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 $\boldsymbol{F}_i^{\text{ext}} + \boldsymbol{R}'_i$ and $\boldsymbol{F}_j^{\text{ext}} + \boldsymbol{R}'_j$ as external forces. Add the new contact's contribution. Continue in the same way with the next contact to be updated.