Exercise 1. Contact Dynamics

Goal: Last week we learned about the Event-Driven MD as a method to model systems of perfectly rigid particles. The Contact Dynamics method is an alternative method to model such systems with the advantage that lasting contacts can be considered as well. The major difference is that the forces are calculated to fulfill given constraints, like the Signorini condition, i.e. particles cannot overlap. More details can be found in the lecture notes, including detailed derivations for simple examples.

Task 1: *Implement the* `Contact Dynamics` *method for a system of spherical particles in one or two dimensions.*

Hint: You may want to recycle several functions that you already implemented for the last exercise sheet(s).

Use the following simplifications:

- *Consider frictionless contacts such that you do not need to consider angular velocities etc.*
- *Assume that the particles have the same mass m and the same radius R.*
- *Consider only single contacts.*

Task 2 (OPTIONAL): *Extend your code by including multiple contacts per particle (contact networks). When calculating the force at one contact, treat the other contact forces acting on the involved particles as external forces.*

It is useful to store the total force $\boldsymbol{R}_i$ acting on a particle i due to all its contacts in a contact network. Before updating the force at one contact (involving particles i and j) one simply subtracts the current contact's contribution to $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$, defining $\boldsymbol{R}'_i$ and $\boldsymbol{R}'_j$. Calculate the force at the contact by setting $\boldsymbol{F}_i^{ext} + \boldsymbol{R}'_i$ and $\boldsymbol{F}_j^{ext} + \boldsymbol{R}'_j$ as external forces. Add the new contact's contribution. Continue in the same way with the next contact to be updated.

Solution. Considering free particle dynamics (i.e. no contacts), we can solve the equations of motion using the `implicit Euler` integration scheme

$$\begin{aligned} \boldsymbol{v}_i(t+\Delta t) &= \boldsymbol{v}_i(t) + \frac{\boldsymbol{F}_i(t+\Delta t)}{m_i}\Delta t \\ \boldsymbol{r}_i(t+\Delta t) &= \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t+\Delta t)\Delta t \end{aligned} \tag{S.1}$$

If we want to consider contact dynamics, we need to include the contact force $\boldsymbol{R}_i$ on a particle i into the total force $\boldsymbol{F}_i(t) = \boldsymbol{F}_i^{\text{ext}}(t) + \boldsymbol{R}_i(t)$. The contact force has to make sure that no overlaps occur (constraints). At the same time, we have to be careful that the contact forces only act during the immediate contact. Here, we only consider fricitonless contacts.

In a first step, we define the normal vector

$$\boldsymbol{n} = \frac{\boldsymbol{r}_2 - \boldsymbol{r}_1}{\|\boldsymbol{r}_2 - \boldsymbol{r}_1\|}$$

between the two particles which are in contact and define the following quantities (`n` for normal)

$$v_n^{\mathrm{loc}} = H^T \begin{pmatrix} \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \end{pmatrix}$$
$$R_n^{\mathrm{loc}} = H^T \begin{pmatrix} \boldsymbol{R}_1 \\ \boldsymbol{R}_2 \end{pmatrix}$$

where $H^T = \begin{pmatrix} -\boldsymbol{n} & \boldsymbol{n} \end{pmatrix}$. The equations of motion are given by

$$d_t \begin{pmatrix} \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \end{pmatrix} = \frac{1}{m} \begin{pmatrix} \boldsymbol{R}_1 + \boldsymbol{F}_1^{\mathrm{ext}} \\ \boldsymbol{R}_2 + \boldsymbol{F}_2^{\mathrm{ext}} \end{pmatrix}$$

or equivalently

$$d_t v_n^{\mathrm{loc}} = \frac{2}{m} R_n^{\mathrm{loc}} + d_t v_n^{\mathrm{free}}$$

where $d_t v_n^{\mathrm{free}} = \frac{1}{m} H^T \begin{pmatrix} \boldsymbol{F}_1^{\mathrm{ext}} & \boldsymbol{F}_2^{\mathrm{ext}} \end{pmatrix}^T$ is the relative acceleration without any contact interaction of the particles. Using the above described Euler scheme (Eq. S.1), we can solve this equation for

$$R_n^{\mathrm{loc}}(t+\Delta t) = \frac{m}{2} \frac{v_n^{\mathrm{loc}}(t+\Delta t) - \left(v_n^{\mathrm{loc}}(t) + d_t v_n^{\mathrm{free}}(t)\Delta t\right)}{\Delta t}$$

Three more conditions have to be fulfilled ($d(t)$ being the distance between the two particle surfaces)

$$\begin{aligned} d(t+\Delta t) = d(t) + v_n^{\mathrm{loc}}(t+\Delta t)\Delta t \geq 0, &\quad \text{volume exclusion} \\ d(t+\Delta t) R_n^{\mathrm{loc}}(t+\Delta t) = 0, &\quad \text{contact condition} \\ R_n^{\mathrm{loc}}(t+\Delta t) \geq 0, &\quad \text{repulsive constraint forces} \end{aligned}$$

The set of allowed pairs $(v_n^{\mathrm{loc}}(t+\Delta t), R_n^{\mathrm{loc}}(t+\Delta t))$ is determined by the `Signorini graph`. Finally, we arrive at

$$\begin{aligned} v_n^{\mathrm{loc}}(t+\Delta t) &= \max\left\{-\frac{d(t)}{\Delta t}, v_n^{\mathrm{loc}}(t) + d_t v_n^{\mathrm{free}}(t)\Delta t\right\} \\ R_n^{\mathrm{loc}}(t+\Delta t) &= \max\left\{0, -\frac{m}{2\Delta t}\left(\frac{d(t)}{\Delta t} + v_n^{\mathrm{loc}}(t) + d_t v_n^{\mathrm{free}}(t)\Delta t\right)\right\} \end{aligned}$$

which only needs to be transformed back via

$$\begin{pmatrix} \boldsymbol{R}_1 \\ \boldsymbol{R}_2 \end{pmatrix} = H R_n^{\mathrm{loc}}$$

Using the above results, we simulate a system of $N = 20$ particles in a box with random initial velocities and gravity acting along the $+x$-direction. We assume only single contacts, i.e. either one particle-wall contact or one particle-particle contact per particle can happen at the same time. In the beginning we observe a realistic/physical behaviour of the particles colliding with each other or with the walls of the box. However, the longer we let the simulation run the more unphysical scenarios can be observed due to the external gravity force. Since the gravity pulls the particles towards one of the walls, the average distance to the neighbors of a particle decreases significantly. This leads to many simultaneous contacts (which is what we neglected beforehand). Consequently, unphysical scenarios like (large) particle overlaps, particle-particle tunneling or particles leaving the box can be observed. There are two possibilities to fix these problems. First, we could introduce multiple contacts per particle as described above (see Task 2). Second, we could decrease the time step size even further. The additional resolution would reduce the number of contacts happening in the same time interval (in this limit we are again in the single-contact case, at least for instantaneous contacts).