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

References:

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, inelastic, inter-particle interactions
- no restitution of particles
- no system dynamics = sequence of binary collisions

Collision Rule:
The collision of two hard spheres and located at traveling at velocities where is described by an instantaneous exchange of momentum:

\[
\mathbf{v}_1' = \mathbf{v}_1 - \frac{m_1}{m_1 + m_2} (\mathbf{v}_1 - \mathbf{v}_2),
\]

\[
\mathbf{v}_2' = \mathbf{v}_2 + \frac{m_2}{m_1 + m_2} (\mathbf{v}_1 - \mathbf{v}_2).
\]

where denotes the center unit vector and the coefficient of normal restitution. This indicates that no post-collisional forces act on particles after the collision.

Soft Spheres

References:

Relevance: In nature collisions are characterized by finite interaction forces (soft sphere). 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:

So far Newton’s (coupled) equations of motion for the many body system:

\[
m_1 \frac{dv_1}{dt} = \mathbf{F}_1,
\]

\[
m_2 \frac{dv_2}{dt} = \mathbf{F}_2,
\]

where \( \mathbf{F}_1, \mathbf{F}_2 \) comprising interaction forces and external forces, forces the act on particle due to inertial, dissipative, and external forces.

Efficient Lookup Tables for the Collision Mapping

To apply the above collision rule for highly efficient soft sphere simulations, a collision rule is needed, which, for a given set of material parameters, particle radii as well as a given directly relates the postcollisional coordinates \((\mathbf{r}_1', \mathbf{v}_1', \mathbf{r}_2', \mathbf{v}_2')\) to the corresponding postcollisional ones \((\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2)\). We consider two coordinate systems: \( \Sigma \) as described left and the laboratory system \( \Sigma' \). indicates that the vector \( \mathbf{x} \) is expressed in \( \Sigma' \).

Position update: The postcollisional inter-center unit vector reads

\[
\mathbf{e}_1' = \frac{\mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1'}{\mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1'},
\]

expressed in \( \Sigma' \) and

\[
\mathbf{e}_2' = \frac{\mathbf{e}_2' \mathbf{e}_2' \mathbf{e}_2' \mathbf{e}_2'}{\mathbf{e}_2' \mathbf{e}_2' \mathbf{e}_2' \mathbf{e}_2'},
\]

with

\[
\frac{\mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1'}{\mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1' \mathbf{e}_1'},
\]

The postcollisional distance between the spheres reads

\[
r_1 = r_1',
\]

The postcollisional impact parameter \( r_1' \) of the spheres reads

\[
\Delta r_1' = -\frac{m_1 v_1 - m_2 v_2}{m_1 + m_2} r_1',
\]

The postcollisional impact parameter \( r_1' \) of the sphere is given by

\[
\mathbf{R}_1' = \mathbf{R}_1 - \mathbf{R}_2, \quad \mathbf{R}_2' = \mathbf{R}_2 + \mathbf{R}_1',
\]

and the postcollisional particle velocities read

\[
\mathbf{v}_1' = \mathbf{v}_1 + \mathbf{R}_1' \mathbf{e}_1', \quad \mathbf{v}_2' = \mathbf{v}_2 - \mathbf{R}_2' \mathbf{e}_2'.
\]

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:


Visualization of two colliding spheres. Red: corresponding collision on the colission plane. Symbols indicate the postcollisional positions at equidistant points in time, and, hence, the system dynamics.

Component of the collision mapping for the linear dashpot model. For various \( \alpha \) (white labels), \( \gamma \) (black labels), \( \kappa \) (red labels). Components of the collision mapping for eMD simulations. A green line indicates postcollisional trajectories of granular matter.