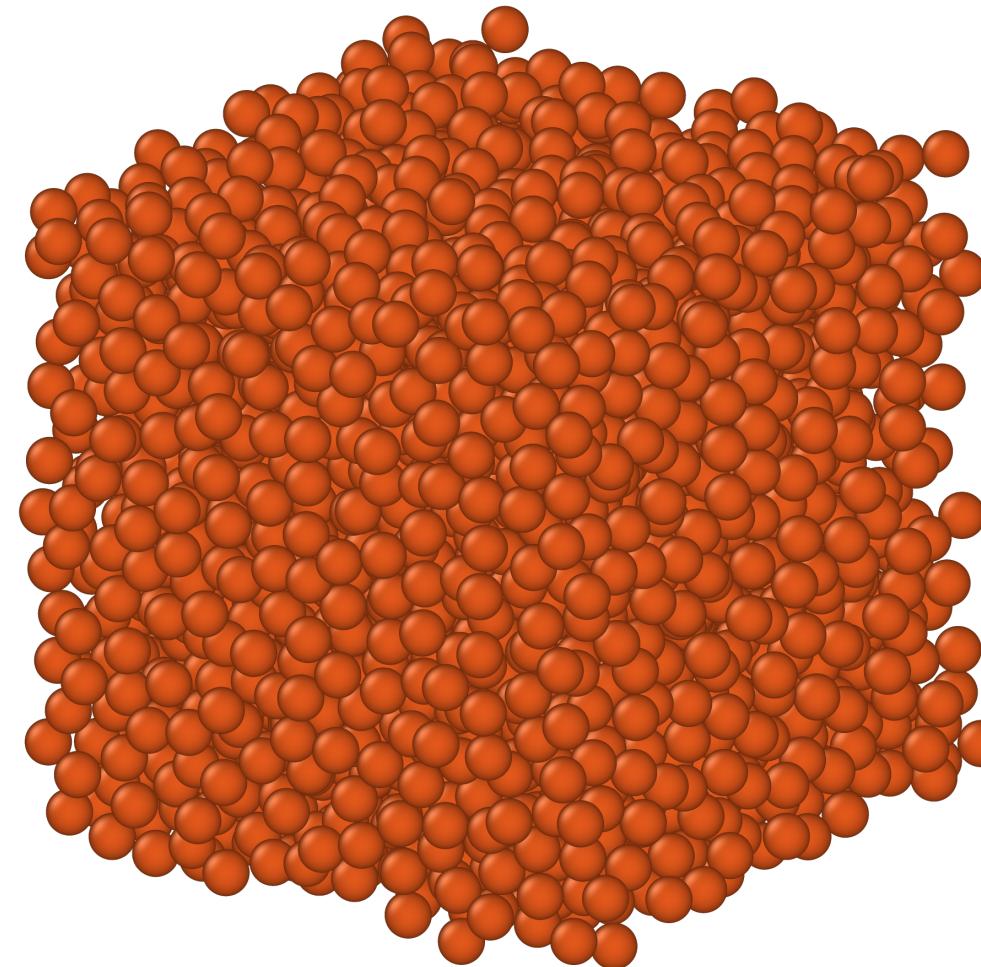


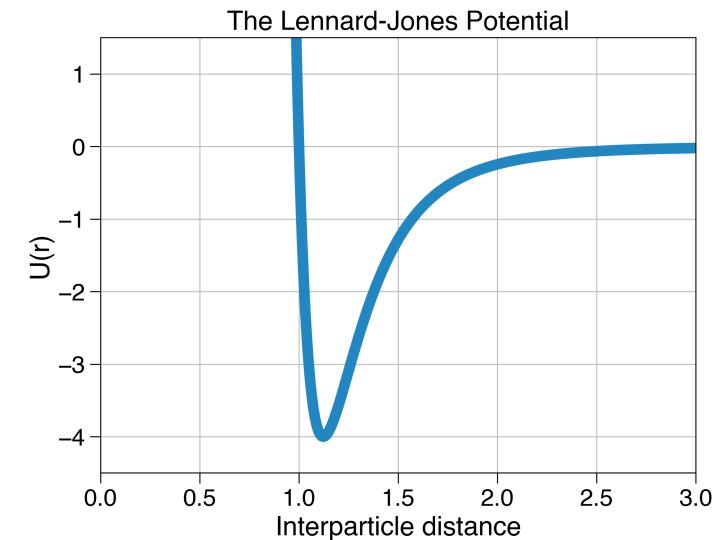
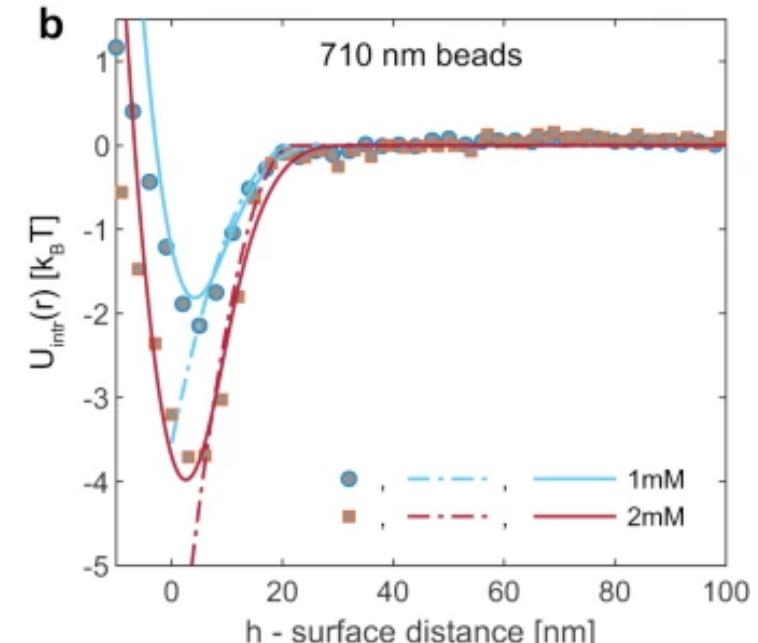
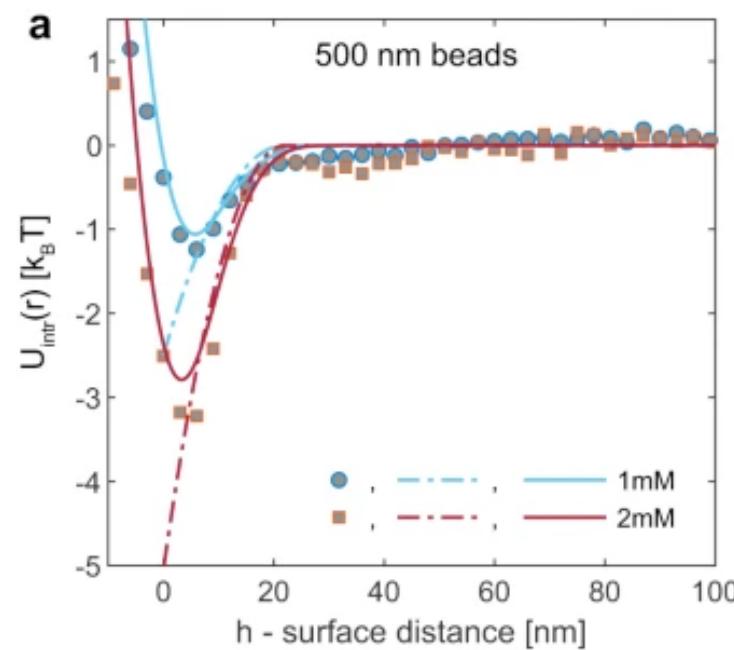
# Simple Fluids



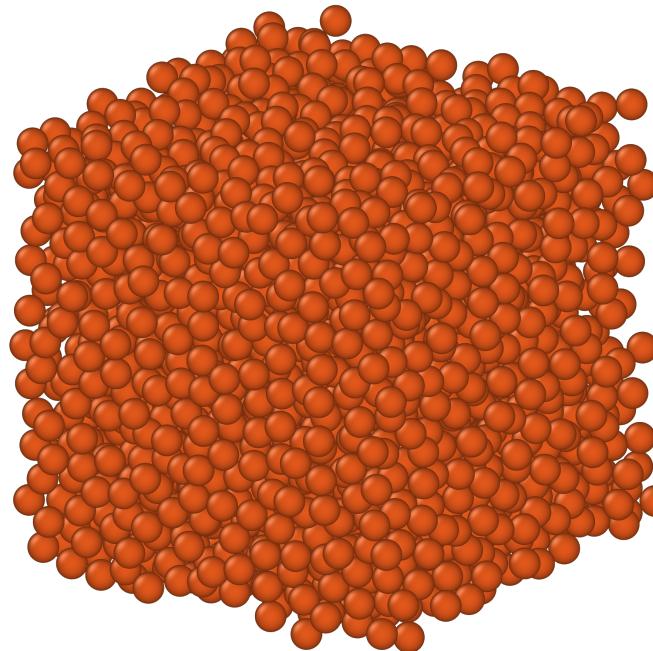
# The Lennard-Jones Model

- 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 Dispersion Forces
- Parameters:
  - $\epsilon$ : strength of attraction
  - $\sigma$ : lengthscale, distance at which energy is 0
  - $r$ : interparticle distance

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



# Units of Measurement in Simulation

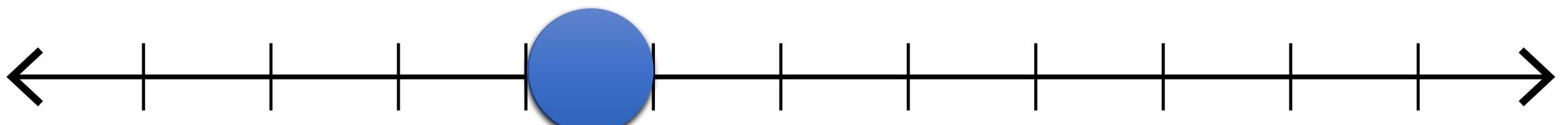


*How big is this box?*

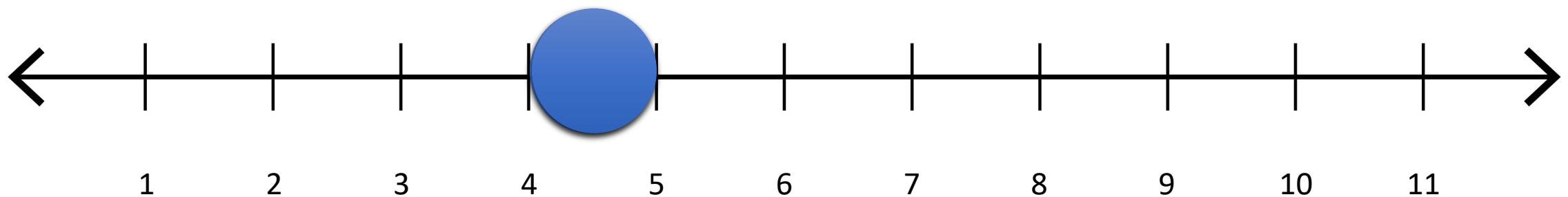
# What is the ball's diameter?



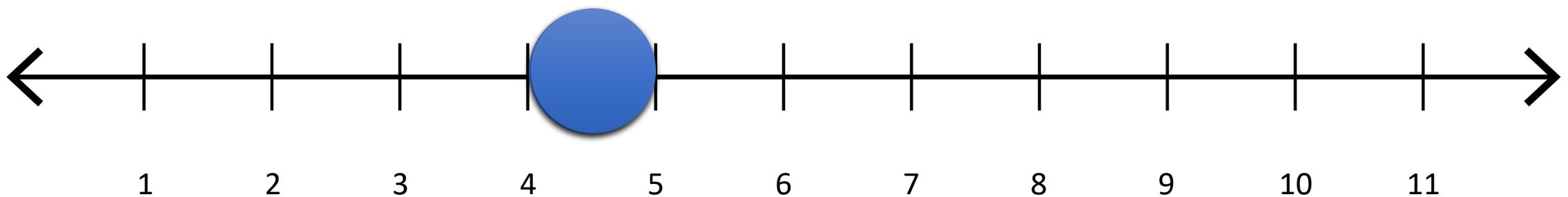
# What is the ball's diameter?



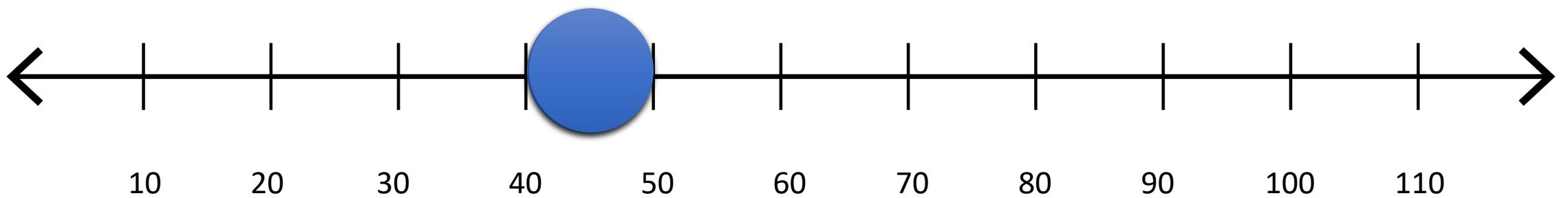
# What is the ball's diameter?



# How far is the ball moving?



# How far is the ball moving?



# 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!*



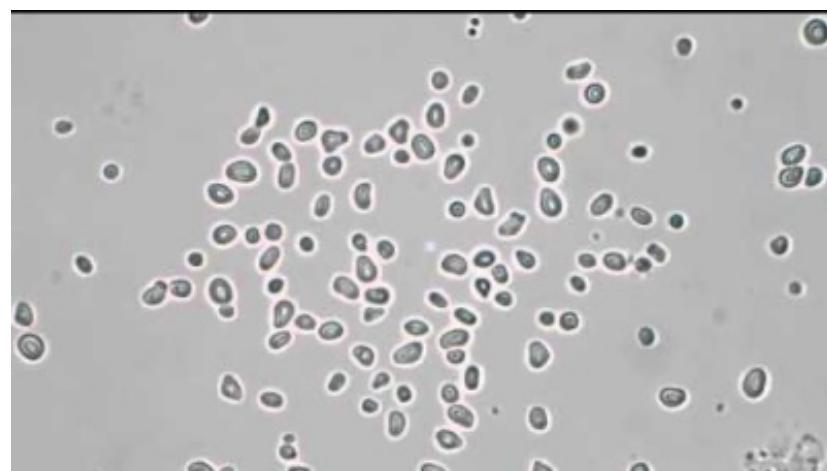
*International standard measures of the meter and kilogram, from Wikipedia*

# Deriving Units

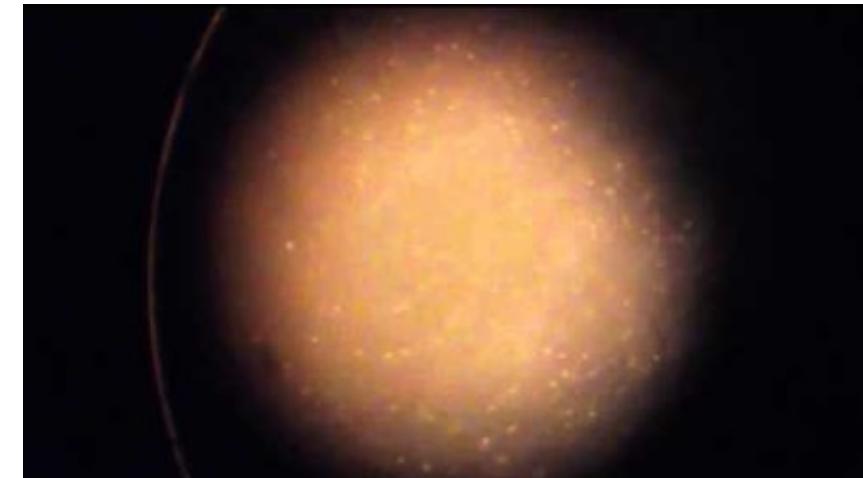
- M → kilograms kg
- D → meters m
- E → joules J → kg m<sup>2</sup> s<sup>-2</sup>
- It is often useful to *not* explicitly choose units!

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

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



Pollen grains in water  
Source: Yeo Yong Kat

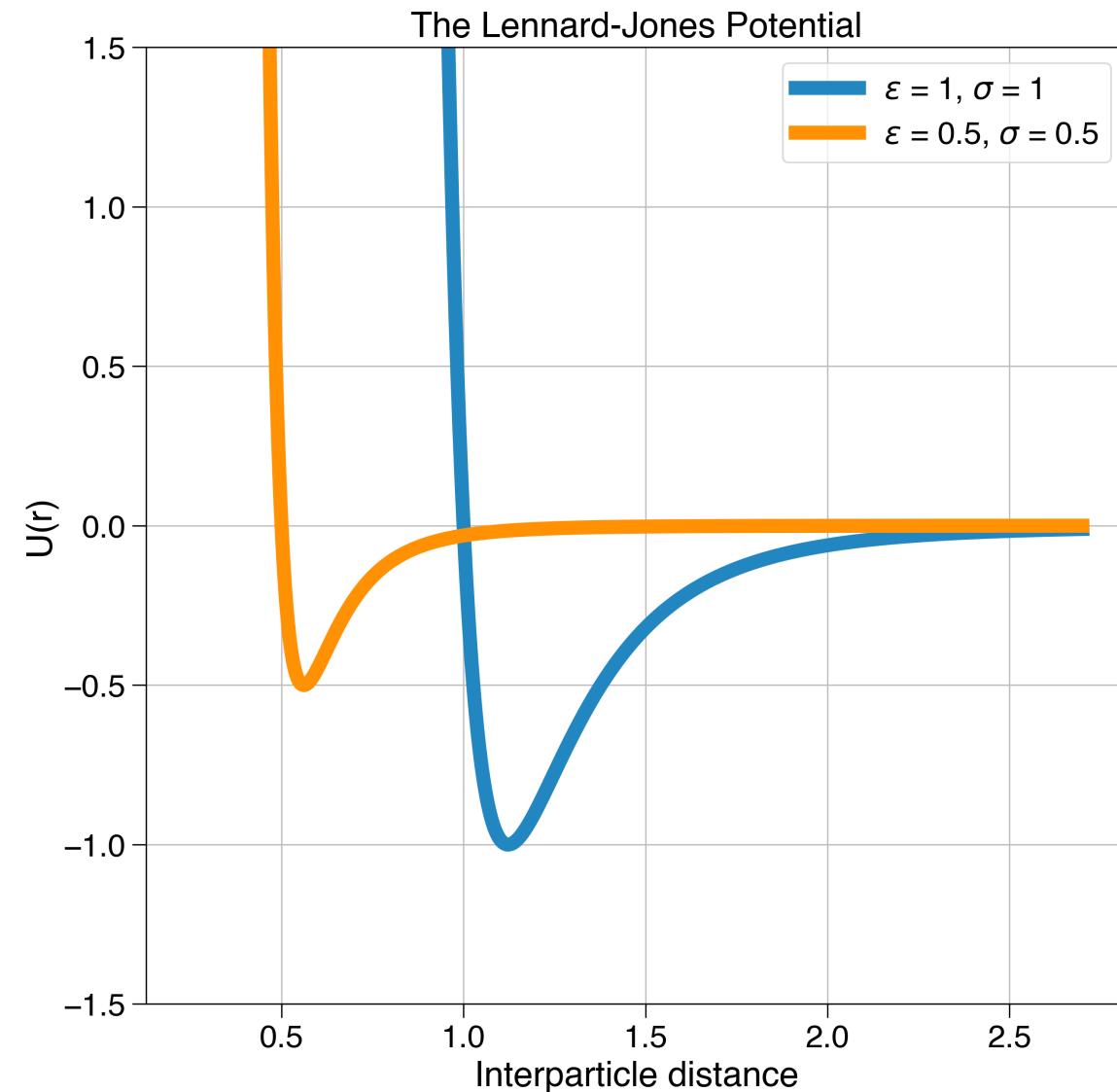


Smoke in air  
Source: FranklyChemistry

# 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:
  - $\epsilon$ : fundamental energy
  - $\sigma$ : fundamental length
- Reduced temperature  $T^*$ :  $kT/\epsilon$
- Reduced length:  $r/\sigma$
- Reduced pressure  $P^*$ :  $E/\sigma^3$

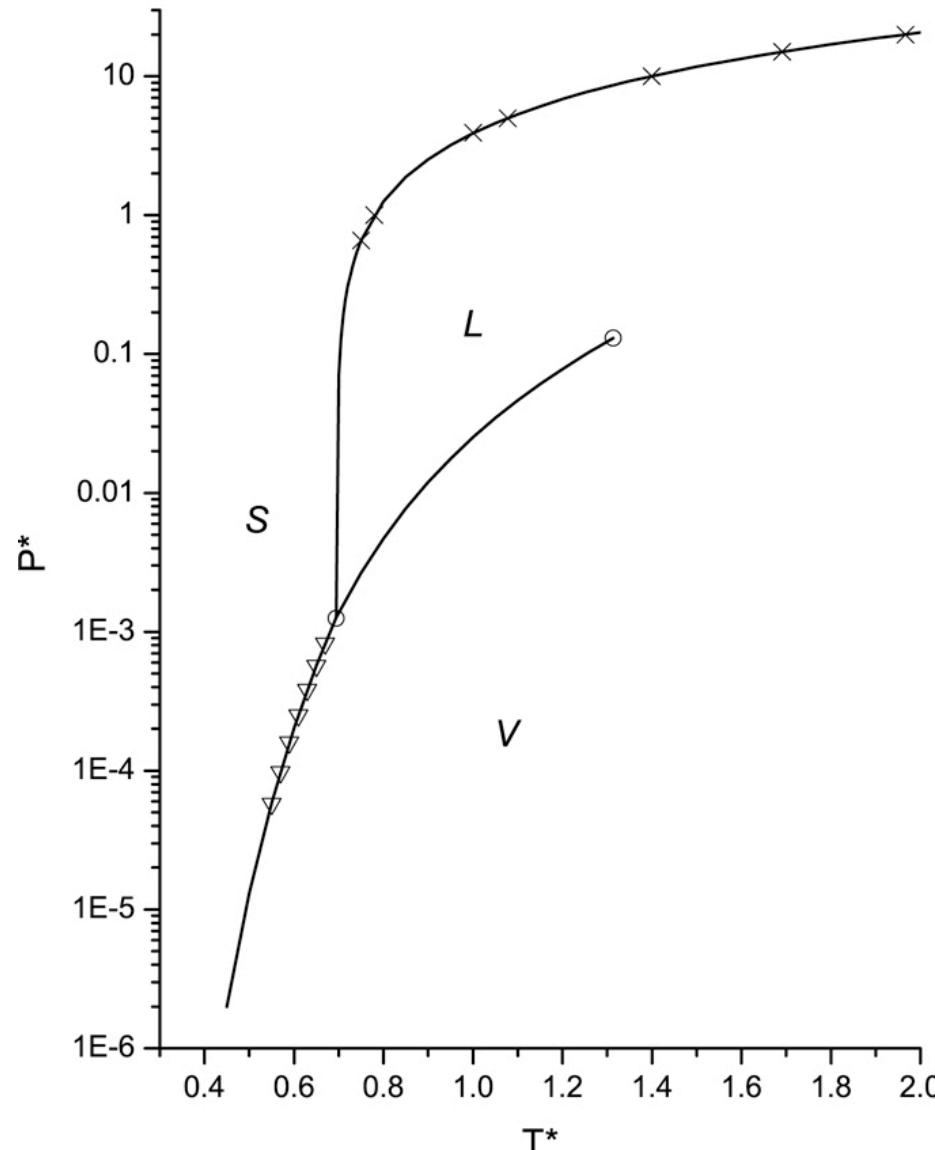
$$V_{\text{LJ}}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$



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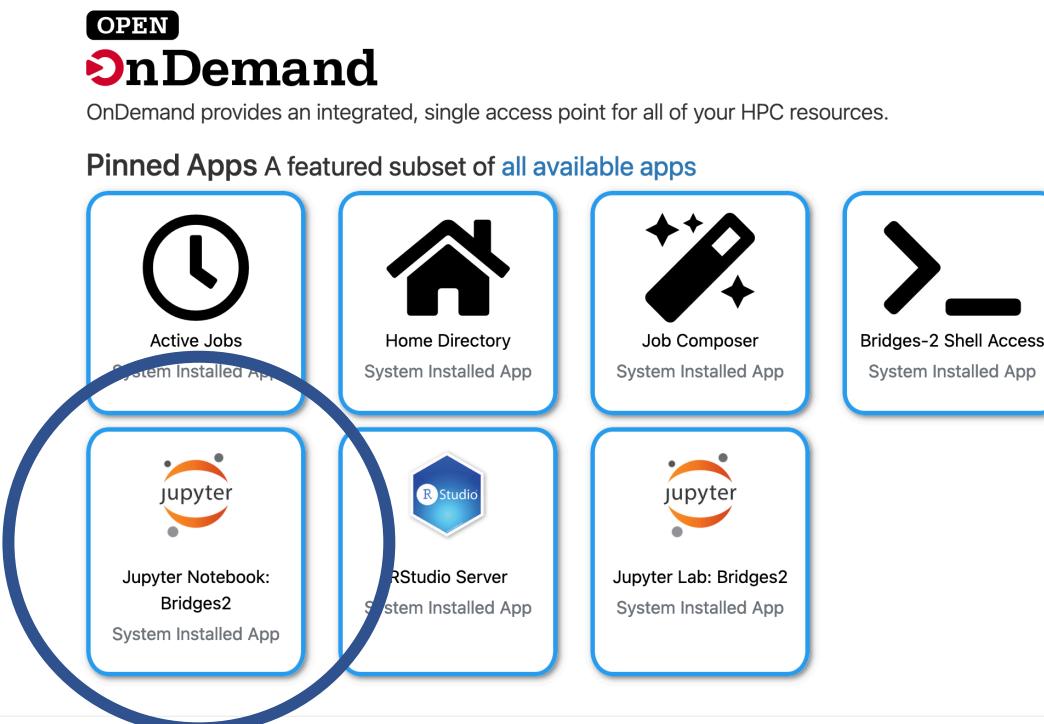
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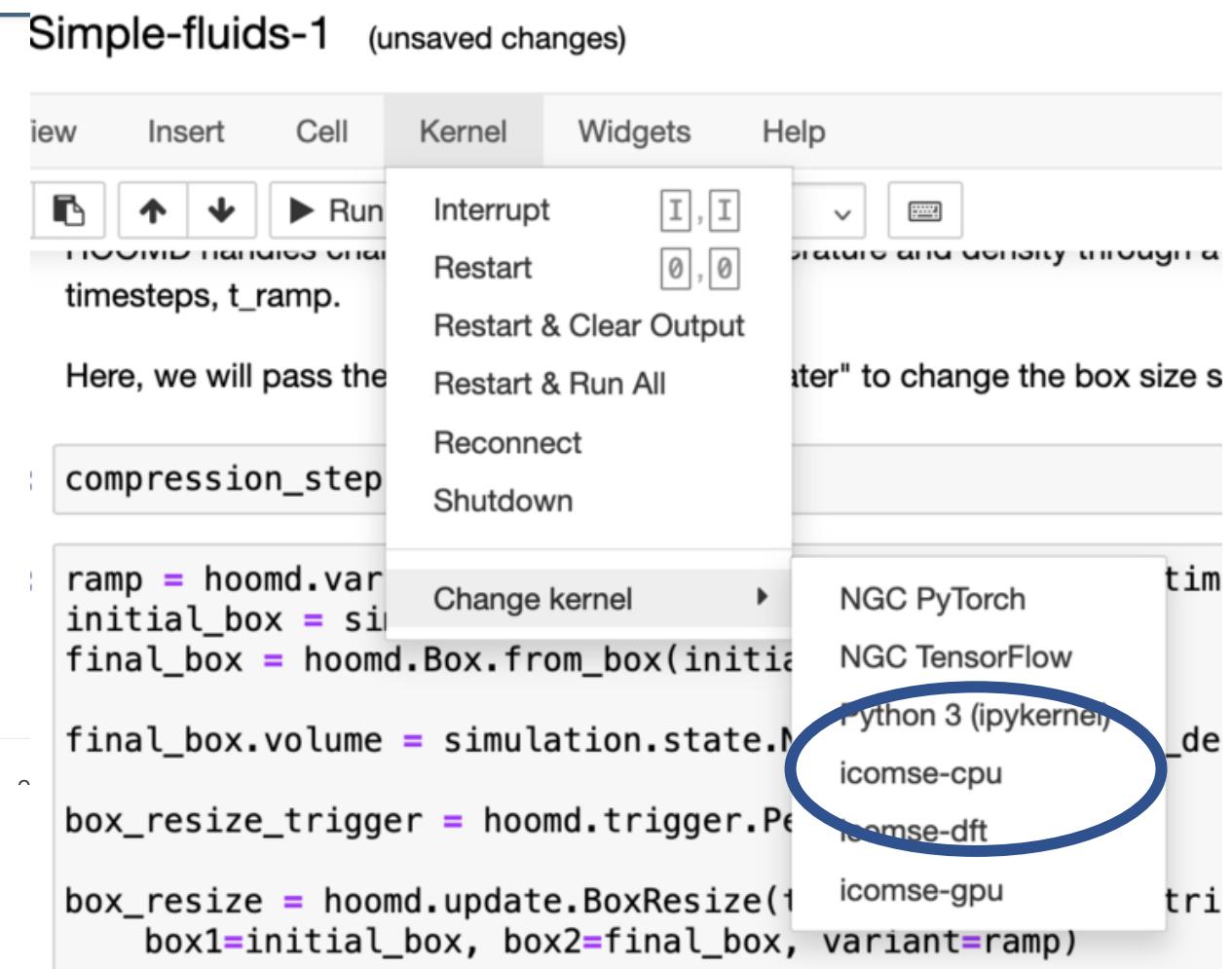
# Simple Fluids 1 Notebook

# 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

Number of nodes

Account

Partition

For help please review the available [Bridges Partitions](#).

Extra Slurm Args

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:  
Rachael@Home:~$
```

Through OnDemand:

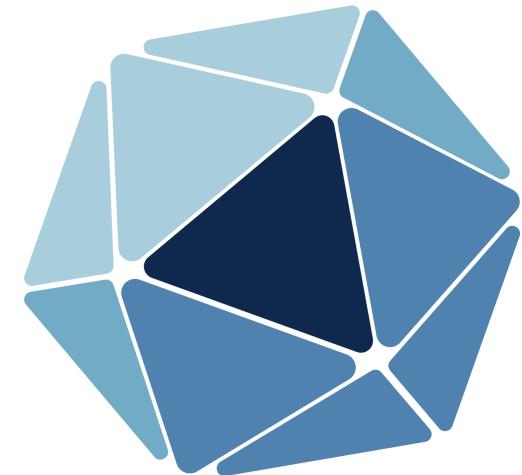
The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with links for Open OnDemand, Apps, Files, Jobs, Clusters, Interactive Apps, and a user icon. Below the navigation bar is a toolbar with buttons for Open in Terminal, Refresh, New File, New Directory, Upload, Download, Copy/Move, and Delete. On the left, there is a sidebar labeled "Home Directory" with options for Ocean and Examples. The main area shows a file list in a terminal window. The terminal window has a title bar with an up arrow, the path /jet/home/rss364/, a "Change directory" button, and a "Copy path" button. Below the title bar are checkboxes for Show Owner/Mode, Show Dotfiles, and a Filter input field. A message indicates "Showing 4 of 21 rows - 1 rows selected". The file list table has columns for Type, Name, Size, and Modified at. The table contains the following rows:

Type	Name	Size	Modified at
□	ondemand	-	7/3/2024 11:08:19 AM
□	tmp_ondemand_ocean_see220002p_symlink	-	7/3/2024 11:47:12 AM
✓	Simple-fluids-1.ipynb	38.6 KB	7/3/2024 6:19:12 PM
□	Untitled.ipynb	1.34 KB	7/3/2024 11:48:23 AM

A red arrow points to the "Simple-fluids-1.ipynb" row, which is highlighted with a blue background. At the bottom of the page, there is a footer with the text "powered by OPEN OnDemand" and "OnDemand version: 3.0.3".

# 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

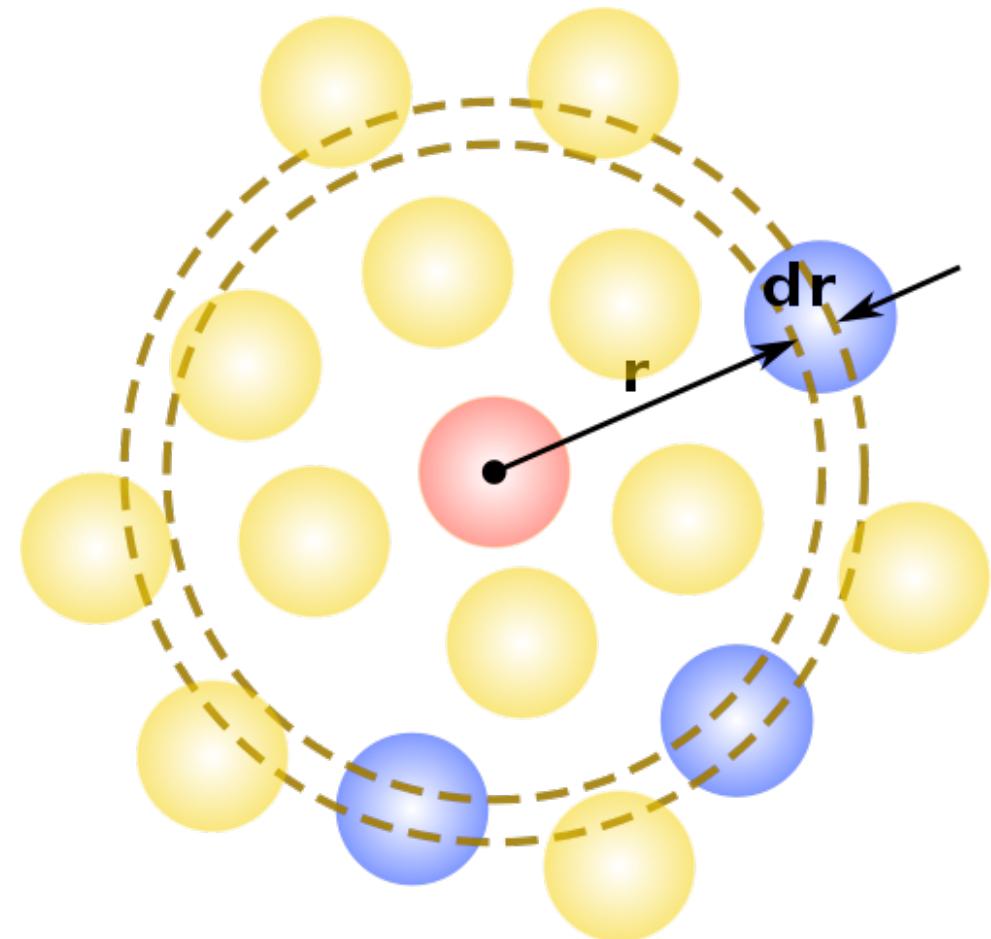
# Radial Distribution Function (RDF)

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

$$g(r) = \frac{\langle \rho(r) \rangle}{\rho}$$

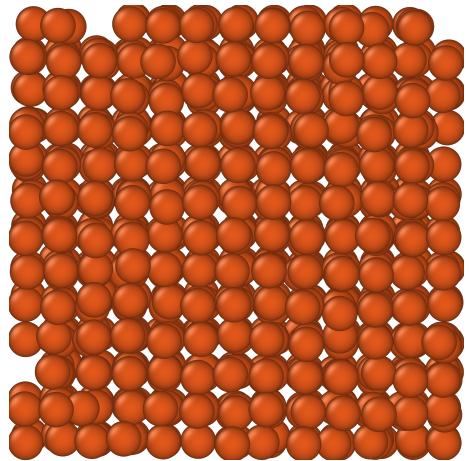
$$g(r) = V \frac{N_{\text{reference particles}}}{N_{\text{particles}}} \langle \delta(r) \rangle$$

- 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

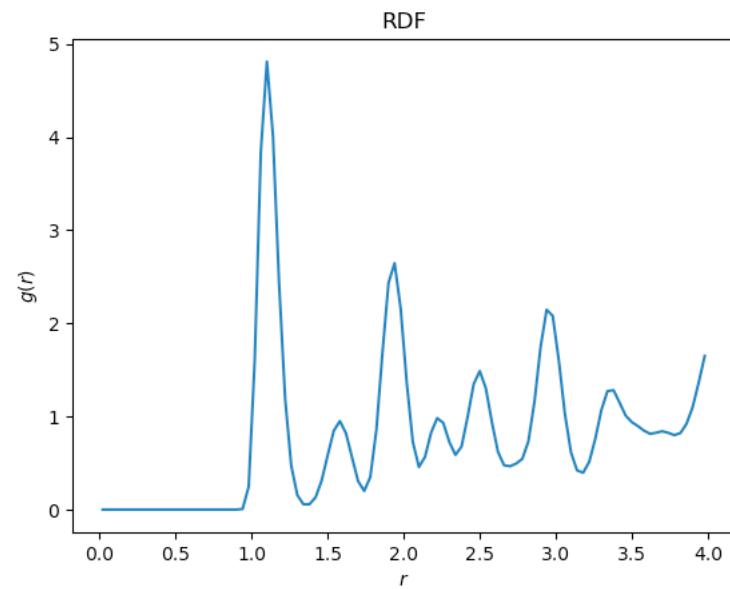


*Graphical depiction of calculating the RDF, from Wikipedia*

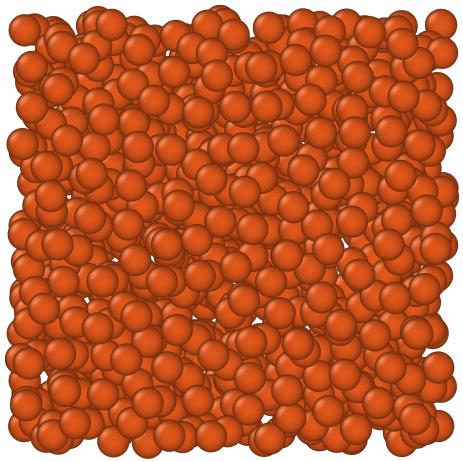
# Sample RDFs



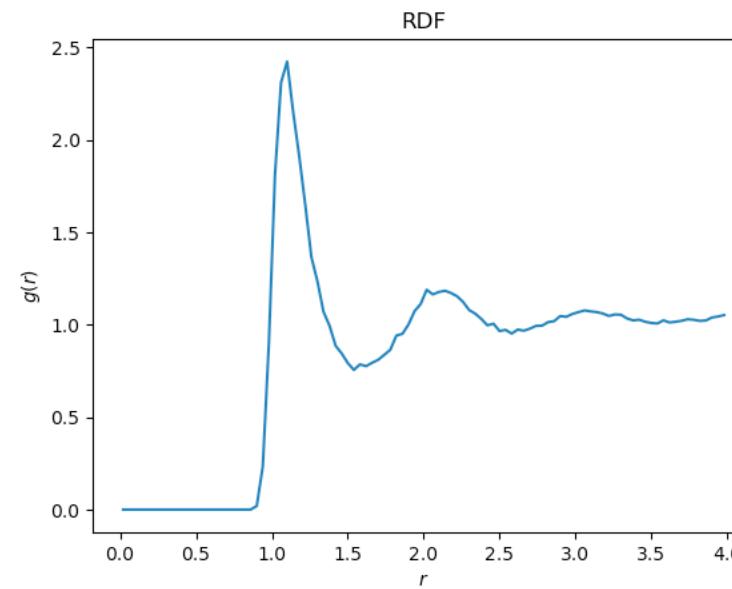
RDF



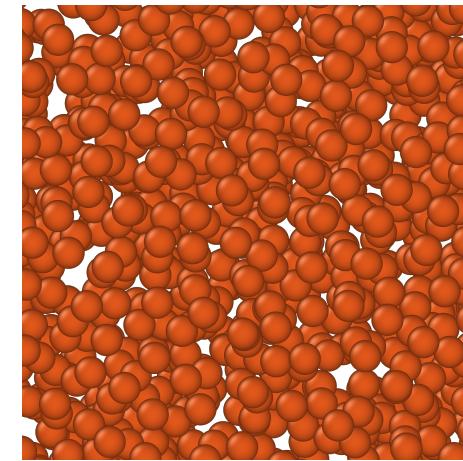
Ordered Solid/Crystal



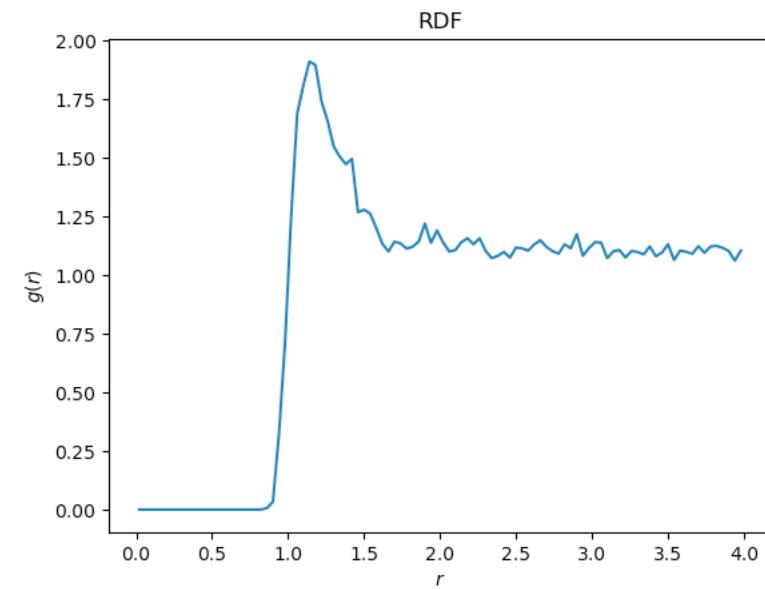
RDF



Liquid



RDF



Gas

# Viewing RDF in Ovito

