11th i-CoMSE Workshop: Mesoscale Particle-Based Modeling

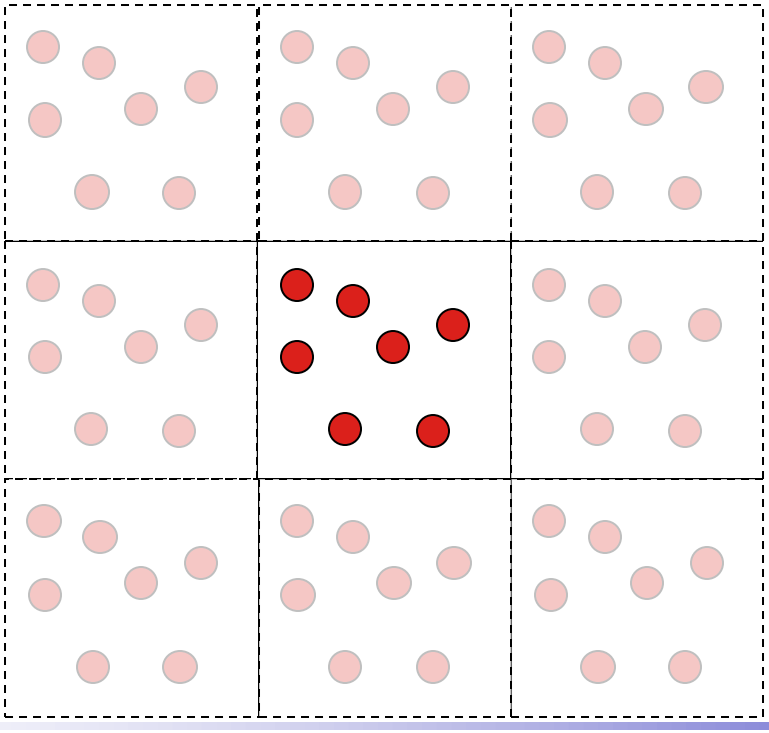
Mississippi State University
July 21–25, 2025

Session 9: Walls

PBCs

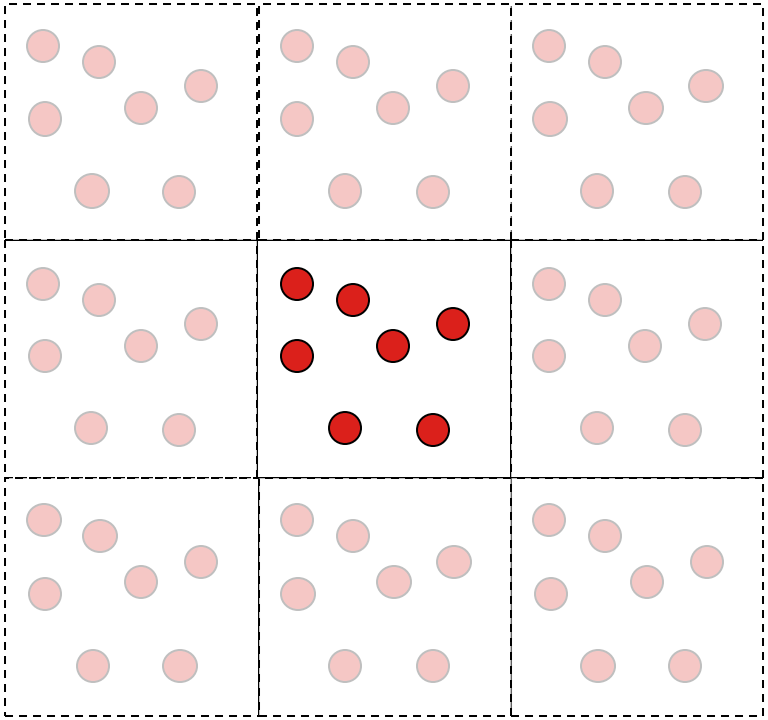
- Periodic boundary conditions (PBCs) allow for simulation of “infinite systems” using a finite number of particles

- $r^{cutoff} \leq \frac{1}{2} L_x$ to be consistent with minimum image convention



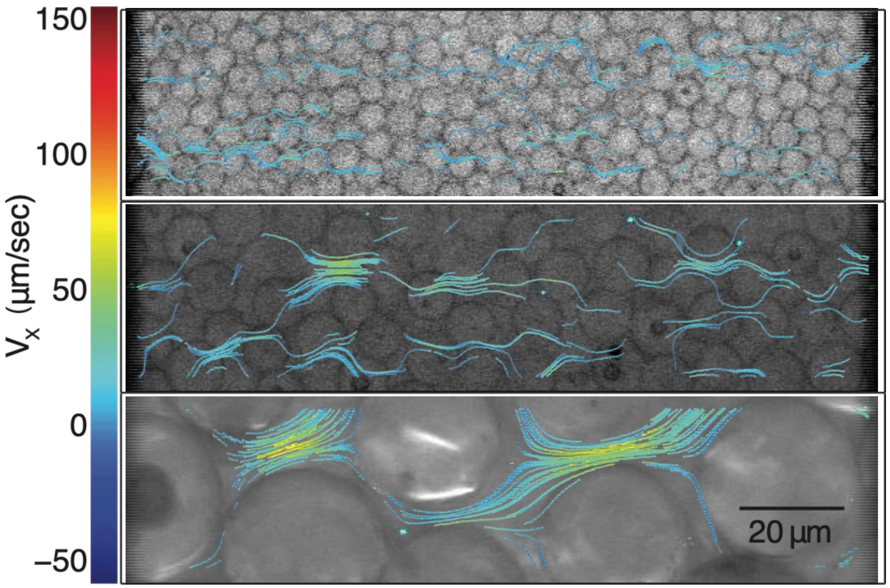
PBCs

- Caution:
  - Correlations between particles can still exits beyond r^{cutoff}
  - Finite size effects can thus still be significant → processes where correlations occur on length scales $\gtrsim L_x$ (e.g., transport properties and phase transitions)



Confined systems

- Many cases where we want to simulate systems with reduced dimensionality that are confined in one or more directions
- Ubiquitous in technological applications where systems interact with solid surfaces

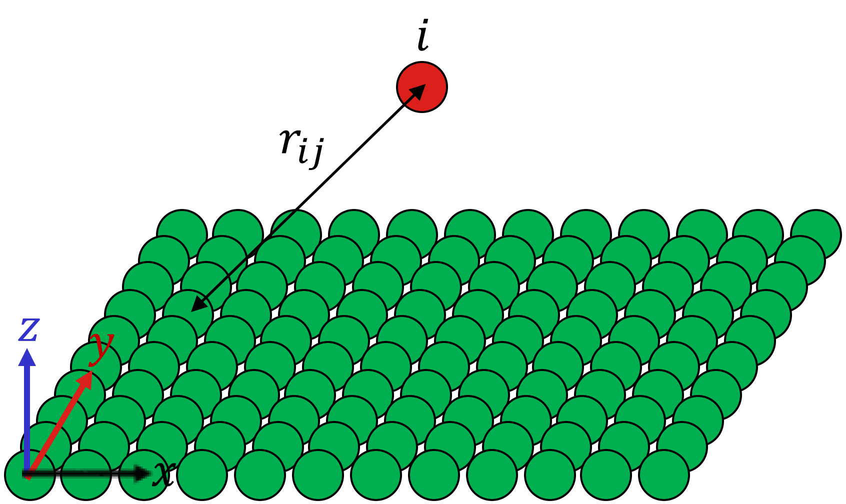


(Courtesy Jacinta Conrad at the University of Houston)

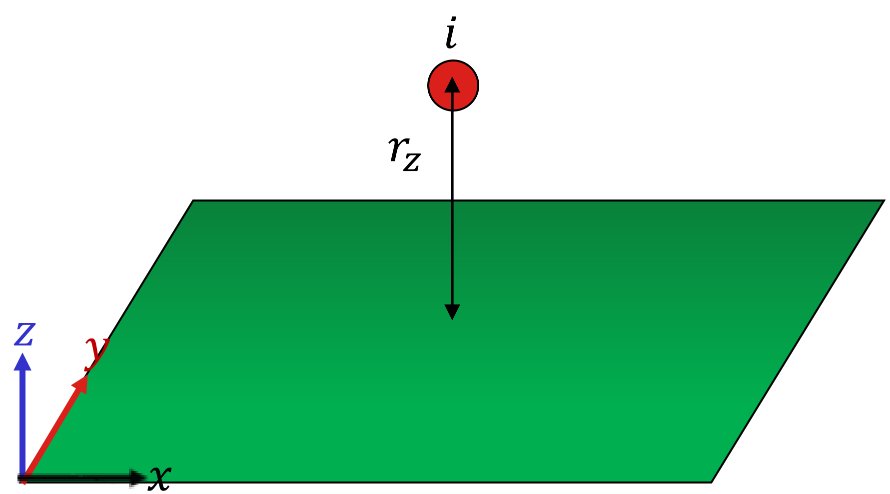
- We can model these types of systems using walls to create solid boundaries

Particle vs. smooth walls

- Particle walls: e.g., planar wall that spans *x-y* dimensions of cell
  - n^{wall} particles arranged in a regular geometry (e.g., cubic lattice)
  - Particle-wall interaction: $u_i^{p,wall} = \sum_j^{n^{wall}} u(r_{ij})$
  - Requires n^{wall} energy/force calculations
  - $u_i^{p,wall}$ varies in *x*, *y*, and *z* directions viz r_{ij}



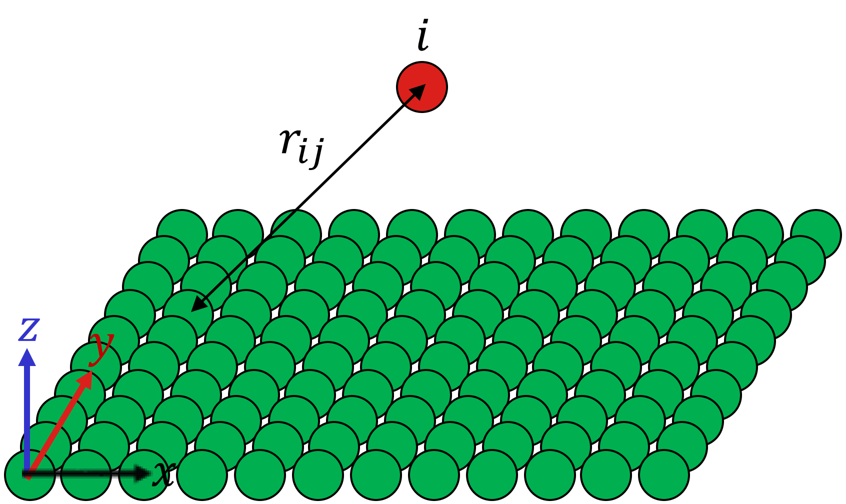
Particle wall



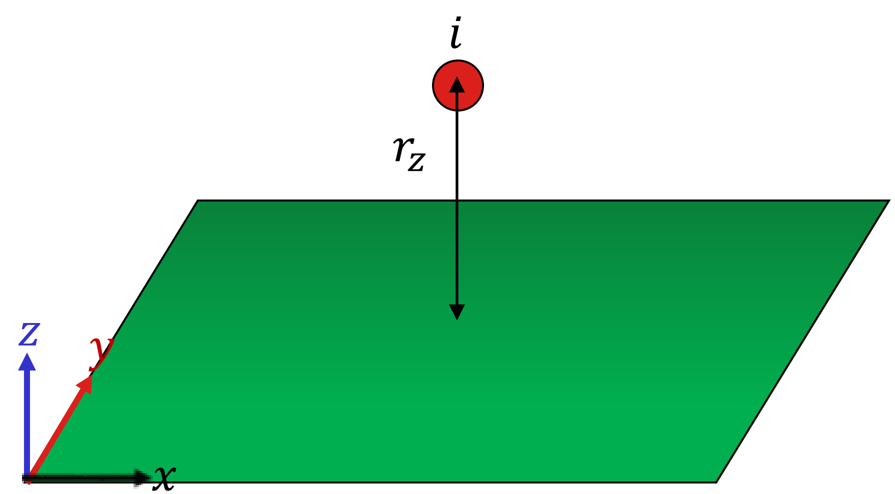
Smooth wall

Particle vs. smooth walls

- Smooth walls: e.g., planar wall that spans *x-y* dimensions of cell
  - Featureless wall modeled as an infinite plane
  - Particle-wall interaction: $u_i^{s,wall}(r_z)$
  - Requires 1 energy/force calculations
  - $u_i^{s,wall}(r_z)$ varies only in the *z* direction viz r_z
- Smooth walls can be thought of effective potentials obtained by integrating over interactions with particles in the wall



Particle wall

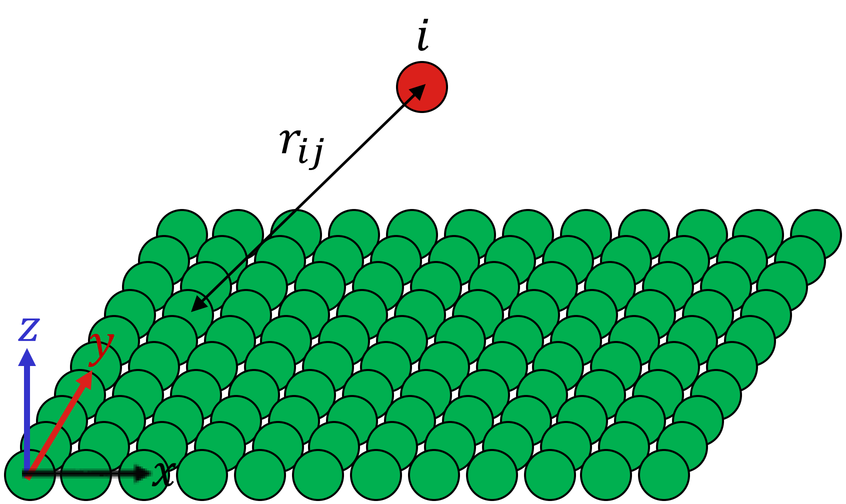


Smooth wall

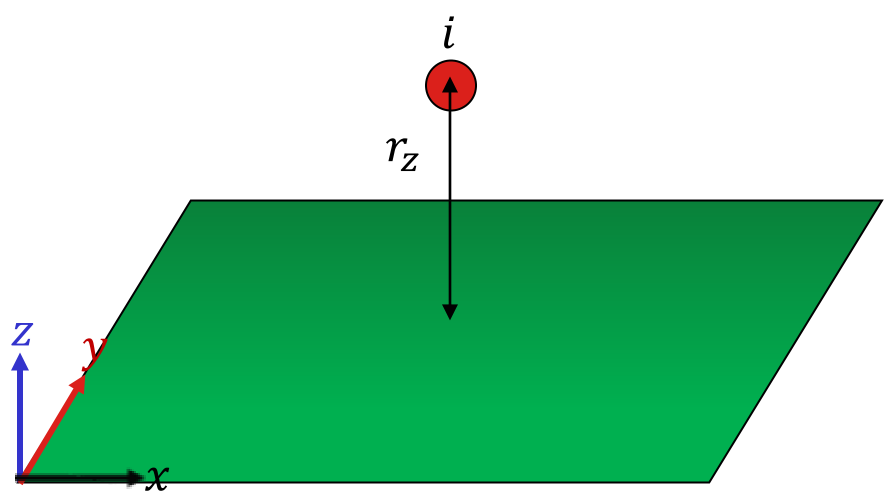
Particle vs. smooth walls

HOOMD-blue

- Particle walls can be implemented by placing the particles manually; wall particles are typically fixed in space and thus their positions are not updated via MD integration
- Smooth walls are easily defined by specifying
  - (i) geometry (hoomd.wall)
  - (ii) potential $u_i^{s,wall}$ (md.external.wall for MD)



Particle wall

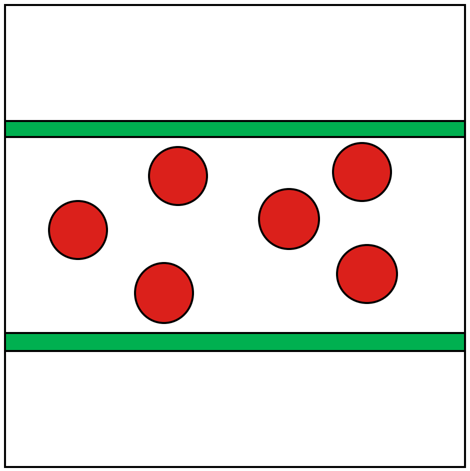


Smooth wall

Quasi-2D geometries

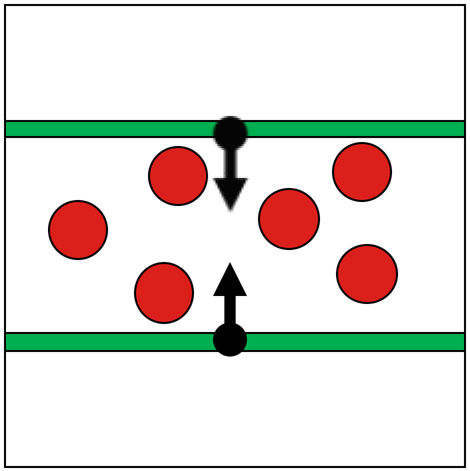
- Quasi-2D geometries can be created by using two parallel planar walls (also called a parallel plate or ”slit pore” geometry)

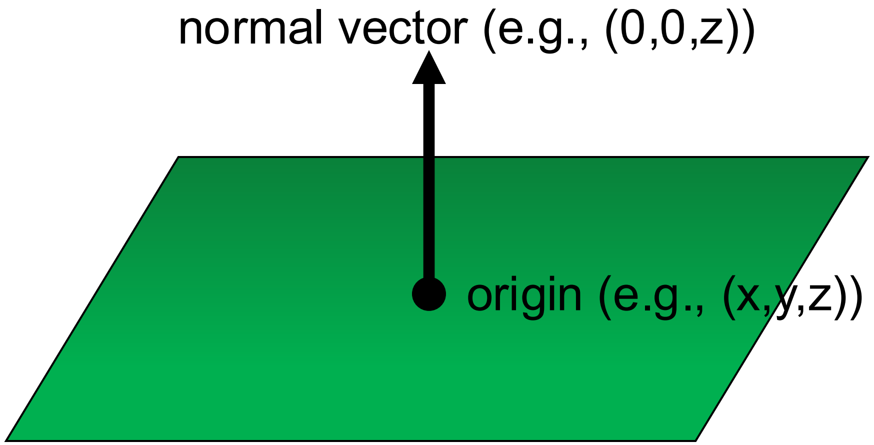
- Particles can move in the plane parallel to the walls but are confined in the direction normal to the walls



Quasi-2D geometries

- Quasi-2D geometries can be created by using two parallel planar walls (also called a parallel plate or “slit pore” geometry)
- hoomd.wall.plane(origin,normal,open)
  - origin: (x,y,z) position of a point that lies in the plane
  - normal: (x,y,z) components of vector normal to the plane
  - open: include (true) or exclude (false) the plane in the space
- $u_i^{s,wall}$ for each wall only depends the normal distance

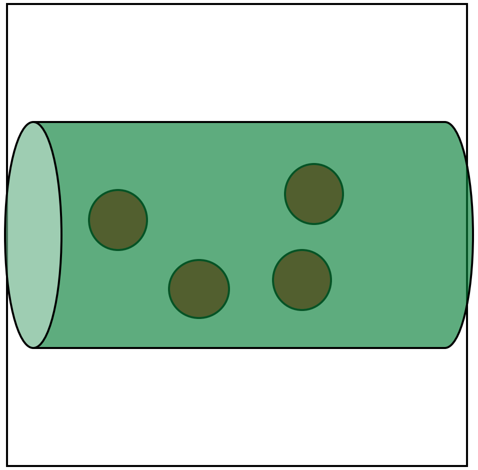




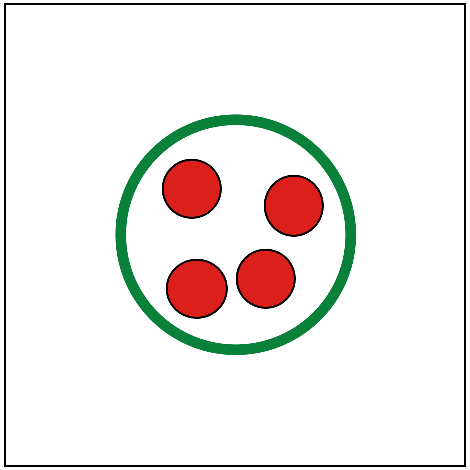
Quasi-1D geometries

- Quasi-1D geometries can be created by using a cylindrical wall

- Particles can move along the major axis of the cylinder but are confined in the radial direction



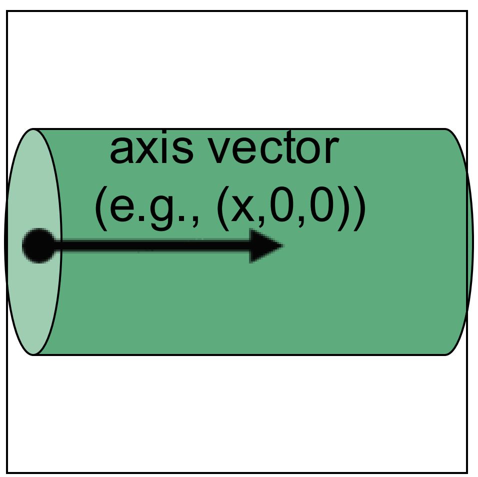
Side view



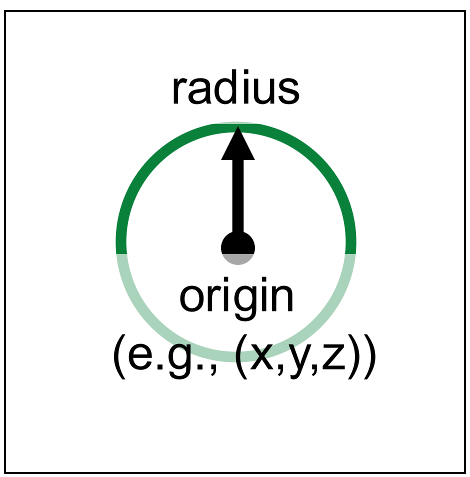
Front view

Quasi-1D geometries

- Quasi-1D geometries can be created by using a cylindrical wall
- hoomd.wall.cylinder(radius, axis, origin, inside, open)
  - radius: radius *r* of the cylinder's circular faces
  - axis: (x,y,z) components of vector normal to the cylinder's circular faces
  - origin: (x,y,z) origin of the cylinder defined as the center of the circle along the cylinder's axis
  - inside: whether positive signed distances are inside or outside the cylinder.
  - open: include (true) or exclude (false) the surface of the cylinder in the space



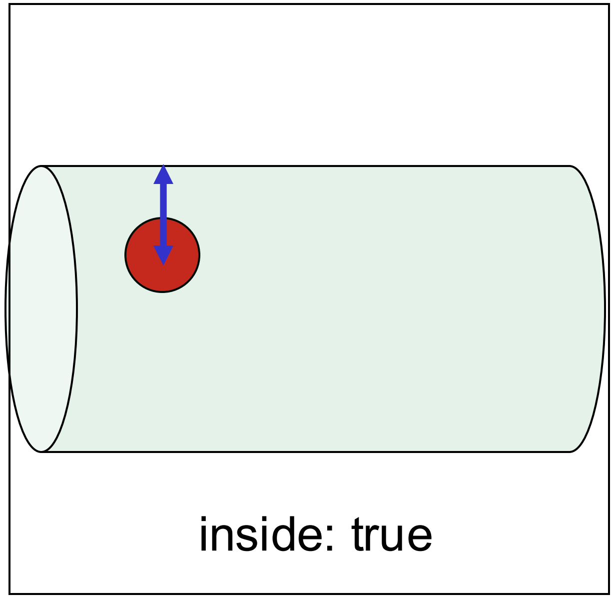
Side view



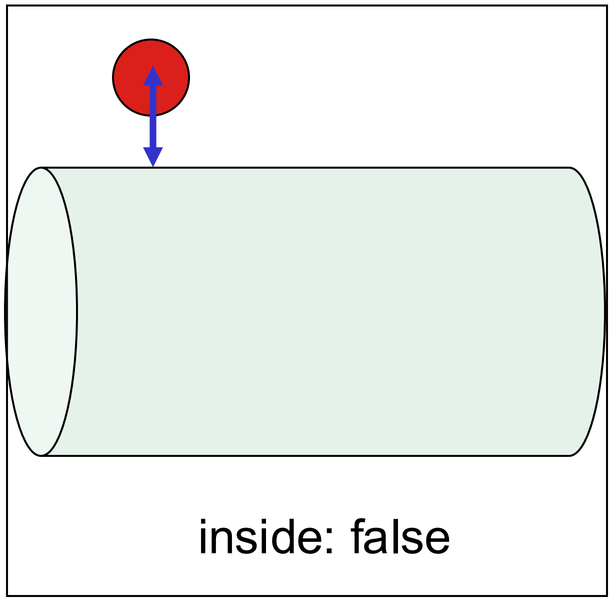
Front view

Quasi-1D geometries

- Quasi-1D geometries can be created by using a cylindrical wall
- hoomd.wall.cylinder(radius, axis, origin, inside, open)
- $u_i^{s,wall}$ only depends the distance from the cylinder's surface
- inside: positive signed distances are inside or outside the cylinder? Cases of positive distances are shown below.



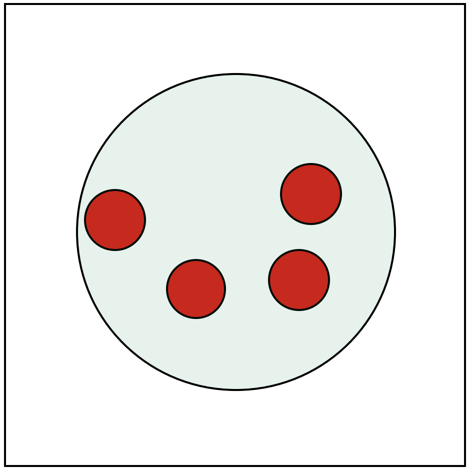
Side view



Side view

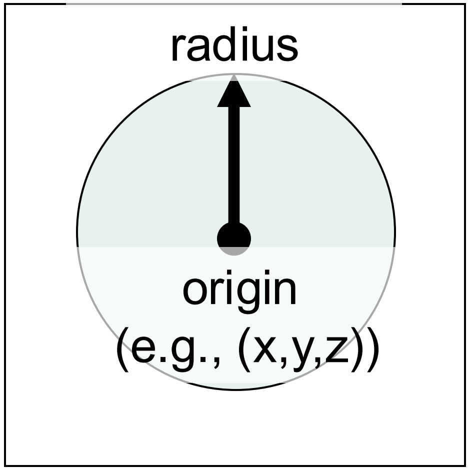
Quasi-0D geometries

- Quasi-0D geometries can be created by using a spherical wall
- Particles are confined in the radial direction



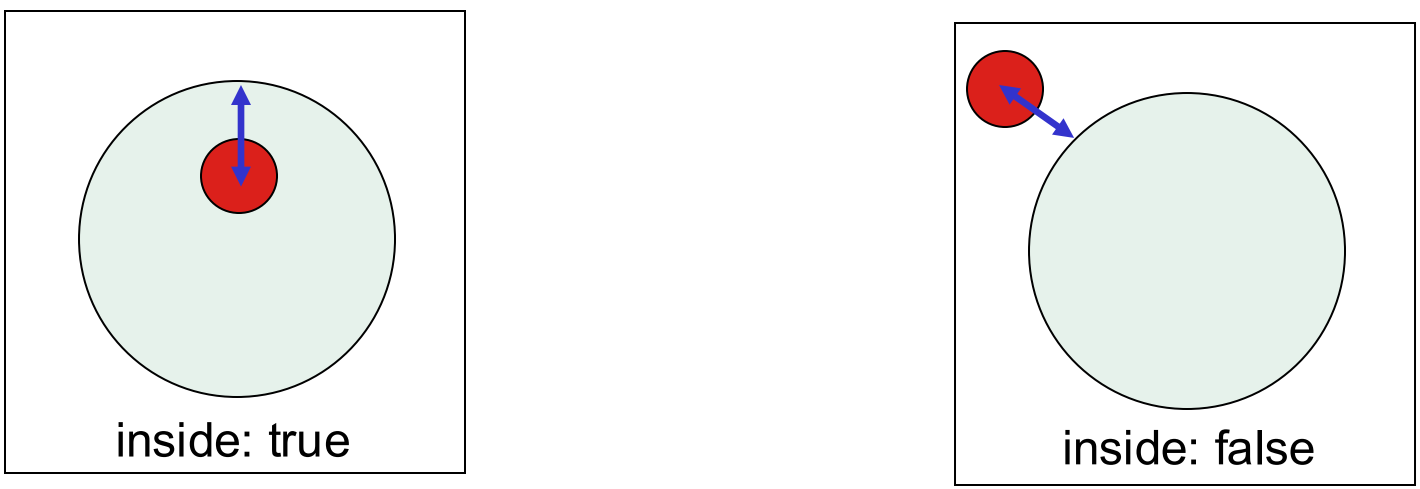
Quasi-0D geometries

- Quasi-0D geometries can be created by using a spherical wall
- hoomd.wall.sphere(radius, axis, origin, inside, open)
  - radius: radius *r* of the sphere
  - origin: (x,y,z) origin of the sphere
  - inside: whether positive signed distances are inside or outside the sphere.
  - open: include (true) or exclude (false) the surface of the sphere in the space



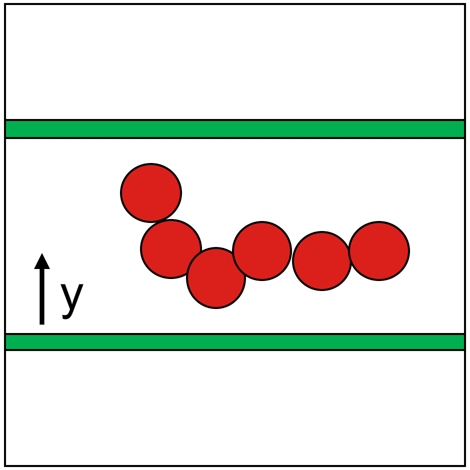
Quasi-0D geometries

- Quasi-0D geometries can be created by using a spherical wall
- hoomd.wall.sphere(radius, axis, origin, inside, open)
- $u_i^{s,wall}$ only depends the distance from the sphere’s surface
- inside: positive signed distances are inside or outside the cylinder? Cases of positive distances are shown below.



Exercise

- Langevin dynamics simulations of a 30-mer FENE polymer chain between repulsive parallel walls (WCA potential for monomer-wall interactions)
- Wall surface normal is oriented along the y-direction of the simulation cell



- Compute histograms for the monomer positions and polymer center of mass position ($H(y_m)$ and $H(y_{COM})$)

- Can also see how these distributions change upon varying wall spacing and the interaction potential (LJ vs WCA)