Event-Driven Simulation of Soft Spheres

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The dynamics of dissipative soft-sphere gases obeys Newton's equation of motion which are commonly solved numerically by (force-based) Molecular Dynamics schemes. With the assumption of instantaneous, pairwise collisions, the simulation can be accelerated considerably using event-driven Molecular Dynamics, where the coefficient of restitution is derived from the interaction force between particles. Recently it was shown [1], however, that this approach may fail dramatically, that is, the obtained trajectories deviate significantly from the ones predicted by Newton's equations. In this paper, we generalize the concept of the coefficient of restitution and derive a numerical scheme which allows us to perform highly efficient event-driven Molecular Dynamics simulations even for non-instantaneous collisions. We show that the particle trajectories predicted by the new scheme agree perfectly with the corresponding (force-based) Molecular Dynamics, except for a short transient period whose duration corresponds to the duration of the contact. Thus, the new algorithm solves Newton's equations of motion like force-based MD while preserving the advantages of event-driven simulations.

Hard Spheres

Relevance:
The hard sphere model is the foundation of both: Kinetic theory of granular matter based on the Boltzmann equation as well as event-driven Molecular Dynamics (eMD) of granular matter.

Assumptions:
• *infinite*, *delta-shaped* interaction forces
→ *instantaneous* collisions.
→ system dynamics = sequence of *binary collisions*

Collision Rule:
The collision of two hard spheres i and j located at $\vec{r}_{i,j}$ traveling at velocities $\dot{\vec{r}}_{i,j}$ is described by an instantaneous exchange of momentum:

$$(\dot{\vec{r}}_i' - \dot{\vec{r}}_j') \cdot \hat{e}_r' = -\varepsilon(\dot{\vec{r}}_i^{\,0} - \dot{\vec{r}}_j^{\,0}) \cdot \hat{e}_r^{\,0}$$

Where $\hat{e}_r$ denotes the inter center unit vector and ε the coefficient of normal restitution. Primes indicate post- and zeros precollisional values. Note that we have $\hat{e}_r' = \hat{e}_r^{\,0}$ due to instantaneous collisions

Soft Spheres

Relevance:
In nature collisions are characterized by finite interaction forces (soft spheres). Soft sphere modeling is the bedrock of (force-based) Molecular Dynamics.

Assumptions:
• *finite* interaction forces
→ *finite* contact duration.
→ system dynamics governed by Newton's equations of motion.

Collision Rule:
• Solve Newton's (coupled) equations of motion for the many body system:

$$m_i \ddot{\vec{r}}_i = \vec{F}_i$$

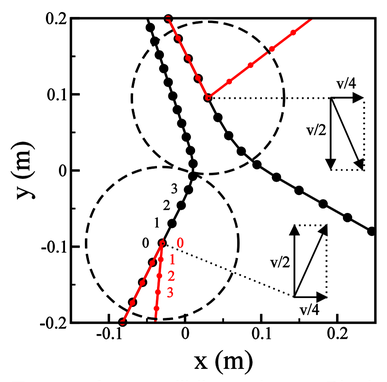
Where $\vec{F}_i$, comprising interaction forces and external forces, denotes the force acting on particle i.

Hard Spheres vs. Soft Spheres

The hard sphere model is a simplification which is commonly assumed to hold true for systems whose dynamics are constituted by a series of binary interactions (dilute systems).

Recently it was shown, that even under this precondition the hard sphere model may fail dramatically if compared to more physical soft sphere models.

Actually, collisions are governed by finite interaction forces in nature. Hence, the soft sphere model is the benchmark by which the hard sphere approximation has to be justified.

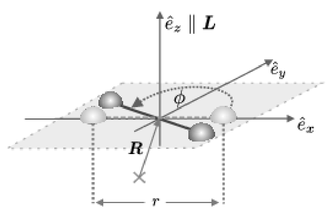


Traces of two colliding spheres. Black: Soft spheres. Red: corresponding hard spheres. Symbols indicate the particle positions at equidistant points in time , and, hence, the system dynamics

Mapping Soft Sphere Collisions to Instantaneous

Equation of Motion for Soft Spheres

The collision of two smooth spheres takes place in a plane.



Within the collision plane we formulate the equation of motion in polar coordinates.

$$\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}} = \frac{c_\varphi}{\tilde{r}^2} \qquad c_\varphi = \frac{T}{\Phi X^2}\frac{L}{m_{\mathrm{eff}}}$$

$$\frac{\mathrm{d}^2\tilde{r}}{\mathrm{d}\tilde{t}^2} = \tilde{r}\left(\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}}\right)^2 \Phi^2 + \frac{F_n}{m_{\mathrm{eff}}}\frac{T^2}{X}$$

Where time is measured in units of T, length in units of X and angles in units of Φ.

$$\tilde{r} = \frac{r}{X},\ \tilde{t} = \frac{t}{T},\ \tilde{\varphi} = \frac{\varphi}{\Phi}$$

F_n normal component of interaction force

$m_{\mathrm{eff}} = \frac{m_i m_j}{m_i + m_j}$ effective mass

Collision Mapping

The collision terminates at $\tilde{t} = \tilde{\tau}$, where

$$\dot{\tilde{r}}(\tilde{\tau}) > 0, \qquad F_n = 0.$$

Solving the equation of motion till $\tilde{t} = \tilde{\tau}$, we obtain $\tilde{\varphi}(\tilde{\tau})$, $\dot{\tilde{\varphi}}(\tilde{\tau})$, $\tilde{r}(\tilde{\tau})$ and $\dot{\tilde{r}}(\tilde{\tau})$, which fully determine the system configuration at the end of the collision. We define:

$$\varepsilon_r \equiv \frac{\tilde{r}'}{\tilde{r}^{\,0}}, \quad \varepsilon_{\dot{r}} \equiv \frac{\dot{\tilde{r}}'}{\dot{\tilde{r}}^{\,0}}, \quad \varepsilon_\varphi \equiv \tilde{\varphi}', \quad \varepsilon_{\dot{\varphi}} \equiv \frac{\dot{\tilde{\varphi}}'}{\dot{\tilde{\varphi}}^{\,0}}, \quad \varepsilon_t \equiv \tilde{\tau}.$$

with

$$\chi(0) \equiv \begin{pmatrix} r^0 \\ \dot{r}^0 \\ \Phi \\ \dot{\varphi}^0 \\ T \end{pmatrix} \qquad \tilde{\varepsilon} \equiv \begin{pmatrix} \varepsilon_r & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_{\dot{r}} & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_\varphi & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_{\dot{\varphi}} & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_t \end{pmatrix}$$

The complete collision dynamics are exactly mapped to an instantaneous event by:

$$\chi(\tau) = \tilde{\varepsilon}\chi(0)$$

Collision Rule

To apply the collision mapping in eMD simulations, a collision rule is needed, which, for a given set of material parameters, particle radii as well as a given $\tilde{\varepsilon}$ directly relates the precollisional coordinates $\vec{r}_i^{\,0}$ and $\dot{\vec{r}}_i^{\,0}$ to the corresponding postcollisional ones $\vec{r}_i'$ and $\dot{\vec{r}}_i'$. We consider two coordinate systems: Σ as described left and the laboratory system Σ^{L}. $\hat{X}$ indicates that the vector X is expressed in Σ.

Position update:
The postcollisional inter-center unit vector reads

$\hat{e}_r' = (\cos(\varepsilon_\varphi\Phi), \sin(\varepsilon_\varphi\Phi), 0)$ expressed in Σ and

$e_r' = \left(\hat{e}_r'\hat{e}_x^{\,L},\ \hat{e}_r'\hat{e}_y^{\,L},\ \hat{e}_r'\hat{e}_z^{\,L}\right)$ expressed in Σ^{L}.

The postcollisional distance between the spheres reads

$$r' = r^{\,0}\varepsilon_r$$

The vectors pointing from the origin of Σ to the spheres read

$$\Delta\vec{r}_1' = -\frac{m_2}{m_1+m_2} r' e_r' \qquad \Delta\vec{r}_2' = \frac{m_1}{m_1+m_2} r' e_r'$$

the postcollisional position of the origin of Σ is given by

$$\vec{R}' = \vec{R}^{\,0} + \dot{\vec{R}}^{\,0}\varepsilon_t T$$

and the postcollisional particle positions read

$$\vec{r}_i' = \vec{R}' + \Delta\vec{r}_i'$$

Velocity update:
The postcollisional angular velocity reads

$$\dot{\varphi}' = \varepsilon_{\dot{\varphi}}\,\dot{\varphi}^{\,0}$$

The derivative of postcollisional inter-center unit vector reads

$\dot{\hat{e}}_r' = (-\dot{\varphi}'\sin(\varepsilon_\varphi\Phi),\ \dot{\varphi}'\cos(\varepsilon_\varphi\Phi),\ 0)$ in Σ and

$e_{\dot{r}}' = \left(\dot{\hat{e}}_r'\hat{e}_x^{\,L},\ \dot{\hat{e}}_r'\hat{e}_y^{\,L},\ \dot{\hat{e}}_r'\hat{e}_z^{\,L}\right)$ in Σ^{L}.

The postcollisional normal relative velocity reads

$$\dot{r}' = \dot{r}^{\,0}\,\varepsilon_{\dot{r}}$$

The postcollisional particle velocities with respect to the origin of Σ read

$$\Delta\vec{v}_1' = -\frac{m_2}{m_1+m_2}(\dot{r}' e_r' + r' e_{\dot{r}}')$$

$$\Delta\vec{v}_2' = \frac{m_1}{m_1+m_2}(\dot{r}' e_r' + r' e_{\dot{r}}')$$

and the postcollisional particle velocities are given by

$$\vec{v}_i' = \dot{\vec{R}}' + \Delta\vec{v}_i'$$

Efficient Lookup Tables for the Collision Mapping

To apply the above collision rule for highly efficient soft sphere eMD, efficient lookup tables for the collision mapping $\tilde{\varepsilon}$ are needed. Here we show how these may be obtained for two widely used interaction forces: The linear dashpot model and viscoelastic spheres. In booth cases we reduce the problem to three free parameters.

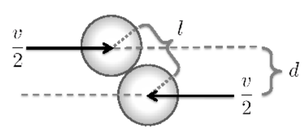
Linear Dashpot Model

$F_n = k(l - r) - \gamma\dot{r}$ $\quad l = R_1 + R_2$, k spring constant and the dissipative parameter γ.

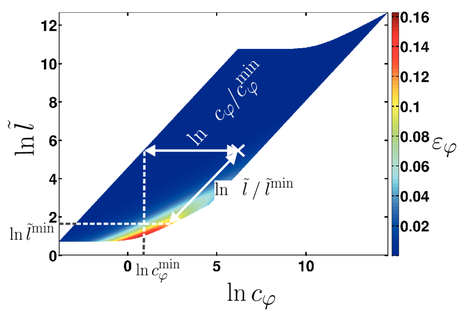
Scaling by $\Phi \equiv 1, \quad T \equiv \frac{1}{\omega}, \quad X \equiv \frac{\dot{r}^{\,0}}{\omega}, \quad \omega = \sqrt{\frac{k}{m_{\mathrm{eff}}}}$ we obtain

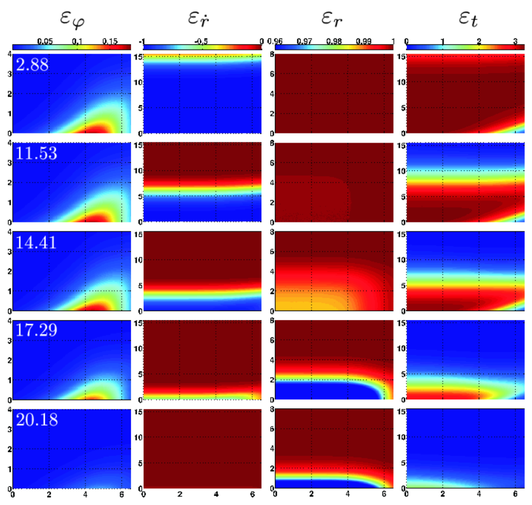
$$\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}} = \frac{c_\varphi}{\tilde{r}^2}$$

$$\frac{\mathrm{d}^2\tilde{r}}{\mathrm{d}\tilde{t}^2} = \frac{c_\varphi^2}{\tilde{r}^3} + (\tilde{l} - \tilde{r}) - c_{\mathrm{dis}}\frac{\mathrm{d}\tilde{r}}{\mathrm{d}\tilde{t}} \quad \text{where} \quad \tilde{l} \equiv \frac{l}{X} \quad \text{and} \quad c_{\mathrm{dis}} \equiv \gamma\frac{T}{m_{\mathrm{eff}}}$$



	unit	min.	max.
k	$[10^3$ N/m$]$	1	1000
R	[m]	0.001	0.1
ρ_m	[kg/m^3]	250	3250
γ	[kg/s]	0.01	1.25
v	[m/s]	0.001	25
d/l	-	0.01	0.99





Components of the collision mapping $\tilde{\varepsilon}$ for the linear dashpot model. For various $\ln c_{\mathrm{dis}}$ (white labels). x-axis $\ln c_\varphi / c_\varphi^{\min}$, y-axis $\ln \tilde{l}/\tilde{l}^{\min}$.

Viscoelastic Spheres

$F_n = \rho_{\mathrm{el}}(l - r)^{3/2} - \frac{3}{2}A\rho_{\mathrm{el}}\dot{r}\sqrt{l - r}$ with $\rho_{\mathrm{el}} = \frac{2Y\sqrt{R_{\mathrm{eff}}}}{3(1-\nu^2)}$ where

Y, ν, A and $R_{\mathrm{eff}} = R_1R_2/(R_1 + R_2)$ denote the Young modulus, the Poisson ratio the dissipative parameter and the effective mass respectively.

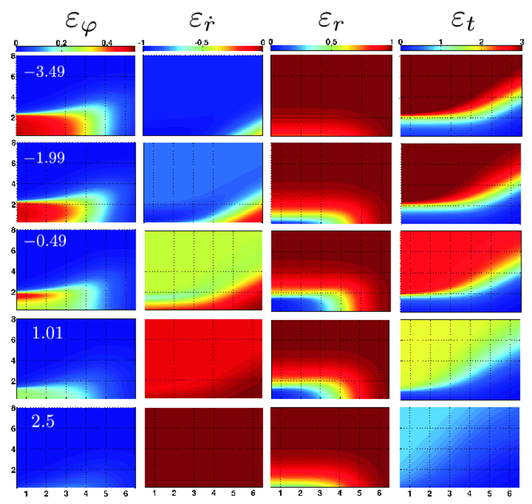
Scaling by $\Phi \equiv 1, \quad T \equiv \frac{1}{k^{\frac{2}{5}}(-\dot{r}^{\,0})^{\frac{1}{5}}}, \quad X \equiv \frac{(-\dot{r}^{\,0})^{\frac{4}{5}}}{k^{\frac{2}{5}}}, \quad k = \frac{\rho}{m_{\mathrm{eff}}}$ we obtain

$$\frac{\mathrm{d}\tilde{\varphi}}{\mathrm{d}\tilde{t}} = \frac{c_\varphi}{\tilde{r}^2}$$

$$\frac{\mathrm{d}^2\tilde{r}}{\mathrm{d}\tilde{t}^2} = \frac{c_\varphi^2}{\tilde{r}^3} + (\tilde{l} - \tilde{r})^{\frac{3}{2}} - c_{\mathrm{dis}}\frac{\mathrm{d}\tilde{r}}{\mathrm{d}\tilde{t}}\sqrt{\tilde{l} - \tilde{r}} \quad \text{where} \quad c_{\mathrm{dis}} \equiv \frac{3A}{2T}$$

In contrast to linear dashpot model, we here have $c_{\mathrm{dis}} = c_{\mathrm{dis}}(\tilde{l}, c_\varphi)$. Similar to c_φ and $\tilde{l}$ we switch to $\ln c_{\mathrm{dis}}/c_{\mathrm{dis}}^{\min}$ to fully rectify the parameter space.

	unit	min.	max.
Y	$[10^9$ N/m$^2]$	0.01	100
ν	-	0.2	0.5
R	[m]	0.001	0.1
ρ_m	[kg/m^3]	250	3250
A	[s]	$1.0e^{-6}$	1.0
v	[m/s]	0.001	25
d/l	-	0.01	0.99



Components of the collision mapping $\tilde{\varepsilon}$ for viscoelastic spheres for various $\ln c_{\mathrm{dis}}/\ln c_{\mathrm{dis}}^{\min}$ (white labels). x-axis $\ln c_\varphi/c_\varphi^{\min}$, y-axis $\ln \tilde{l}/\tilde{l}^{\min}$.

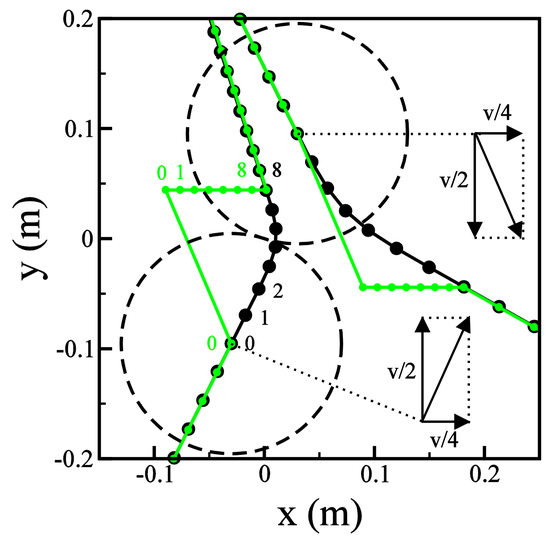
Simulation Algorithm

Idea:

1. Compute the collision mapping $\tilde{\varepsilon}$. Using lookup tables this may be done in a convenient and efficient way.
2. By applying the above collision rule with $\varepsilon_t = 0$ we rotate the two particles around their center of mass by the angle $\varphi = \varepsilon_\varphi\,\Phi$, and compute their postcollisional velocities $\vec{v}_{1,2}'$.
3. Then the particle velocities are set to the center of mass velocity: $\vec{v}_{1,2} = \dot{\vec{R}}^{\,0}$.
4. At time $t = t^{\,0} + \tau$ $(\tau = \varepsilon_t T)$ we schedule an event setting the particle velocities to the above postcollisional values $\vec{v}_{1,2}'$.

Exceptions:

1. The rotation step (step 2) leads to overlapping particles.
→ perform a regular hard sphere collision with $\varepsilon = -\varepsilon_{\dot{r}}$.
2. While the particles artificially propagate with center of mass velocity (step 3) they might collide with surrounding particles.
→ directly set the velocity of the afffected particle i to the above value $\vec{v}_i$ and perform a collision according to the above algorithm.



Scetch of the simulation algorithm. Traces of two colliding spheres. Black: Soft sphere benchmark. Green: corresponding collision as resolved by the above algorithm. Symbols indicate the particle positions at equidistant points in time , and, hence, the system dynamics.

We present an algorithm, which at least for dilute systems, exactly maps the collision dynamics to two instantaneous events. It thus allows for the highly efficient event-driven simulation of granular systems of soft spheres. All impact details are mapped to four scalar numbers only depending on three free parameters. These numbers may be precomputed and used in terms of efficient lookup tables.

References:

[1] P. Müller and T. Pöschel, Granular Matter **14**, 115-120 (2012).