1 Introduction

The DEM can be used to simulate the interaction of multiple bodies in contact. Under the assumption that the radius of the bodies are not larger than half the cell size, the forces acting at the contact points can be considered to be of short range and thus we can conveniently reuse our acceleration structure from the last assignment.

With the DEM we are now able to simulate particles with actual shape and volume (rigid bodies) instead of just point masses. For simplicity we will only use spheres in this assignment. Therefore we need one additional parameter in the input file: the radius of each particle. Choose the second value in each input line to be the radius r.

Since our objects now have a shape they can also rotate. To model these rotations every sphere has to store its current rotation (quaternion) and its angular velocity (vector). The direction of the angular velocity vector is the rotation axis the sphere is rotating around.

2 Contact Resolution

The contact resolution has two parts. The normal force and the tangential force. The simplest DEM approach for the normal force is to insert spring-dampers at each contact point in order to prevent penetrations. Assuming two bodies a and b collide then the spring-damper is inserted along the surface normal $\mathbf{n}$, which is the direction vector pointing from particle b to particle a and having unit length. A spring-damper is described by the equation

$$\begin{aligned} &\text{(A)} \quad \mathbf{F_n} = +k_s p \hat{n} - k_{dn} \mathbf{v}_n, \\ &\text{(B)} \quad \mathbf{F_n} = -k_s p \hat{n} - k_{dn} \mathbf{v}_n, \end{aligned}$$

where p is the (positive) penetration depth at the contact in normal direction and k_{dn} the damping coefficient in normal direction. **Pay attention to apply the forces with the right signs.** But since we are also including rotations we have a tangential force as well. The tangential force is just a damping term depending on the relative tangential contact velocity which is limited by the previously calculated normal force.

$$\mathbf{F_t} = \min\left(k_{dt}|\mathbf{v}_t|, k_f F_n\right)\hat{t},$$

where k_{dt} is the damping coefficient in tangential direction and k_f is the friction coefficient. Again the direction of the force matters! The tangential force is then applied to both bodies like the normal force. Both contact forces act at the contact point resulting in a force contribution

$$\mathbf{F} = \mathbf{F_n} + \mathbf{F_t}$$

and a torque contribution

$$\tau_\mathbf{a} = (\mathbf{x} - \mathbf{x_a}) \times \mathbf{F_t}$$

with the contact position $\mathbf{x} = \mathbf{x_b} + \frac{r_b}{r_a + r_b}\left(\mathbf{x_a} - \mathbf{x_b}\right)$.

3 Contact Detection

For two spheres with radii r_a and r_b and positions $\mathbf{x}_a$ and $\mathbf{x}_b$ the penetration depth p can be easily determined to be

$$p = r_a + r_b - |\mathbf{x}_a - \mathbf{x}_b|.$$

Note that if $p < 0$ then there is no contact and consequently no spring-damper active and thus no resulting contact force present. To calculate the contact velocity $\mathbf{v}$ the velocity difference of the involved bodies must be evaluated:

$$\mathbf{v} = [\mathbf{v_a} + \omega_\mathbf{a} \times (\mathbf{x} - \mathbf{x_a})] - [\mathbf{v}_b + \omega_\mathbf{b} \times (\mathbf{x} - \mathbf{x_b})],$$

with the contact position $\mathbf{x} = \mathbf{x_b} + \frac{r_b}{r_a + r_b}(\mathbf{x_a} - \mathbf{x_b})$, the body positions $\mathbf{x_a}$ and $\mathbf{x_b}$, the linear body velocities $\mathbf{v_a}$ and $\mathbf{v_b}$ and the angular velocities $\omega_\mathbf{a}$ and $\omega_\mathbf{b}$.

4 Details

The spring-damper forces should be computed in your force calculation kernel and replace the forces resulting from the Lennard-Jones potential. Add the spring constant k_s and damping coefficients k_{dn} and k_{dt} as additional parameters `k_s`, `k_dn` and `k_dt` to the parameter file. Also add the parameters `g_x`, `g_y` and `g_z` for a gravitational acceleration applied to all particles that have not infinite mass in each time step. The parameter `r_cut` is no longer relevant in this assignment.

The general idea of treating the reflecting boundary conditions works equivalently to sphere-sphere collisions: As soon as a particle overlaps with the boundary plane a spring-damper starts to counteract the overlap in normal direction and a damping occurs in tangential direction. In order to specify the type of boundary conditions we introduce a new set of parameters `reflect_x`, `reflect_y` and `reflect_z`. A non-zero value indicates reflecting boundary conditions on both boundaries of the respective direction. A zero value indicates periodic boundary conditions.

The visualization must be extended so that particles of different sizes can be visualized. Thus the VTK file writer should also output a scalar field containing the particles' radii in each time step. Also output the current rotation of the particle and visualize it using for example a second arrow glyph.

To support arbitrary obstacle geometries there exists a simple approach: The obstacles can be decomposed into a set of particles of infinite mass. The infinite mass prevents the obstacle particles from moving in the position update but the particles still contribute to the force calculation of the other particles. Extend your input file reader so that it is able to read in `inf` mass values and store them appropriately. Make sure that gravitational acceleration is *not* applied to these particles.