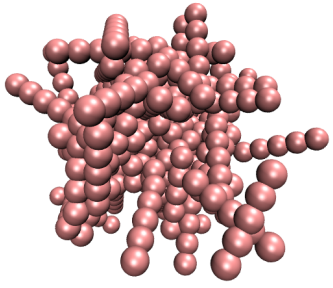
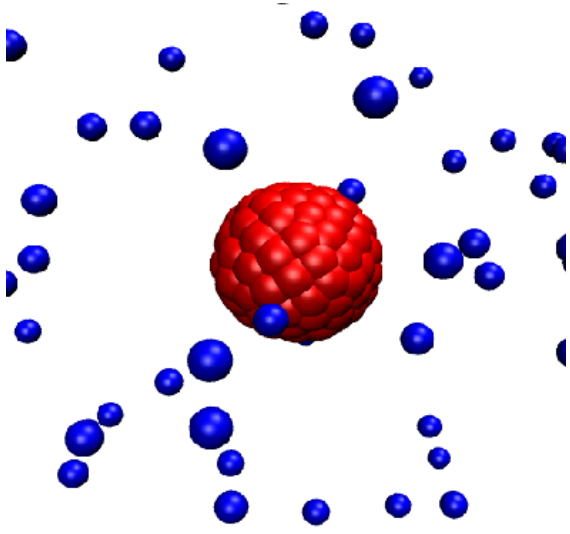
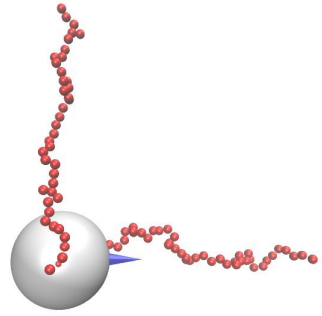
Rigid Bodies in MD Simulations



Rod-like particles



Raspberry particles



Polymer attached to the surface of a colloid

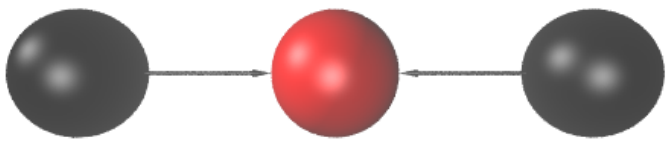
Virtual sites: Introduction

- Derive position and velocities from other particles
  $\Rightarrow$ Not propagated using Newton's equations
- Interact with the rest of the system via the usual interactions
- Transfer the forces they feel onto the particles from which they were derived

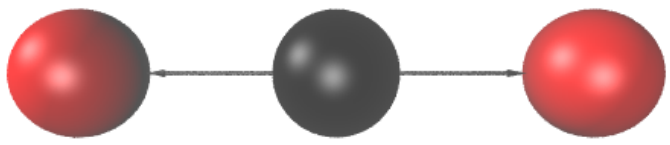
Algorithm

1. Place virtual particles according to the positions of the non-virtual particles
2. Calculate all forces in the system, including those on virtual particles
3. Transfer forces from the virtual particles to the non-virtual particles
4. Integrate Newton's equations of motion for the non-virtual particles

Virtual sites: Implementations in ESPResSo

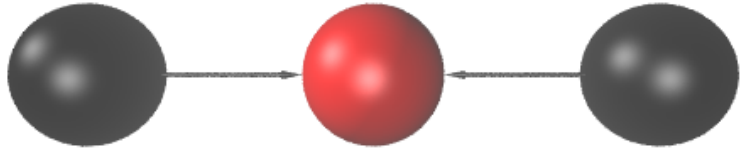


Virtual site at the center of mass of a molecule (COM)



Virtual site relative to the position and orientation of an other particle (RELATIVE)

Virtual sites: Center of mass



Position and velocity of virtual site

$$\vec{x}_v = \frac{\sum_i m_i \vec{x}_i}{\sum_i m_i}$$

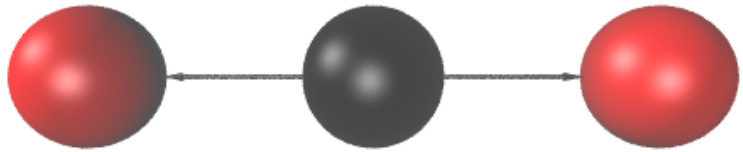
$$\vec{v}_v = \frac{\sum_i m_i \vec{v}_i}{\sum_i m_i}$$

Transferring forces from the virtual site to the particles of the molecule

$$\vec{F}_i = \frac{m_i \vec{F}_v}{\sum_i m_i}$$

- Subscript v denotes the virtual particle
- Subscript i denotes non-virtual particles forming the molecule

Virtual sites for rigid bodies



- All particles forming the rigid body are defined *relative* to the center of mass.
- The center of mass is propagated using Newton's equations.

Position of the virtual site

$\vec{x}_v = \vec{x}_c + r_v O_c O_v \vec{e}_z$

Transferring forces from the virtual particle onto the center of mass

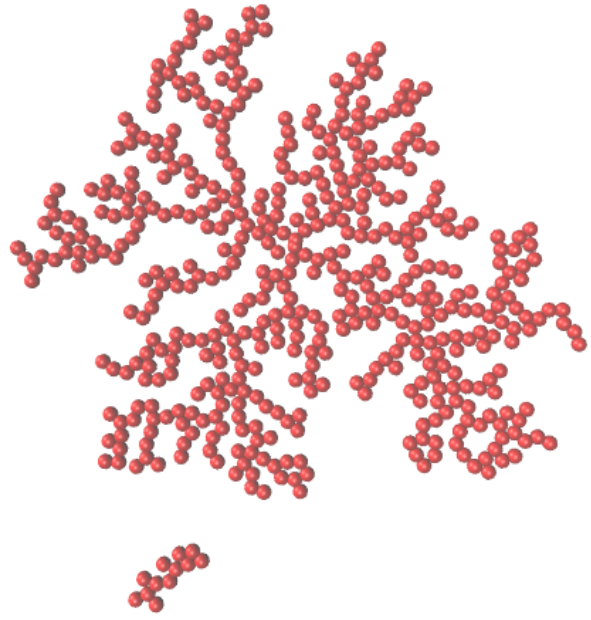
Force: $\vec{F}_c = \vec{F}_v$ Torque: $\vec{T}_c = (\vec{x}_v - \vec{x}_c) \times \vec{F}_v$

- Subscript c: center of mass particle
- Subscript v: virtual site
- r_v: Distance between center of mass and virtual site
- O_c: Rotation operator which rotates the co-rotating frame of the rigid body onto the lab frame
- O_v: Rotation operator which rotates z-axis in co-rotating frame onto the vector from center of mass to virtual site

Rigid bodies: Usage

- Compile ESPResSo with ROTATION and VS_RELATIVE
- *First* place the particle at the center of mass
- Then place the remaining particles of the rigid body and relate them to the center of mass:
  part *id* virtual 1 vs_auto_relate_to *id*
- Assign the center of mass particle the mass and inertial tensor of the entire rigid body.

Dynamic bonding

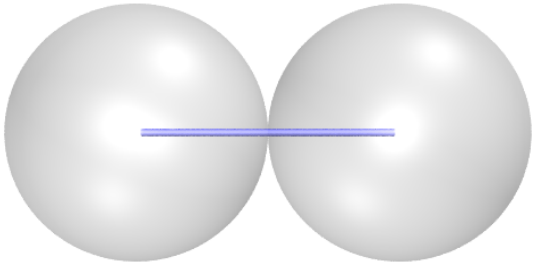


Diffusion limited aggregation

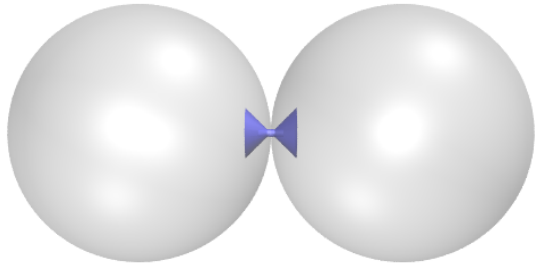
When a particle collides with the cluster, it sticks.

Then a new particle is added, consecutively.

Dynamic bonding: Modes



Bind centers
Distance dependent bond between the centers of the colliding particles.



Bind at point of collision
Two virtual sites are placed at the point of collision and related to the colliding particles, respectively.
The virtual sites are bound with a zero-length bond.

Dynamic bonding: Usage

- Make sure, a non-bonded interaction is defined for the particles that should be bound
- Make sure the minimum global cutoff (setmd min_global_cut) is larger than the bonding distance
- Define a bonded interaction which will connect the centers of the colliding particles
- For the case of bonding at point of collision: Define a bonded interaction between the virtual sites with equilibrium length of zero.
- Enable collision detection via the on_collision command