Computational Statistical Physics

Part II: Interacting particles and molecular dynamics

Marina Marinkovic

May 18, 2022

ETH Zürich
Institute for Theoretical Physics
HIT G 41.5
Wolfgang-Pauli-Strasse 27
8093 Zürich

402-0812-00L
FS 2022

Elastic Collisions

One of the first examples for event-driven programming applied to molecular dynamics is a work by Alder in 1957.

In this method only the exchange of the particles' momenta is taken into account and no forces are calculated. Furthermore, only binary collisions are considered and interactions between three or more particles are neglected. Between two collision events, the particles follow ballistic trajectories. To perform an event-driven MD simulation, we need to determine the time t_c between two collisions to then obtain the velocities of the two particles after the collision from the velocities of the particles before the collision using a look-up table.

Elastic Collisions

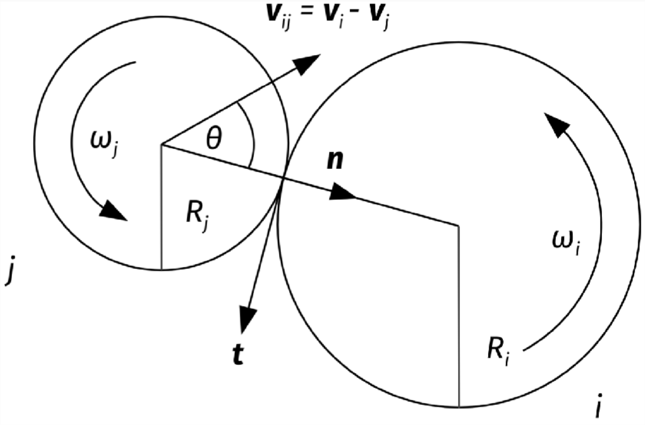

Figure 1: Two particles collide elastically.

Elastic Collisions

For the moment, we are not taking into account the influence of friction and thus neglect the exchange of angular momentum. We compute the times t_{ij}, at which the next collision between the particle i and the particle j would occur. At time t_{ij}, the distance between the two particles is

$$|\mathbf{r}_{ij}\left(t_{ij}\right)| = |R_i + R_j| \tag{1}$$

Given a relative velocity v_{ij} at time t_0, the contact time t_{ij} of two particles can be obtained from

$$v_{ij}^2 t_{ij}^2 + 2\left[\mathbf{r}_{ij}\left(t_0\right)\mathbf{v}_{ij}\right]t_{ij} + \left[r_{ij}\left(t_0\right)\right]^2 - \left(R_i + R_j\right)^2 = 0. \tag{2}$$

Elastic Collisions

We should bear in mind that Eq. (2) are only meaningful if the trajectories of particles i and j cross with each other. The time t_c when the next collision occurs, is the minimum over all pairs, i.e.,

$$t_c = \min_{ij} \left(t_{ij} \right) . \tag{3}$$

Thus, in the time interval $[t_0, t_c]$ the particles' positions and angular orientations evolve according to

$$\mathbf{r}_i \left(t_0 + t_c \right) = \mathbf{r}_i \left(t_0 \right) + \mathbf{v}_i \left(t_0 \right) t_c \quad \text{and} \quad \phi_i \left(t_0 + t_c \right) = \phi_i \left(t_0 \right) + \omega_i \left(t_0 \right) t_c . \tag{4}$$

Lubachevsky method

Instead of going through all the particle pairs ($\mathcal{O}\left(N^2\right)$), we create a list of events for each particle. The reordering of the event list takes a time in the order of $\mathcal{O}\left(N \log N\right)$.

In practice, this can be implemented in six arrays (event times, new partners, positions and velocities) of dimension N (number of particles in the system). Alternatively, one creates a list of pointers pointing to a data structure for each particle consisting of six variables.

Lubachevsky method

Storing the last event is needed as particles are only updated after being involved in an event. For each particle i, the time $t^{(i)}$ is the minimal time of all possible collisions involving this particle, i.e.,

$$t^{(i)} = \min_j \left(t_{ij}\right). \tag{5}$$

Comparing particle i with $N-1$ others can be improved by dividing the systems in sectors such that only neighboring sectors have to be considered in this step.

Lubachevsky method

These sector boundaries have to be treated similar to obstacles such that when particles cross sector boundaries a collision event happens. For each particle i, this step would then be of order $\mathcal{O}(1)$ instead of $\mathcal{O}(N)$. The next collision occurs at time

$$t_c = \min_i \left(t^{(i)} \right). \tag{6}$$

Lubachevsky method

We store $t^{(i)}$ in increasing order in a stack:

- The vector $\mathrm{part}[m]$ points to particle i which is at position m in the stack. (Sometimes also a vector $\mathrm{pos}[i]$ is used to store position m of particle i in the stack.)
- This constitutes an implicit ordering of the collision times $t^{(i)}$, where $m = 1$ points to the smallest time.
- $\mathrm{part}[1]$ is the particle with minimal collision time: $t_c = t^{(\mathrm{part}[1])}$
- After the event for both particles all 6 entries (event times, new partners, positions and velocities) have to be updated. Additionally, the vector $\mathrm{part}[m]$ has to be reordered.

Lubachevsky method

We store $t^{(i)}$ in increasing order in a stack:

- The vector $\mathrm{part}[m]$ points to particle i which is at position m in the stack. (Sometimes also a vector $\mathrm{pos}[i]$ is used to store position m of particle i in the stack.)
- This constitutes an implicit ordering of the collision times $t^{(i)}$, where $m = 1$ points to the smallest time.
- $\mathrm{part}[1]$ is the particle with minimal collision time: $t_c = t^{(\mathrm{part}[1])}$
- After the event for both particles all 6 entries (event times, new partners, positions and velocities) have to be updated. Additionally, the vector $\mathrm{part}[m]$ has to be reordered.

Lubachevsky method

We store $t^{(i)}$ in increasing order in a stack:

- The vector $\mathrm{part}[m]$ points to particle i which is at position m in the stack. (Sometimes also a vector $\mathrm{pos}[i]$ is used to store position m of particle i in the stack.)
- This constitutes an implicit ordering of the collision times $t^{(i)}$, where $m = 1$ points to the smallest time.
- $\mathrm{part}[1]$ is the particle with minimal collision time: $t_c = t^{(\mathrm{part}[1])}$
- After the event for both particles all 6 entries (event times, new partners, positions and velocities) have to be updated. Additionally, the vector $\mathrm{part}[m]$ has to be reordered.

Lubachevsky method

We store $t^{(i)}$ in increasing order in a stack:

- The vector $\mathrm{part}[m]$ points to particle i which is at position m in the stack. (Sometimes also a vector $\mathrm{pos}[i]$ is used to store position m of particle i in the stack.)
- This constitutes an implicit ordering of the collision times $t^{(i)}$, where $m = 1$ points to the smallest time.
- $\mathrm{part}[1]$ is the particle with minimal collision time: $t_c = t^{(\mathrm{part}[1])}$
- After the event for both particles all 6 entries (event times, new partners, positions and velocities) have to be updated. Additionally, the vector $\mathrm{part}[m]$ has to be reordered.

Lubachevsky method

Reordering the times $t^{(i)}$ after each event is of order $\mathcal{O}(\log N)$ when using, e.g., binary trees for sorting. The advantages of this method are that it is not necessary to minimize all the collision times of all the pairs at every step, and that it is unnecessary to update the positions of particles that do not collide. Only the position and velocity of the particle involved in the collision event are updated.

Collision with perfect slip

We now approximate a collision by neglecting the tangential exchange of momentum – i.e. we assume a perfect slip. Only linear momentum and no angular momentum is exchanged. The conservation of momentum leads to

$$\mathbf{v}_i{}^{\text{after}} = \mathbf{v}_i{}^{\text{before}} + \frac{\Delta \mathbf{p}}{m_i}, \tag{7}$$

$$\mathbf{v}_j{}^{\text{after}} = \mathbf{v}_j{}^{\text{before}} - \frac{\Delta \mathbf{p}}{m_j}, \tag{8}$$

and energy conservation:

$$\frac{1}{2} m_i \left(\mathbf{v}_i^{\text{before}}\right)^2 + \frac{1}{2} m_j \left(\mathbf{v}_j^{\text{before}}\right)^2 = \frac{1}{2} m_i \left(\mathbf{v}_i^{\text{after}}\right)^2 + \frac{1}{2} m_j \left(\mathbf{v}_j^{\text{after}}\right)^2. \tag{9}$$

Collision with perfect slip

The exchanged momentum is

$$\Delta \mathbf{p} = -2m_{\text{eff}} \left[\left(\mathbf{v}_i^{\text{before}} - \mathbf{v}_j^{\text{before}} \right) \cdot \mathbf{n} \right] \mathbf{n} \tag{10}$$

with $m_{\text{eff}} = \frac{m_i m_j}{m_i + m_j}$ being the *effective mass* and $\mathbf{n} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$. If $m_i = m_j$, the velocity updates are

$$\mathbf{v}_i{}^{\text{after}} = \mathbf{v}_i^{\text{before}} - v_{ij}^n \cdot \mathbf{n}, \tag{11}$$

$$\mathbf{v}_j{}^{\text{after}} = \mathbf{v}_j^{\text{before}} + v_{ij}^n \cdot \mathbf{n}, \tag{12}$$

with $v_{ij}^n = \left(\mathbf{v}_i^{\text{before}} - \mathbf{v}_j^{\text{before}} \right) \cdot \mathbf{n}$.

Collision with rotation

We now consider two spheres i and j of the same radius R and mass m. Due to friction, angular momentum is exchanged if particles collide with nonzero tangential velocity. The equations of motion for rotation are

$$I \frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \mathbf{r} \wedge \mathbf{f}_i, \tag{13}$$

where I denotes the moment of inertia and $\mathbf{f}_i$ the forces exerted on particle i.

In the case of two colliding disks of radius R, moment of inertia I and mass m, the exchange of angular momentum is

$$\begin{aligned} I\left(\boldsymbol{\omega}_i' - \boldsymbol{\omega}_i\right) &= -Rm\mathbf{n} \wedge \left(\mathbf{v}_i' - \mathbf{v}_i\right), \\ I\left(\boldsymbol{\omega}_j' - \boldsymbol{\omega}_j\right) &= Rm\mathbf{n} \wedge \left(\mathbf{v}_j' - \mathbf{v}_j\right), \end{aligned} \tag{14}$$

with the primed velocities representing the ones after the collision.

Collision with rotation

Together with the conservation of momentum

$$\mathbf{v}_i' + \mathbf{v}_j' = \mathbf{v}_i + \mathbf{v}_j, \tag{15}$$

we obtain the rule for computing the new angular velocities after the collision, i.e.,

$$\boldsymbol{\omega}_i' - \boldsymbol{\omega}_i = \boldsymbol{\omega}_j' - \boldsymbol{\omega}_j = -\frac{Rm}{I}\left(\mathbf{v}_i' - \mathbf{v}_i\right) \wedge \mathbf{n}. \tag{16}$$

The relative velocity between particles i and j is

$$\mathbf{u}_{ij} = \mathbf{v}_i - \mathbf{v}_j - R(\boldsymbol{\omega}_i + \boldsymbol{\omega}_j) \wedge \mathbf{n}. \tag{17}$$

We decompose the relative velocities $\mathbf{u}$ of the particles into their normal and tangential components $\mathbf{u}^n$ and $\mathbf{u}^t$, respectively.

Collision with rotation

It is important to keep in mind that we are at this point not interested in the relative velocities of the centers of mass of the particles. For the angular momentum exchange, the relevant quantity to consider is the relative velocity of the particle surfaces at the contact point. The normal and tangential velocities are given by

$$\begin{aligned} \mathbf{u}_{ij}^{n} &= (\mathbf{u}_{ij}\mathbf{n})\,\mathbf{n}, \\ \mathbf{u}_{ij}^{t} &= \mathbf{u}_{ij} \wedge \mathbf{n} = [(\mathbf{v}_i - \mathbf{v}_j) - R\,(\boldsymbol{\omega}_i + \boldsymbol{\omega}_j)] \wedge \mathbf{n}. \end{aligned} \tag{18}$$

Collision with rotation

General slips are described by

$$\mathbf{u}_{ij}^{t\,\prime} = e_t \mathbf{u}_{ij}^{t}, \tag{19}$$

where the the *tangential restitution coefficient* e_t accounts for different slip types. The perfect slip collision is recovered for $e_t = 1$ which implies that no rotation energy is transferred from one particle to the other. No slip at all corresponds to $e_t = 0$. Energy conservation only holds if $e_t = 1$. In the case of $e_t < 1$, energy is dissipated.

If we compute the difference of the relative tangential velocities before and after the slip we get

$$\begin{aligned}(1 - e_t)\,\mathbf{u}_{ij}^{t} &= \mathbf{u}_{ij}^{t} - \mathbf{u}_{ij}^{t\,\prime} \\ &= -\left[\left(\mathbf{v}_i' - \mathbf{v}_i - \mathbf{v}_j' + \mathbf{v}_j\right) - R\left(\boldsymbol{\omega}_i' - \boldsymbol{\omega}_i + \boldsymbol{\omega}_j' - \boldsymbol{\omega}_j\right) \wedge \mathbf{n}\right].\end{aligned} \tag{20}$$

Collision with rotation

Combining the previous equation with Eq. (16), we obtain an expression without angular velocities

$$\mathbf{u}_{ij}^t - \mathbf{u}_{ij}^{t\,\prime} = (1 - e_t)\,\mathbf{u}_{ij}^t \tag{21}$$

$$= -\left[2\left(\mathbf{v}_i^{t\prime} - \mathbf{v}_i^t\right) + 2q\left(\mathbf{v}_i^{t\prime} - \mathbf{v}_i^t\right)\right] \tag{22}$$

and finally

$$\mathbf{v}_i^{t\prime} = \mathbf{v}_i^t - \frac{(1 - e_t)\,\mathbf{u}_{ij}^t}{2\,(1 + q)} \quad \text{with} \quad q = \frac{mR^2}{I}. \tag{23}$$

Collision with rotation

Analogously, we find for the remaining quantities

$$\begin{aligned} \mathbf{v}_j^{t\,\prime} &= \mathbf{v}_j^t + \frac{(1-e_t)\,\mathbf{u}_{ij}^t}{2\,(1+q)}, \\ \boldsymbol{\omega}_i' &= \boldsymbol{\omega}_i - \frac{(1-e_t)\,\mathbf{u}_{ij}^t \wedge \mathbf{n}}{2R\,(1+q^{-1})}, \\ \boldsymbol{\omega}_j' &= \boldsymbol{\omega}_j - \frac{(1-e_t)\,\mathbf{u}_{ij}^t \wedge \mathbf{n}}{2R\,(1+q^{-1})}. \end{aligned} \tag{24}$$

And the updated velocities are

$$\begin{aligned} \mathbf{v}_i{}' &= \mathbf{v}_i - \mathbf{u}_{ij}^n - \frac{(1-e_t)\,\mathbf{u}_{ij}^t}{2\,(1+q)}, \\ \mathbf{v}_j{}' &= \mathbf{v}_j + \mathbf{u}_{ij}^n + \frac{(1-e_t)\,\mathbf{u}_{ij}^t}{2\,(1+q)}. \end{aligned} \tag{25}$$

Inelastic collisions

The kinetic energy of interacting and colliding particles is not constant due to friction, plastic deformation or thermal dissipation. We account for energy dissipation effects in an effective manner by introducing the *restitution coefficient*. The restitution coefficient is defined as the ratio of the energy before and after the interaction event, and it describes multiple physical effects, i.e.,

$$r = \frac{E^{\text{after}}}{E^{\text{before}}} = \left(\frac{v^{\text{after}}}{v^{\text{before}}}\right)^2, \tag{26}$$

where E^{after} and E^{before} are the energies before and after the interaction event, and v^{after} and v^{before} are the corresponding velocities.

Inelastic collisions

Elastic collisions correspond to $r = 1$ whereas perfect plasticity is described by $r = 0$. Similar to our previous discussion of collisions with rotations, we also distinguish between normal and tangential energy transfer and define the corresponding coefficients

$$e_n = \sqrt{r_n} = \frac{v_n^{\text{after}}}{v_n^{\text{before}}}, \tag{27}$$

$$e_t = \sqrt{r_t} = \frac{v_t^{\text{after}}}{v_t^{\text{before}}}. \tag{28}$$

In the case of a bouncing ball, the restitution coefficient accounts for effects such as air friction, deformations and thermal dissipation.

Inelastic collisions

These coefficients strongly depend on the material, the shape of the particles, the energies involved in the events, the angle of impact and other factors. Usually, they are determined experimentally.

The relative velocity of the particles at their contact point is

$$\mathbf{u}_{ij}^{n} = (\mathbf{u}_{ij}\mathbf{n})\,\mathbf{n} = [(\mathbf{v}_i - \mathbf{v}_j)\,\mathbf{n}]\,\mathbf{n}. \tag{29}$$

The normal velocity components are affected by inelasticity. In the case of an inelastic collision, dissipation effects lead to reduced normal velocities

$$\mathbf{u}_{ij}^{n\,\prime} = -e_n \mathbf{u}_{ij}^{n} \tag{30}$$

Inelastic collisions

For $e_n = 1$, there is no dissipation whereas dissipation effects occur for $e_n < 1$.

Similar to Eq. (19) and following derivations, we obtain the expressions for the velocities of each particle after the collision

$$\begin{aligned} \mathbf{v}_i{}' &= \mathbf{v}_i - \frac{(1+e_n)}{2}\mathbf{u}_{ij}^n, \\ \mathbf{v}_j{}' &= \mathbf{v}_j + \frac{(1+e_n)}{2}\mathbf{u}_{ij}^n. \end{aligned} \tag{31}$$

In the case of perfect slip, the momentum exchange is

$$\Delta\mathbf{p}_n = -m_{\text{eff}}(1+e_n)\left[(\mathbf{v}_i - \mathbf{v}_j)\,\mathbf{n}\right]\mathbf{n}. \tag{32}$$

Inelastic collisions

With $q = \frac{m_{\text{eff}} R^2}{I_{\text{eff}}}$, the equations for the velocities after the collision are

$$\begin{aligned}
\mathbf{v}'_i &= \mathbf{v}_i - \frac{(1+e_n)}{2}\mathbf{u}^n_{ij} - \frac{(1-e_t)\,\mathbf{u}^t_{ij}}{2\,(1+q)}, \\
\mathbf{v}'_j &= \mathbf{v}_j + \frac{(1+e_n)}{2}\mathbf{u}^n_{ij} + \frac{(1-e_t)\,\mathbf{u}^t_{ij}}{2\,(1+q)}, \\
\boldsymbol{\omega}'_i &= \boldsymbol{\omega}_i - \frac{(1-e_t)\,\mathbf{u}^t_{ij} \wedge \mathbf{n}}{2R\,(1+q^{-1})}, \\
\boldsymbol{\omega}'_j &= \boldsymbol{\omega}_j + \frac{(1-e_t)\,\mathbf{u}^t_{ij} \wedge \mathbf{n}}{2R\,(1+q^{-1})}.
\end{aligned} \tag{33}$$

These equations describe inelastic collisions of rotating particles.

Inelastic collisions

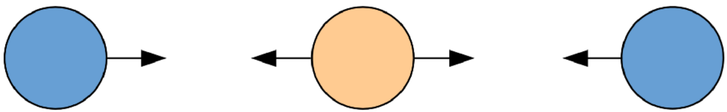

Figure 2: The orange particle at the center is bouncing between the blue particles which approach each other.

Inelastic collisions

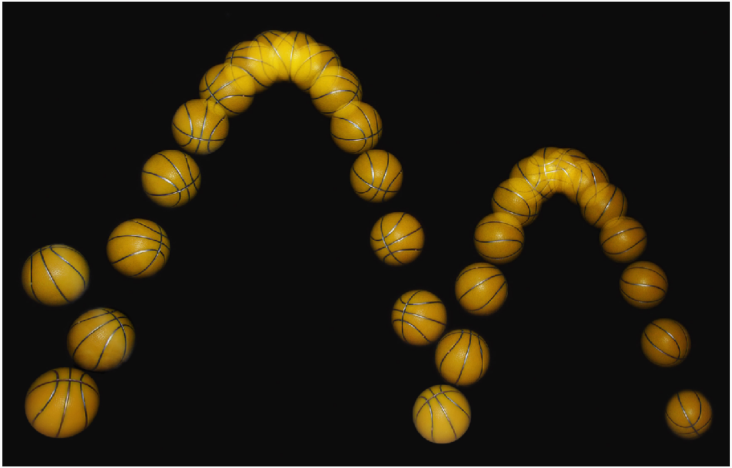

Figure 3: A bouncing ball.

Inelastic collisions

Every time the ball hits the surface its kinetic energy is lowered according to Eq.(26). As a consequence, the ball will not reach the initial height anymore and the time between two contacts with the surface approaches zero. After a finite time, the ball comes to a rest, but the simulation takes infinite time to run. In a event-driven simulation, the ball never stops its motion and the number of events per time step increases. A similar problem is the famous *Zenon Paradox*[1].

[1] https://en.wikipedia.org/wiki/Zeno's_paradoxes

Inelastic collisions

Since the height is directly proportional to the energy, the height also scales with the restitution coefficient at every bounce. Consequently, at the i^{th} bounce the damping of the height is proportional to r^i. The total time is given by

$$\begin{aligned} t_{\mathrm{tot}} &= \sum_{i=1}^{\infty} t_i \\ &= 2\sqrt{\frac{2h^{\mathsf{initial}}}{g}} \sum_{i=1}^{\infty} \sqrt{r^i} \\ &= 2\sqrt{\frac{2h^{\mathsf{initial}}}{g}} \left(\frac{1}{1-\sqrt{r}} - 1 \right). \end{aligned} \tag{34}$$

Inelastic collisions

Luding and McNamara introduced in 1998 a coefficient of restitution that is dependent of the time elapsed since the last event occurred. If the time since the last collision of one of the interacting particles $t^{(i)}$ or $t^{(j)}$ is less than t_{contact}, then the coefficient is set to unity, i.e.,

$$r^{i,j} = \begin{cases} r, & \text{for} \quad t^{(i)} > t_{\text{contact}} \quad \text{or} \quad t^{(j)} > t_{\text{contact}} \\ 1, & \text{otherwise} \ . \end{cases} \tag{35}$$

With this redefinition of the restitution coefficient, the collision type changes from inelastic to elastic if too many collisions occur during t_{contact}.

Inelastic collisions

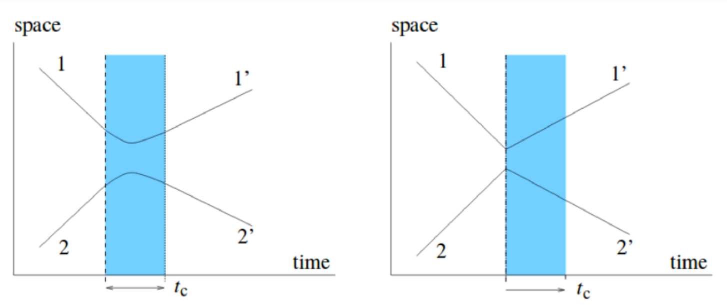

Figure 4: Trajectories of soft (left) and hard (right) particles. The figure is taken from [S. Luding, S. McNamara, *Granul. Matter* (1998).].

Inelastic collisions

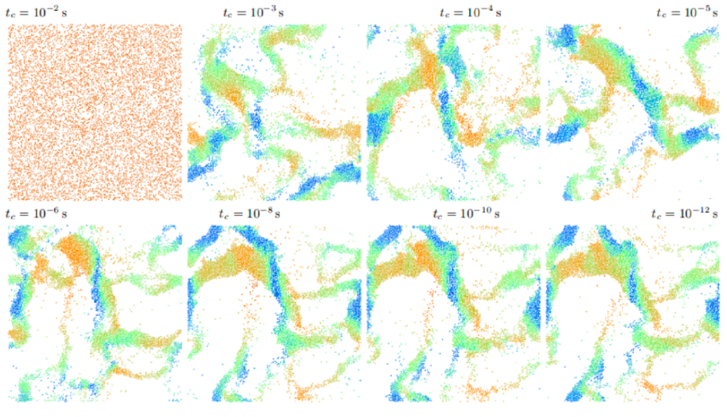

Figure 5: Examples of different contact times t_c. The figure is taken from [S. Luding, S. McNamara, *Granul. Matter* (1998).].

Contact dynamics

Contact Dynamics

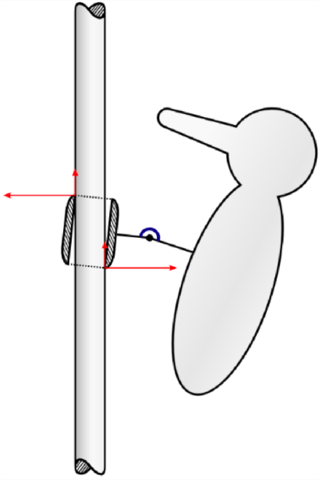

Figure 6: A woodpecker toy as a benchmark example for contact dynamics problems.

Contact Dynamics

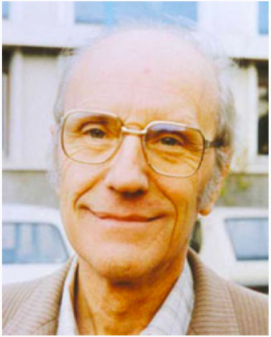

Figure 7: Per Lötstedt and Jean-Jacques Moreau contributed to development of contact dynamics.

Contact Dynamics

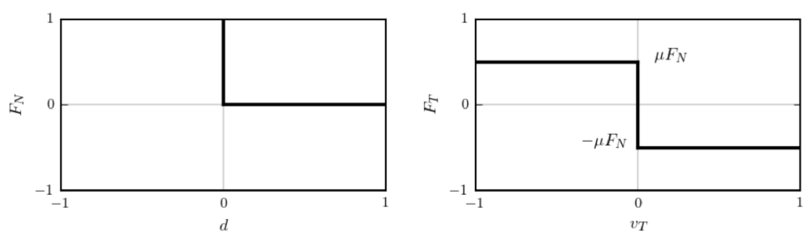

Figure 8: Signorini (left) and Coulomb (right) graphs.

One-dimensional Contact

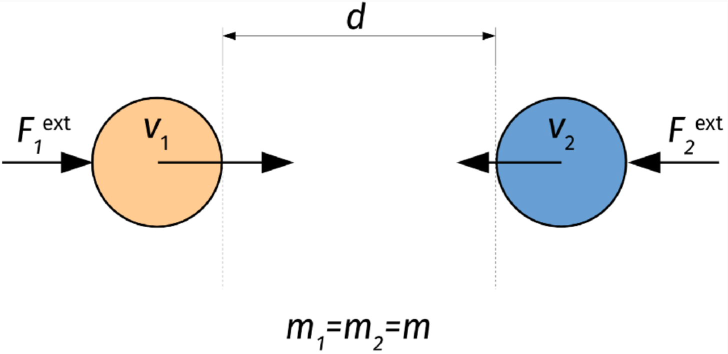

Figure 9: Illustration of a one-dimensional contact.

One-dimensional Contact

We have to make sure that these two particles do not overlap. Therefore, we impose constraint forces in such a way that they compensate all other forces which would lead to overlaps. These constraint forces should be defined in such a way that they have no influence on the particle dynamics before and after the contact. The time evolution of the particles' positions and velocities is described by an implicit Euler scheme which is given by

$$\begin{aligned} \mathbf{v}_i\left(t+\Delta t\right) &= \mathbf{v}_i\left(t\right) + \Delta t \frac{1}{m_i} \mathbf{F}_i\left(t+\Delta t\right), \\ \mathbf{r}_i\left(t+\Delta t\right) &= \mathbf{r}_i\left(t\right) + \Delta t \mathbf{v}_i\left(t+\Delta t\right), \end{aligned} \tag{36}$$

where the force consists of an external and a contact term, i.e., $\mathbf{F}_i\left(t\right) = \mathbf{F}_i^{\text{ext}}\left(t\right) + \mathbf{R}_i\left(t\right)$.

One-dimensional Contact

So far, we only considered forces that act on the center of mass. However, contact forces act locally on the contact point and not on the center of mass. We therefore introduce a matrix H which transforms local contact forces into particle forces, and the corresponding transpose H^T transforms particle velocities into relative velocities.

This leads to

$$v_n^{\mathsf{loc}} = v_2 - v_1 = \begin{pmatrix} -1 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{37}$$

and local forces

$$\begin{pmatrix} R_1 \\ R_2 \end{pmatrix} = \begin{pmatrix} -R_n^{\mathsf{loc}} \\ R_n^{\mathsf{loc}} \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix} R_n^{\mathsf{loc}} = H R_n^{\mathsf{loc}}. \tag{38}$$

One-dimensional Contact

The equations of motion for both particles are

$$\frac{\mathsf{d}}{\mathrm{d}t}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \frac{1}{m}\left[\begin{pmatrix} R_1 \\ R_2 \end{pmatrix} + \begin{pmatrix} F_1^{\mathsf{ext}} \\ F_2^{\mathsf{ext}} \end{pmatrix}\right]. \tag{39}$$

Combining the last equation with the transformation rule of Eq. (38) we find

$$\begin{aligned} \frac{\mathrm{d}v_n^{\mathsf{loc}}}{\mathrm{d}t} &= \begin{pmatrix} -1 & 1 \end{pmatrix} \frac{1}{m}\left[\begin{pmatrix} -1 \\ 1 \end{pmatrix} R_n^{\mathsf{loc}} + \begin{pmatrix} F_1^{\mathsf{ext}} \\ F_2^{\mathsf{ext}} \end{pmatrix}\right] \\ &= \frac{1}{m_{\mathsf{eff}}} R_n^{\mathsf{loc}} + \frac{1}{m}\left(F_2^{\mathsf{ext}} - F_1^{\mathsf{ext}}\right), \end{aligned} \tag{40}$$

where $m_{\mathrm{eff}} = m/2$ is the effective mass and $\frac{1}{m}\left(F_2^{\mathsf{ext}} - F_1^{\mathsf{ext}}\right)$ the acceleration without contact forces.

One-dimensional Contact

We integrate the last equation with an implicit Euler method and find:

$$\frac{v_n^{\mathsf{loc}}(t+\Delta t) - v_n^{\mathsf{loc}}(t)}{\Delta t} = \frac{1}{m_{\mathsf{eff}}} R_n^{\mathsf{loc}}(t+\Delta t) + \frac{1}{m}\left(F_2^{\mathsf{ext}} - F_1^{\mathsf{ext}}\right). \tag{41}$$

The unknown quantities in this equation are v_n^{loc} and R_n^{loc}. To find a solution, we make use of the Signorini constraint and compute

$$R_n^{\mathsf{loc}}(t+\Delta t) = \frac{v_n^{\mathsf{loc}}(t+\Delta t) - v_n^{\mathsf{loc,\ free}}(t+\Delta t)}{\Delta t} \tag{42}$$

with

$$v_n^{\mathsf{loc,\ free}}(t+\Delta t) = v_n^{\mathsf{loc}}(t) + \Delta t \frac{1}{m}\left(F_2^{\mathsf{ext}} - F_1^{\mathsf{ext}}\right). \tag{43}$$

One-dimensional Contact

We distinguish between the possible cases:

- Particles are not in contact,
- Particles are in closing contact,
- Particles are in persisting contact and
- Particles are in opening contact.

Three-dimensional Contact

We now extend the described contact dynamics approach to three dimensions. In particular, we consider particle interactions without friction. Thus, we do not need to take into account angular velocities and torques. In three dimensions, velocities and forces are given by

$$\mathbf{v}_{12} = \begin{pmatrix} v_{12}^x \\ v_{12}^y \\ v_{12}^z \end{pmatrix} \quad \mathbf{R}_{12} = \begin{pmatrix} R_{12}^x \\ R_{12}^y \\ R_{12}^z \end{pmatrix} \quad \mathbf{F}_{12}^{\text{ext}} = \begin{pmatrix} F_{12}^{x,\text{ext}} \\ F_{12}^{y,\text{ext}} \\ F_{12}^{z,\text{ext}} \end{pmatrix}. \qquad (44)$$

Three-dimensional Contact

Only normal components v_n^{loc} and R_n^{loc} have to be considered nn during particle contact. We therefore project all necessary variables onto the normal vector

$$\mathbf{n} = \begin{pmatrix} n^x \\ n^y \\ n^z \end{pmatrix}, \tag{45}$$

and obtain

$$v_n^{loc} = \mathbf{n} \cdot (\mathbf{v}_2 - \mathbf{v}_1) \quad \mathbf{R}_1 = -\mathbf{n} R_n^{loc} \quad \mathbf{R}_2 = \mathbf{n} R_n^{loc}. \tag{46}$$

Three-dimensional Contact

From the projection, we obtain the matrix H for the coordinate transformation

$$v_n^{loc} = H^T \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{pmatrix}, \quad \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{pmatrix} = H R_n^{loc}, \tag{47}$$

with

$$H^T = (-n_x, -n_y, -n_z, n_x, n_y, n_z) \tag{48}$$

Friction can be included by considering angular velocities and torques.