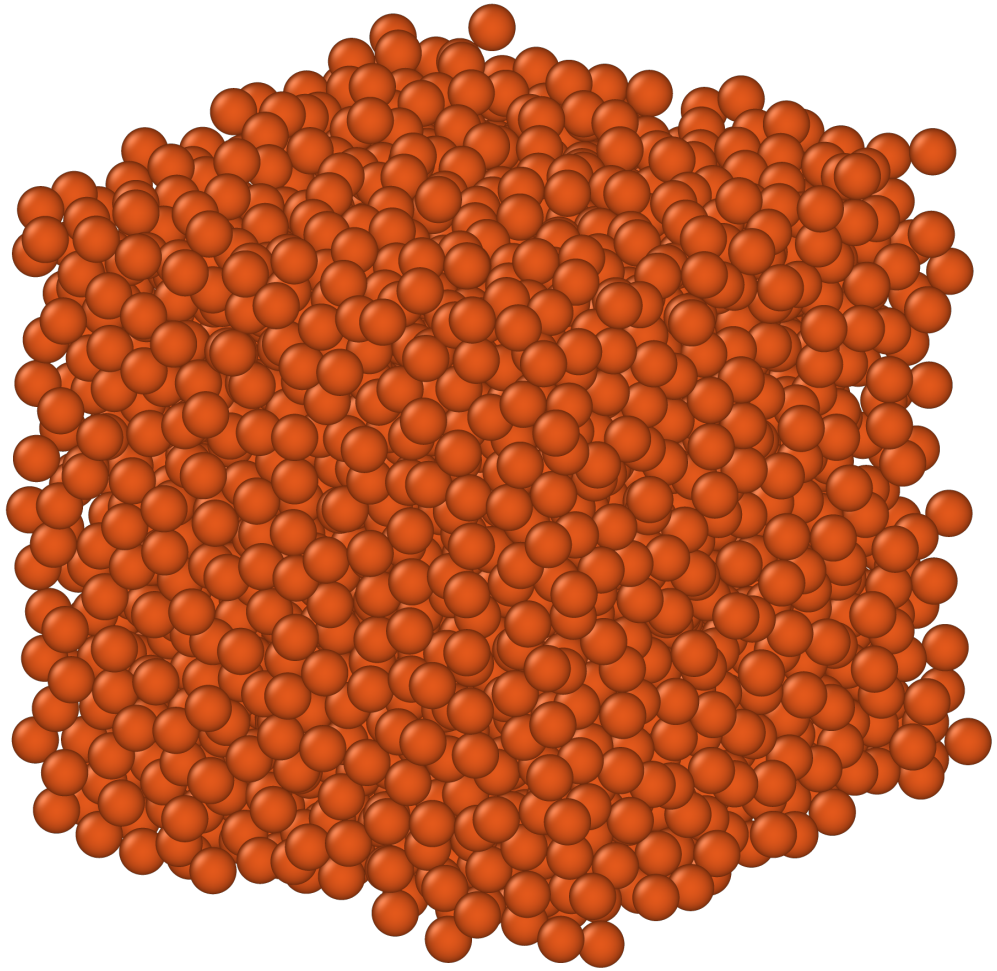
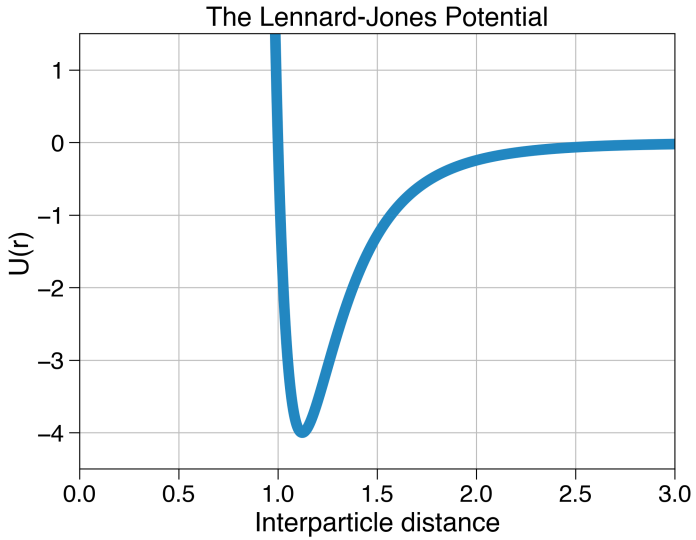
Simple Fluids

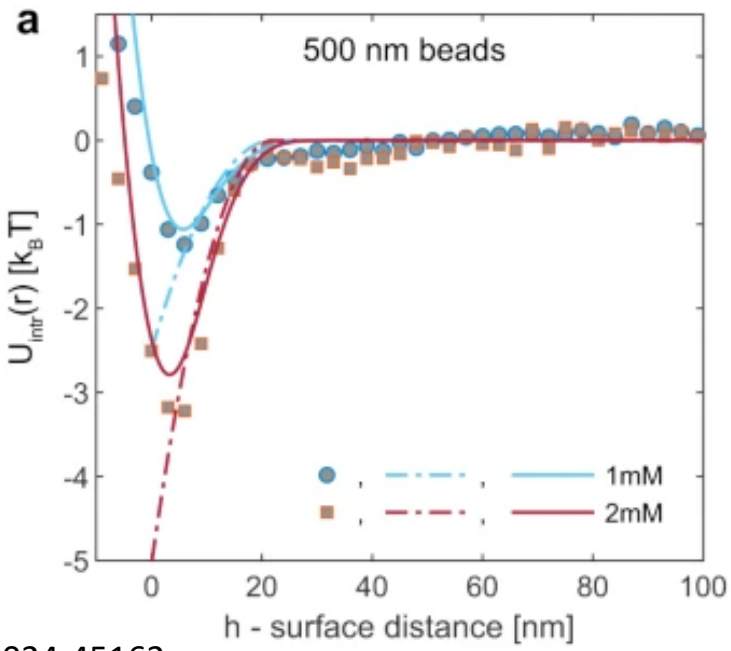


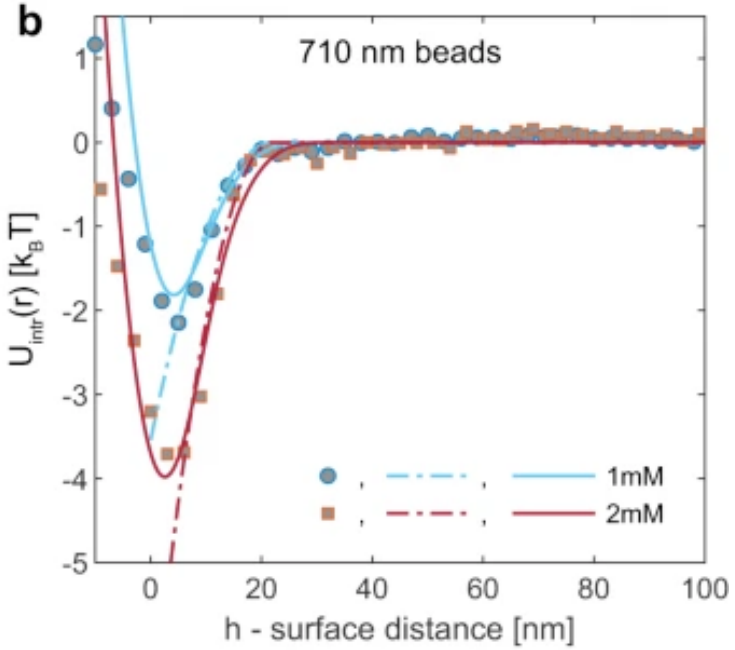
The Lennard-Jones Model

- Used on length scales ranging from atoms to nanoparticles
- Most commonly studied pair potential
- Computationally efficient
- r^{-12}: Repulsion
- $-r^{-6}$: Attractive forces, *e.g.* London Disperson Forces
- Parameters:
  - ϵ: strength of attraction
  - σ: lengthscale, distance at which energy is 0
  - *r:* interparticle distance

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

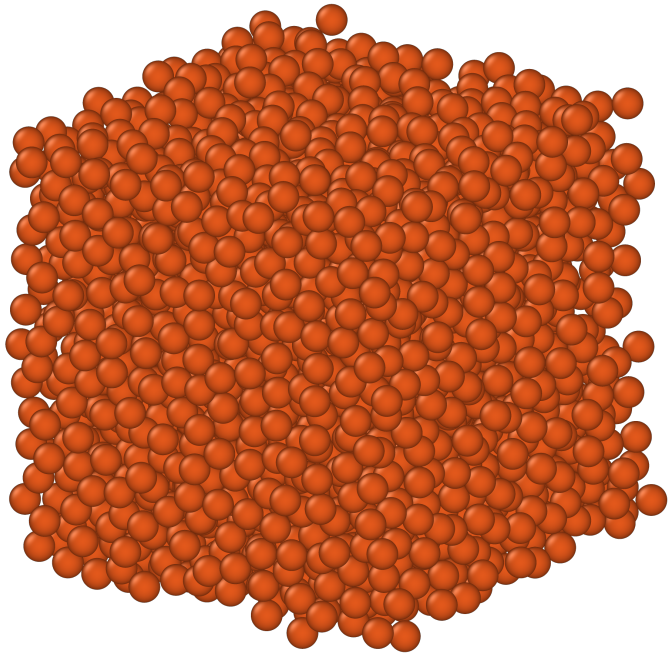






Zhang, C., Muñetón Díaz, J., Muster, A. *et al.*, *Nat Commun* **15**, 1020 (2024). https://doi.org/10.1038/s41467-024-45162-w

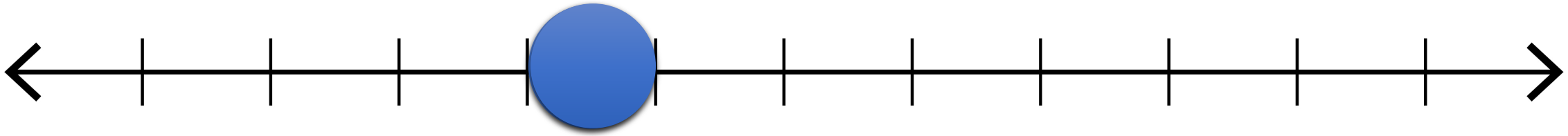
Units of Measurement in Simulation



How big is this box?

What is the ball’s diameter?

What is the ball’s diameter?



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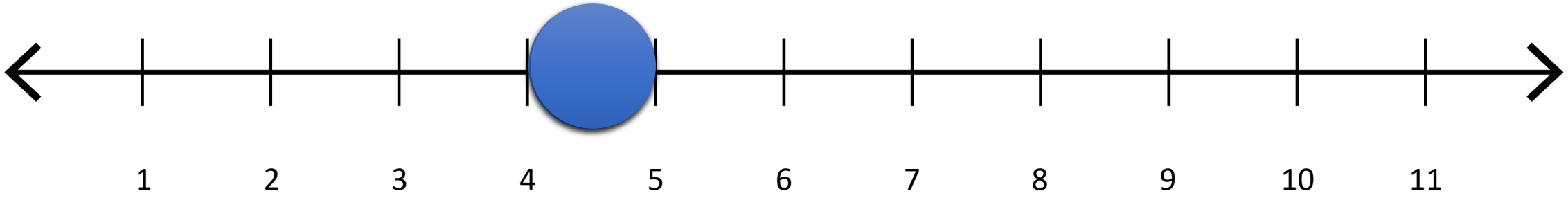
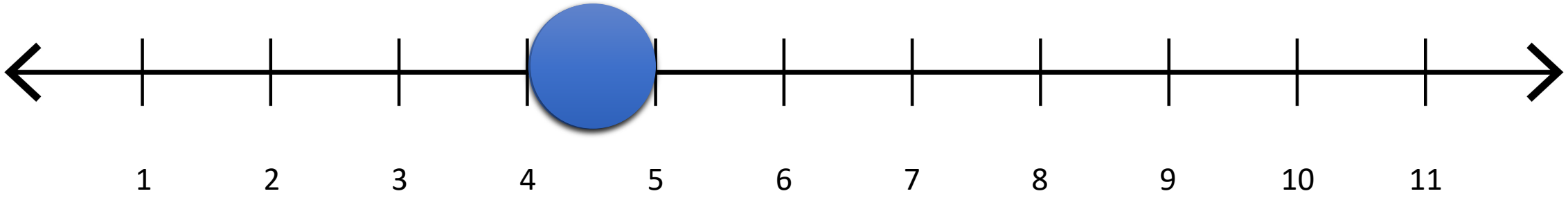


How far is the ball moving?



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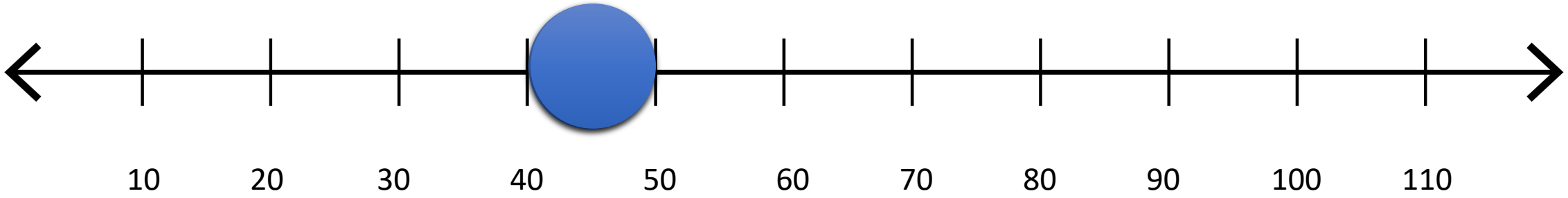


Fundamental Units

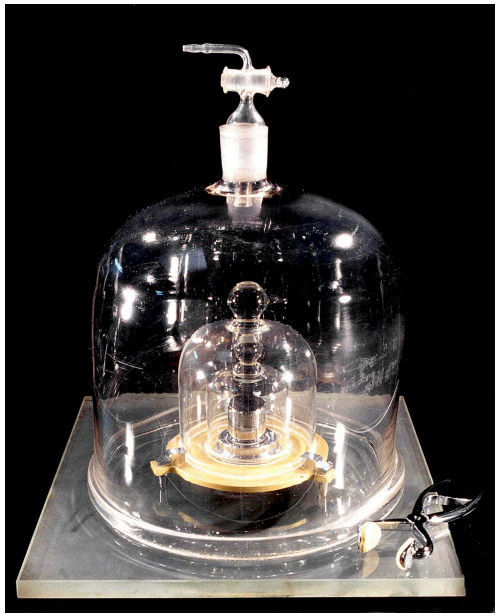
- Describes the units that are used to *set* the values of all others

In the lab, we use..
- Length
- Mass
- Temperature
- Time

To derive…
- Energy
- Pressure
- Velocity

In simulation, we set…
- Length
- Mass
- *Energy!*

To derive…
- Pressure
- Velocity
- *Time!*



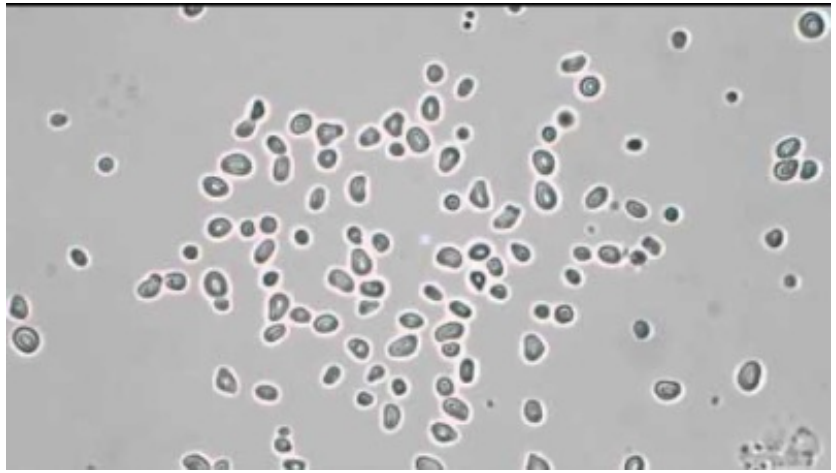
International standard measures of the meter and kilogram, from Wikipedia

Deriving Units

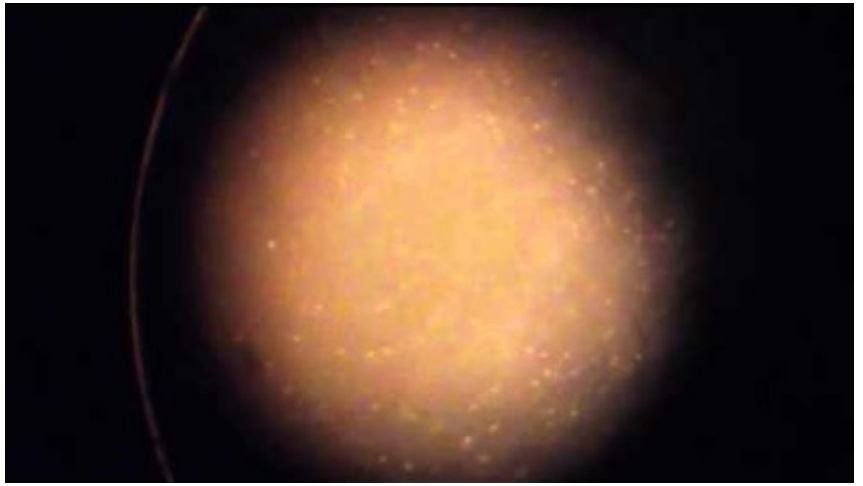
- M → kilograms kg
- D → meters m
- E → joules J → kg m^2 s^{-2}
- It is often useful to *not* explicitly choose units!

$$t = \sqrt{\frac{M\ D^2}{E}} = \sqrt{\frac{kg\ * m^2}{kg * m^2 * s^{-2}}}$$

$$P = \frac{E}{D^3} \qquad T = \frac{E}{k_b}$$



Pollen grains in water
Source: Yeo Yong Kat

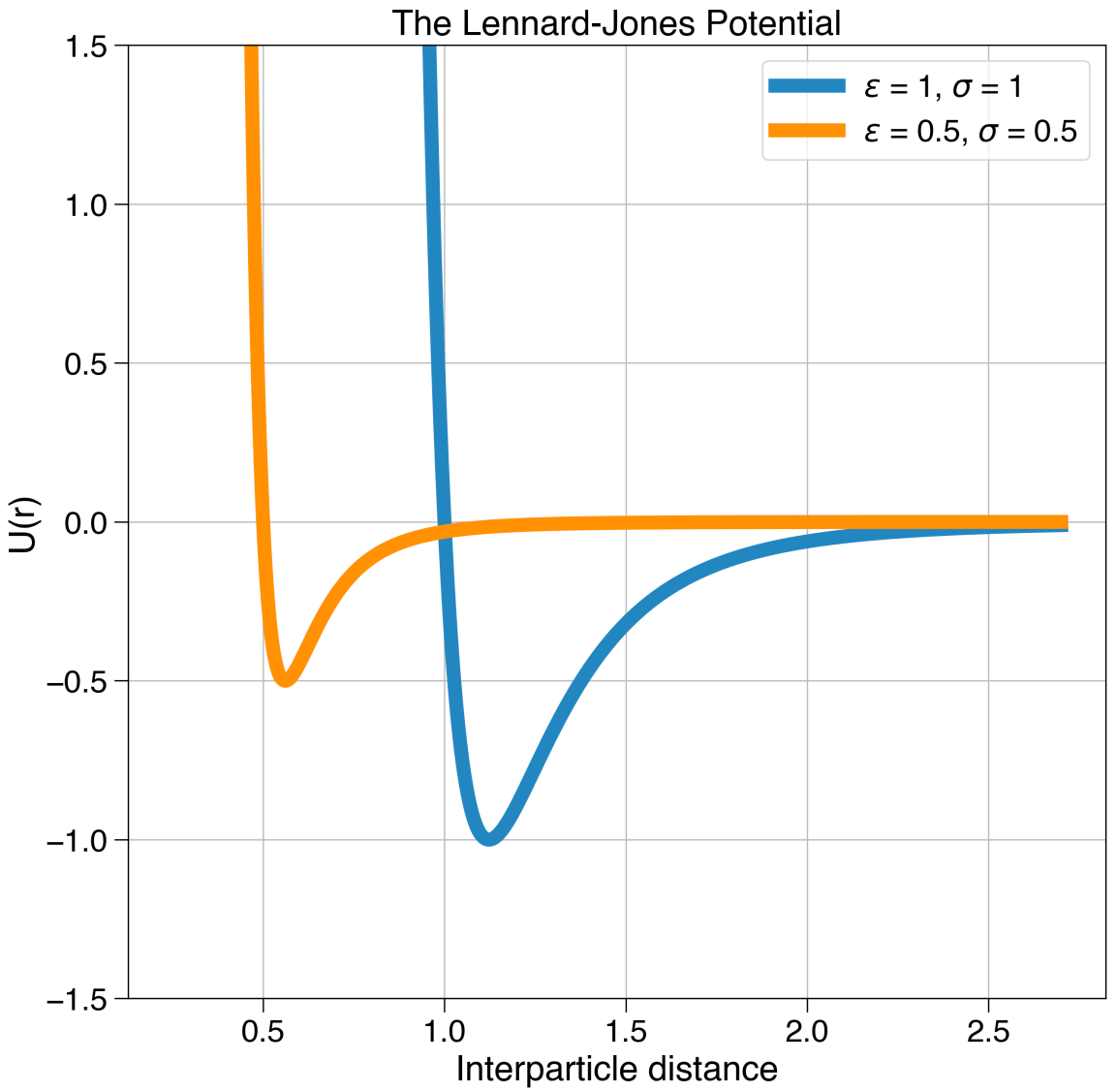


Smoke in air
Source: FranklyChemistry

Lennard-Jones Units

- As long as physics doesn't change, a simulation is valid
- Reduced units: quantities reported in multiples of some fundamental value
- For LJ system:
  - ϵ: fundamental energy
  - σ: fundamental length
- Reduced temperature T*: kT/ϵ
- Reduced length: r/σ
- Reduced pressure P*: E/σ^3

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



J. Chem. Phys. 145, 014503 (2016)

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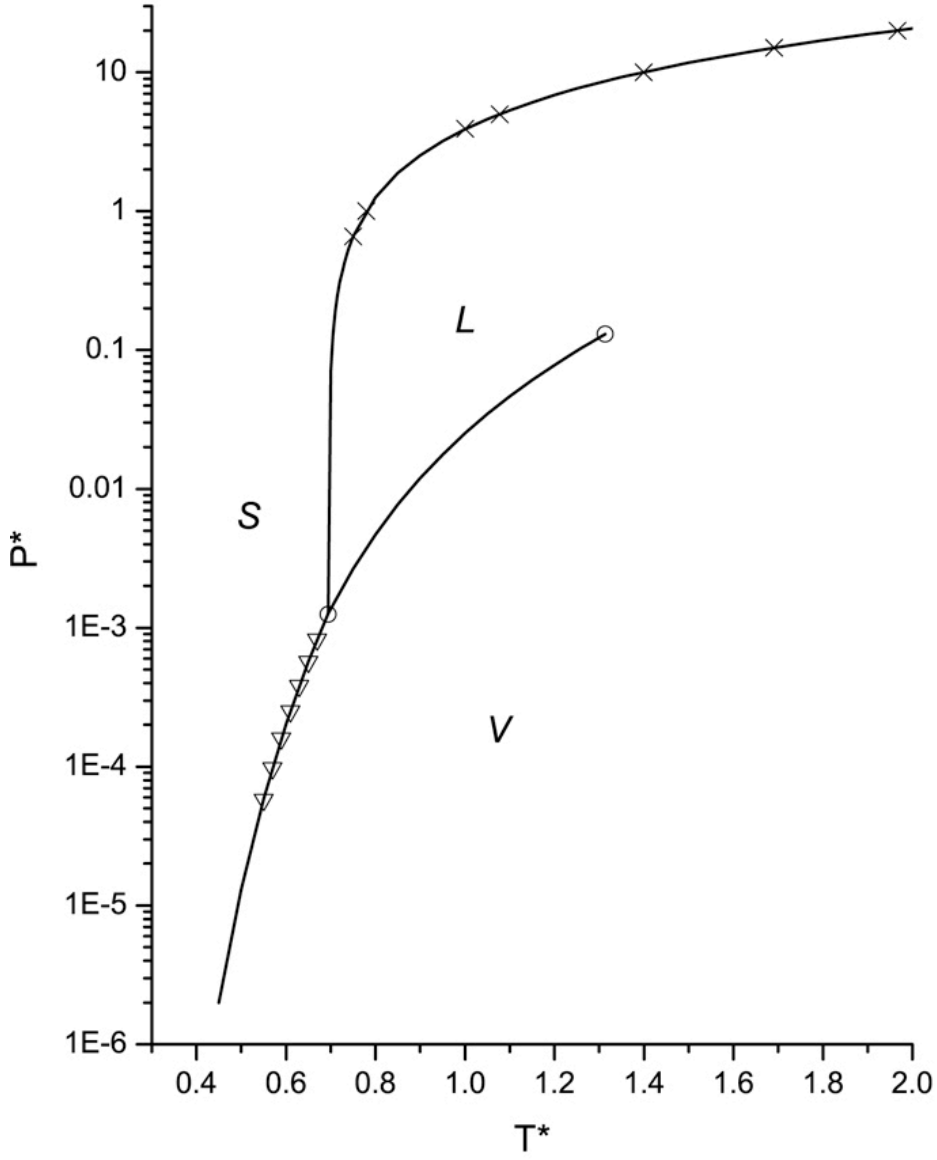
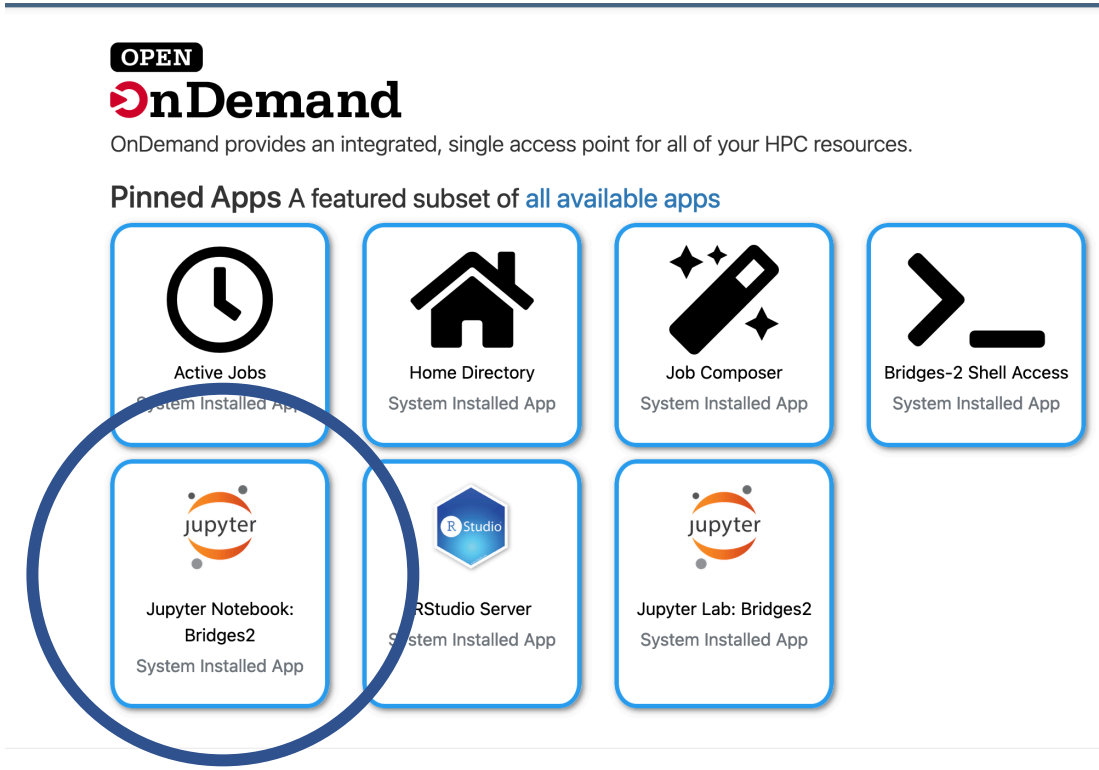


J. Chem. Phys. 145, 014503 (2016)

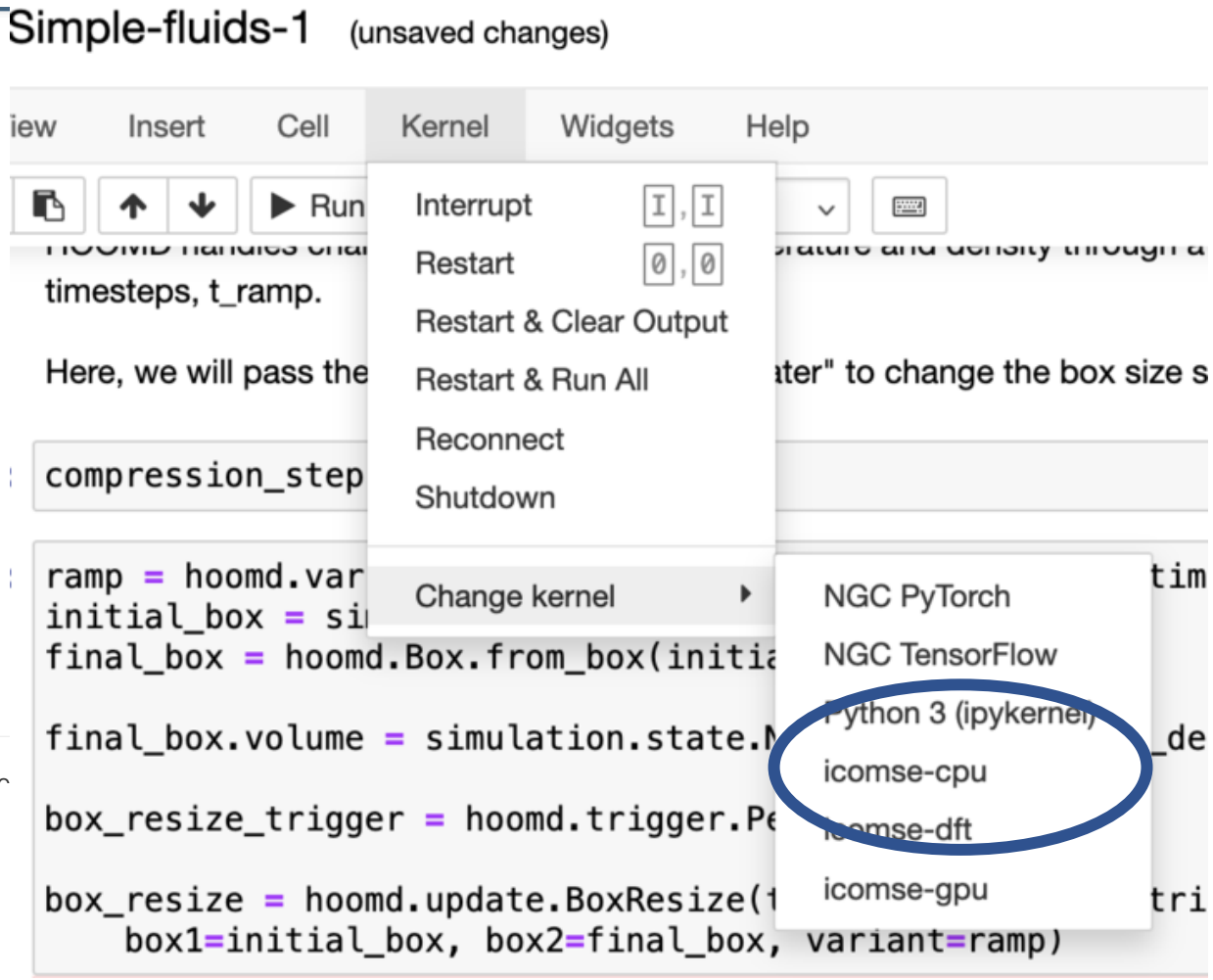
Simple Fluids 1 Notebook

Accessing OnDemand

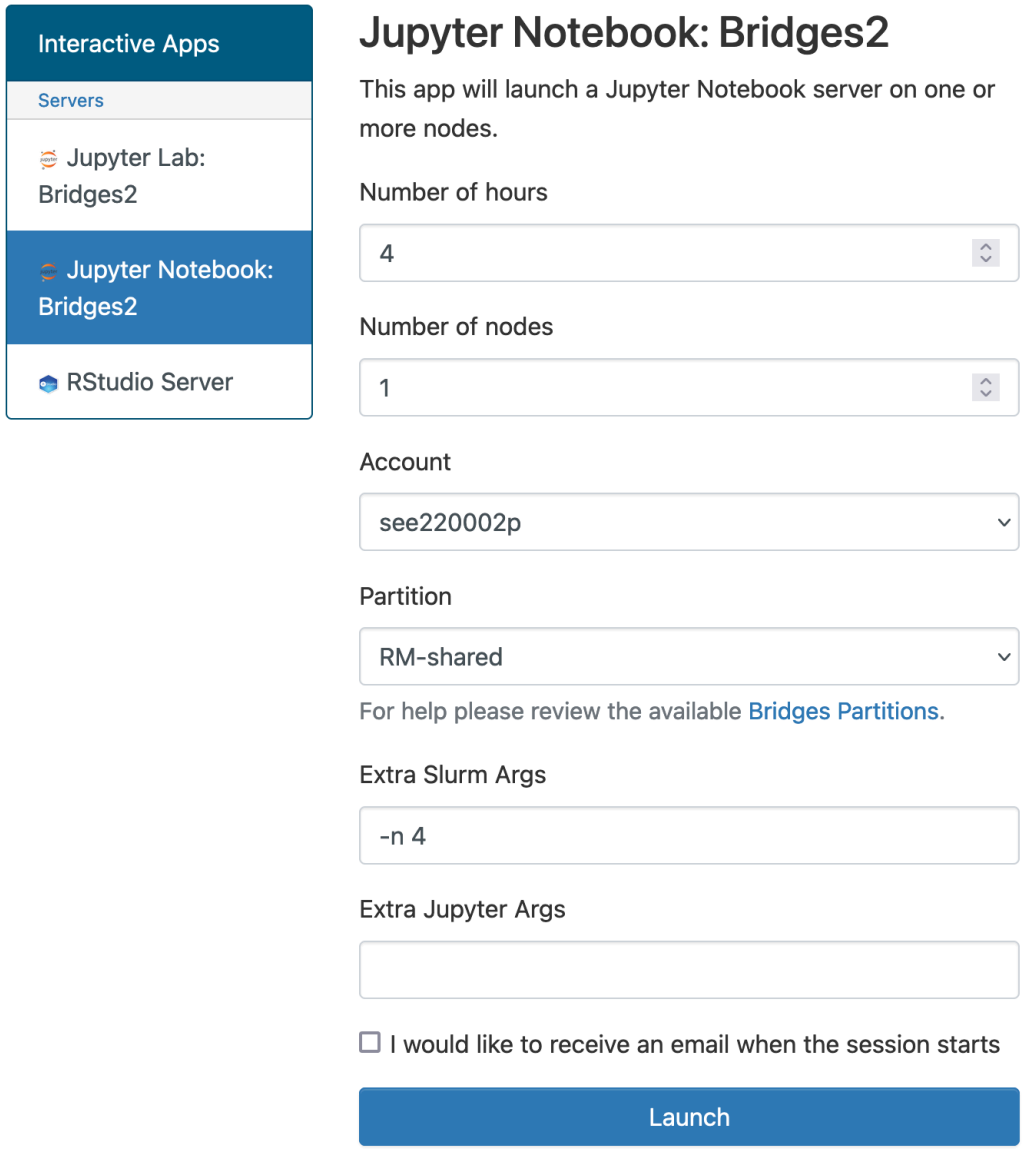
Jupyter Notebook



Choose the correct kernel



Job Request

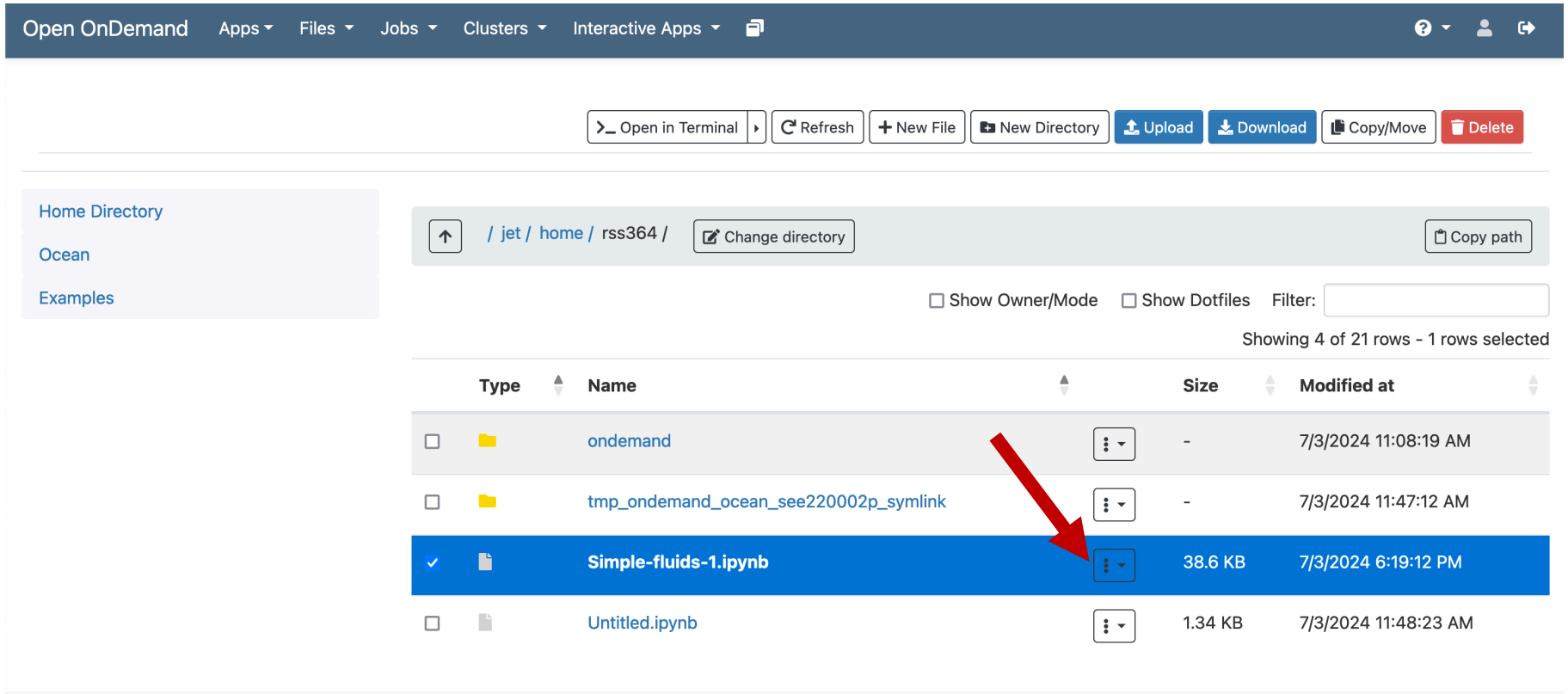

Interactive Apps
Servers
Jupyter Lab: Bridges2
Jupyter Notebook: Bridges2
RStudio Server
Jupyter Notebook: Bridges2
This app will launch a Jupyter Notebook server on one or more nodes.
Number of hours
4
Number of nodes
1
Account
see220002p
Partition
RM-shared
For help please review the available Bridges Partitions.
Extra Slurm Args
-n 4
Extra Jupyter Args
I would like to receive an email when the session starts
Launch

Uploading/Downloading Data

Through the command line:

```
(base) Rachael@Home ~/example_folder $ scp -r username@data.bridges2.psc.edu:path/to/file path/to/destination
username@data.bridges2.psc.edu's password:
```

Through OnDemand:



Steps of a simulation in HOOMD-blue

- Create a *simulation object*
- Initialize the particle positions, simulation box size, etc.
- Set random initial condition
- Choose integrators & thermostats
- Set pair potentials for all particles
- Set up files to record data
- Run the simulation

hoomdblue

Documentation: https://hoomd-blue.readthedocs.io

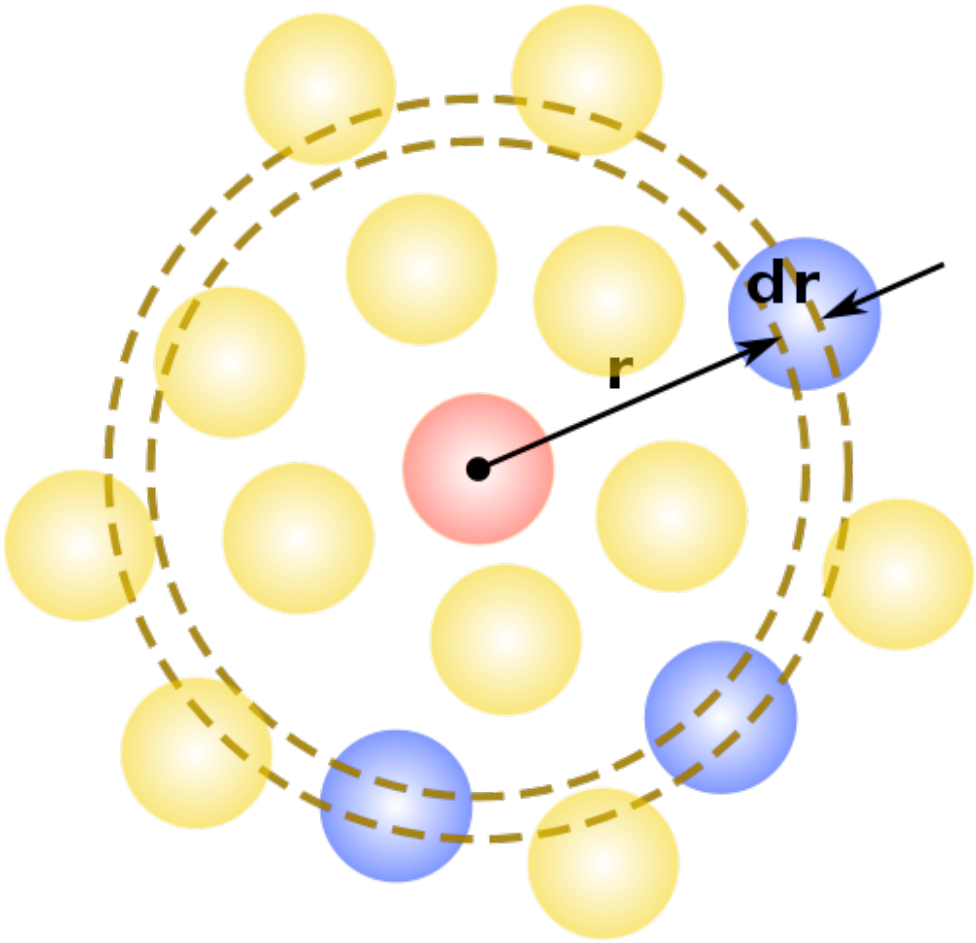
Simulation Analysis:
Radial Distribution Function

Radial Distribution Function (RDF)

- In words: the ratio between the *actual* density and the total system density at a distance *r* away from a particle
- In equations:

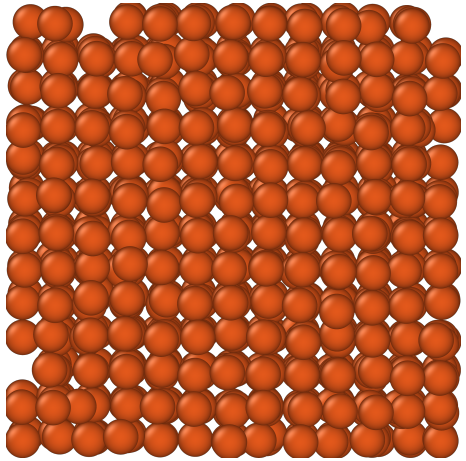
$$g(r) = \frac{\langle \rho(r) \rangle}{\rho} \qquad g(r) = V \frac{N_{\text{reference particles}}}{N_{\text{particles}}} \langle \delta(r) \rangle$$

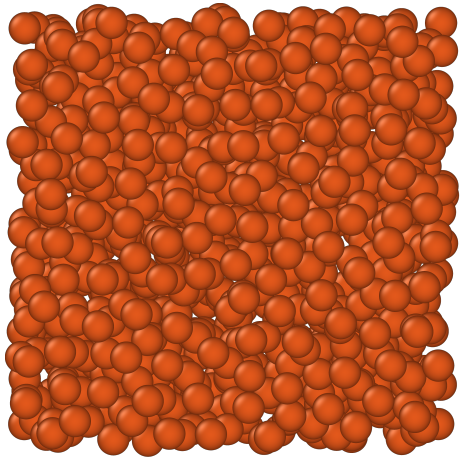
- Algorithm:
  - Choose a "shell width" dr
  - Choose a particle
    - Count the number of particles inside dr and convert to density
    - Move out by *dr* and repeat
  - Repeat for all particles and take the average

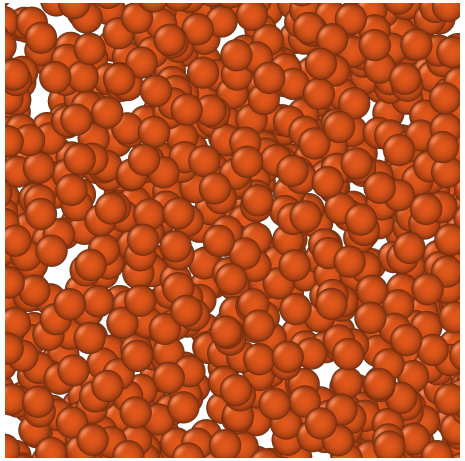


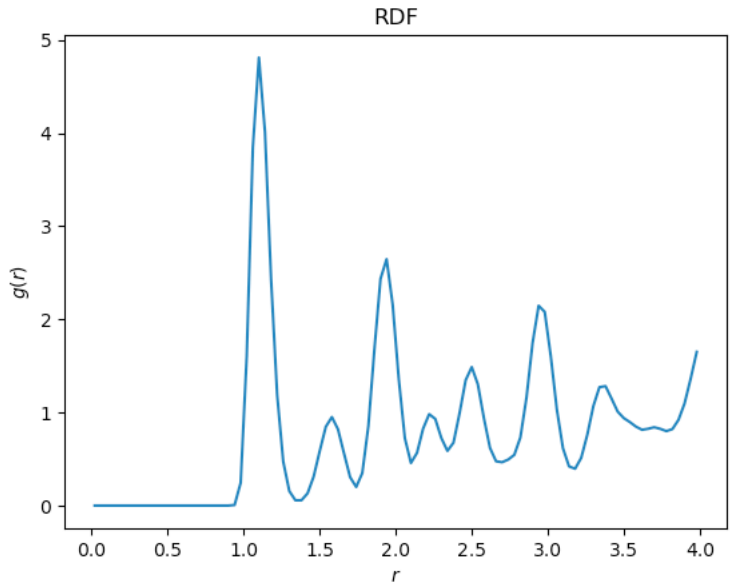
Graphical depiction of calculating the RDF, from Wikipedia

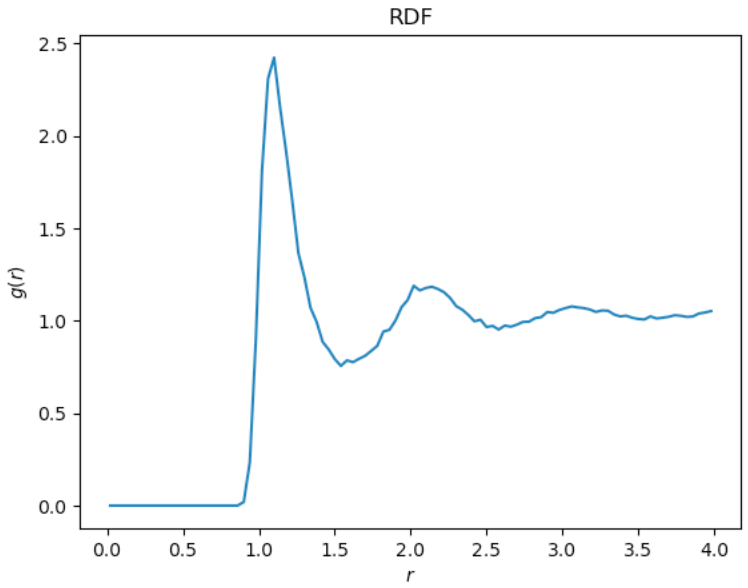
Sample RDFs

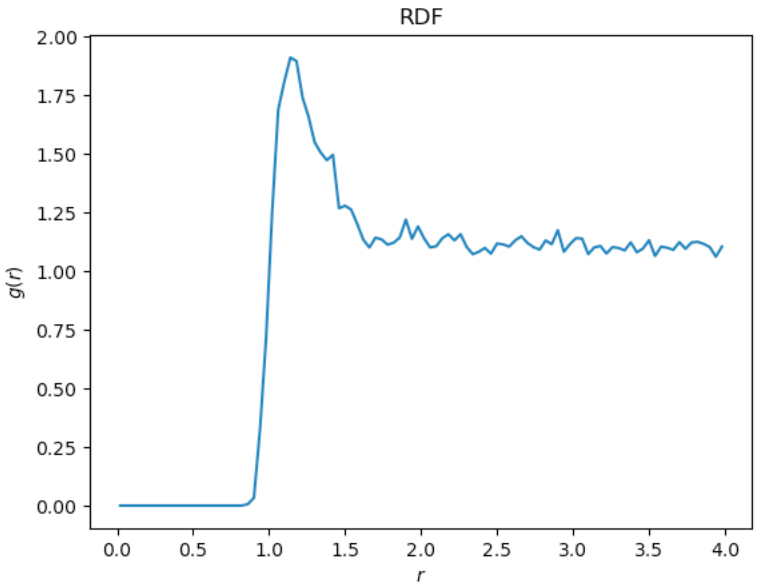












Ordered Solid/Crystal

Liquid

Gas

Viewing RDF in Ovito