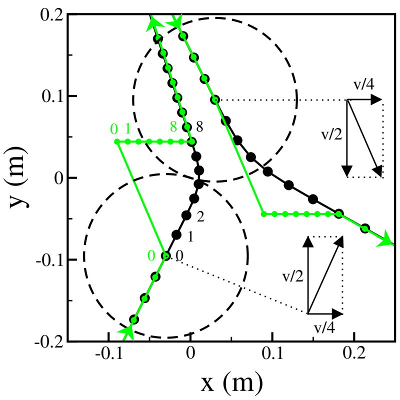

FIGURE 3. Setup and Parameters as detailed in Fig. 1. Green dots/line: traces within the soft sphere eMD algorithm.

simulation of *soft* spheres. It extends classical eMD for granular systems based on the hard sphere model to soft spheres:

1. At the moment of impact, from the particle positions, velocities, radii and material parameters, the collision mapping Eq. (10) is computed (see Sec. "*Linear-Dashpot Model*").
2. By applying the collision rule detailed in Sec. "*Improved Collision Rule*" with $\left\{\varepsilon_\varphi, \varepsilon_t = 0, \varepsilon_r, \varepsilon_{\dot{r}}\right\}$ the two particle dumbbell is rotated by the angle $\varphi = \varepsilon_\varphi \Phi$. Additionally, the particles postcollisional velocities $\vec{v}\,'_{1,2}$ are obtained. While storing the latter, the particle velocities are set to the center of mass velocity $\vec{v}_{1,2} = \dot{\vec{R}}^0$.
3. At time $t = t^0 + \tau$ ($\tau = \varepsilon_t T$) an event is scheduled which sets the particle velocities to the above postcollisional values $\vec{v}\,'_{1,2}$.

Utilizing this algorithm we have to deal with two possible exceptions:

1. The rotation step (item 2 of the above enumeration) may not be executed as it would lead to overlap with surrounding particles. In this case a regular hard sphere collision with the coefficient of restitution $\varepsilon = -\varepsilon_{\dot{r}}$ is performed.
2. During the short transient state where the two colliding particles artificially propagate at the center of mass velocity, they might collide with surrounding particles. In this case, the postcollisional velocity of the affected particle i is immediately set to the above value $\vec{v}\,'_i$ and a collision according to the above algorithm is performed.

Details and a complete description of the algorithm can be found in [7].

Of course, the described exception handling is an approximation. The algorithm is only applicable to systems which are dilute in a way that the above exceptions occur only rarely. A detailed analysis shows that for typical applications (dilute granular gases) only about 0.1% of the collisions lead to the above exceptions ([7]).

CONCLUSION

The hard-sphere model assumes infinte δ-shaped interaction forces between granular particles. This implies that collisions are characterized by instantaneously changing particle velocities, which allows for highly efficient eMD simulation. Contrary, all real granular particles interact with finite interaction forces leading to a finite contact duration, which, in turn, allows for changing particle positions as well. The dynamics of such systems are obtained by (numerically) solving the governing equations of motion which is usually several orders of magnitude less efficient if compared to eMD simulations. The presented algorithm allows for the event-driven simulation of soft frictionless spheres while maintaining the efficieny of classical eMD. The applied linear-dashpot interaction is exemplary. Following the lines of Sec. "*Linear-Dashpot Model*" the collision mapping Eq. 10 may be obtained for any other interaction forces as well.

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REFERENCES

1. B. D. Lubachevsky, *J. Comp. Phys.* **94**, 255 (1991).
2. M. Allen, and D. Tildesley, *Computer Simulation of Liquids*, Oxford University Press, Oxford, Oxford, 1987.
3. P. Müller, and T. Pöschel, *Granular Matter* **14**, 115 (2011).
4. P. Müller, D. Krengel, and T. Pöschel, *Phys. Rev. E* **85**, 041306 (2012).
5. T. Schwager, and T. Pöschel, *Granular Matter* **9**, 465 (2007).
6. N. V. Brilliantov, C. Salueña, T. Schwager, and T. Pöschel, *Phys. Rev. Lett.* **93**, 134301 (2004).
7. P. Müller, and T. Pöschel, *Phys. Rev. E* **87**, 033301 (2013).