REPORT

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0.1 Idea and Motivation

The general idea of molecular dynamics, is to solve numerically Newton's equation of motion simultaneously for all particles i:

$$\ddot{\vec{r_i}} = \frac{1}{m_i}\vec{F_i}(\vec{r_1}, \vec{v_1}, \cdots, \vec{r_N}, \vec{v_N}) \tag{1}$$

This type of Molecular Dynamics is called force-based.This general scheme has been successfully applied to the simulation of granular systems in many situations; however in some cases it is less appropriate:
In systems where the typical duration of a collision is much shorter than the mean time between successive collisions of a particle, particles are very rarely in contact with more than one other particles.Hence, most of the time each of the particles propagates along a ballistic trajectory, interrupted by collisions with other particles of very short duration.Therefore, the pairwise collision of particles may be considered as instantaneous events and each of these events may be treated separately.Examples of such systems are granular gases i.e very dilute granular systems such as cosmic dust clouds. Although force-based Molecular Dynamics is applicable, in principle, to such systems, the computation is very inefficient. If Newton's equation of motion is integrated for an isolated pair of colliding particles, the post-collision velocities $\vec{v}'_{1/2}$are obtained as functions of the pre-collision velocities $\vec{v}_{1/2}$. These functions can be used to set up an event-driven Molecular Dynamics simulation.
In some cases the detailed interaction force of granular particles is not known as a function of the relative position $|\vec{r}_1 - \vec{r}_2|$, velocity $|\vec{v}_1 - \vec{v}_2|$, and orientation because to derive this function, a microscopic description of the particle material is required, i.e., a continuum mechanics description, which may be very complicated, such as those for nonlinear materials or complicated particle shapes. Nevertheless, it is frequently possible to investigate the pairwise particle collision experimentally and, hence, to determine approximations for the post-collision velocities as functions of the pre-collision velocities.
The main assumption for applying event-driven Molecular Dynamics is that at any time instant in the entire system, there occurs at most one collision of infinitesimal duration. This collision alters the velocities of the involved particles according to a collision law which is characterized by coefficients of restitution . With the idealization of infinitesimal duration, these coefficients describe the mechanics of pairwise particle collisions exhaustively. Hence, the time-consuming simultaneous computation of the trajectories of all particles according to 1 is unnecessary. During the time intervals between collisions, the particles move along known ballistic trajectories. Therefore, the positions of the particles at the time of the next collision can be computed in one step. Obviously, this algorithm is much more efficient than force-based algorithms since the numerical integration of the equations of motion is avoided. Instead the dynamics of the system is determined by a sequence of discrete events.

0.1.1 Collision of particles

The relative velocity of colliding particles i and j at the point of contact, $\vec{g}_{ij}$, is determined by the translational and rotational particle velocities:

$$\vec{g}_{ij} = \vec{v}_i - \vec{v}_j = \vec{v}_{ij} \tag{2}$$

with $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$.The normal and tangential collision velocities are given by the projections.