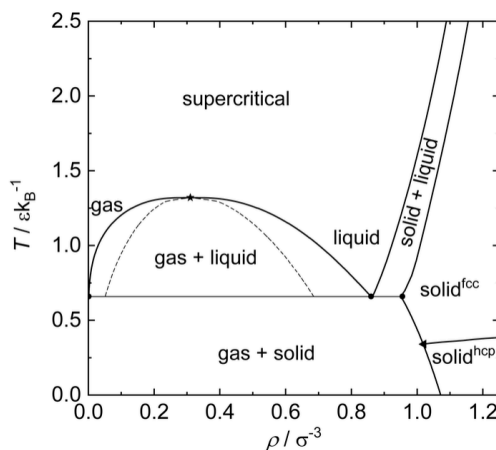


Phases

Using simulations, we can isolate solid, liquid and gas phases. Thinking about these phases, we know that each of these phases is going to look very different. Something in the solid phase will be highly ordered and in a visible crystalline structure. In the gas phase, we expect a disperse system where particles are far apart, while a liquid phase will have some clumps of particles.

Using the phase diagram below:



Source: https://en.wikipedia.org/wiki/Lennard-Jones_potential

you can isolate solid, liquid, and gas regimes. This diagram uses reduced Lennard Jones Units, which takes common units and normalizes them to make comparisons much easier. The relationship between a variety of parameters can be seen here:

Property	Symbol	Reduced form
Length	r^*	$\frac{r}{\sigma}$
Time	t^*	$t \sqrt{\frac{\epsilon}{m\sigma^2}}$
Temperature	T^*	$\frac{k_B T}{\epsilon}$
Force	F^*	$\frac{F\sigma}{\epsilon}$
Energy	U^*	$\frac{U}{\epsilon}$
Pressure	p^*	$\frac{p\sigma^3}{\epsilon}$
Density	ρ^*	$\rho\sigma^3$
Surface tension	γ^*	$\frac{\gamma\sigma^2}{\epsilon}$

Source: https://en.wikipedia.org/wiki/Lennard-Jones_potential

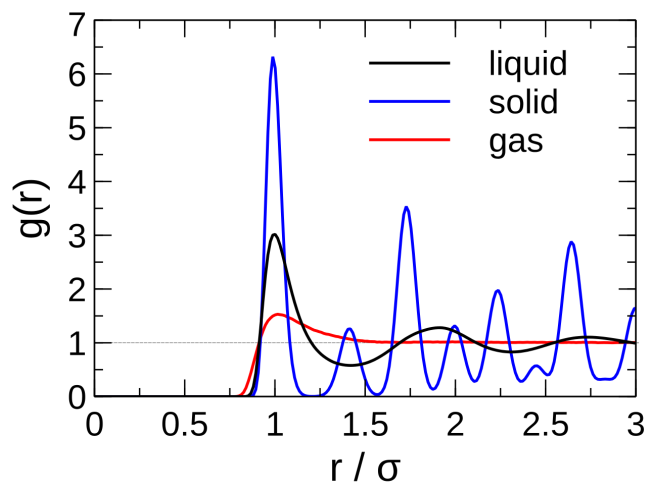
Since sometimes this can be confusing, here's the math behind a density and a temperature calculation for Ar atoms:

Reduced Units

$$\tau^* = \frac{k_B T}{\epsilon} = \frac{(1.38 \times 10^{-23} \text{ J/K})(T)}{1.6502 \times 10^{-21} \text{ J}}$$

$$\rho^* = \frac{N}{V^*} = \frac{N\sigma^3}{V} = \frac{\# \text{ Atoms}}{V} \sigma^3$$

Using this conversion, you should be able to figure out a configuration where you reach solid, liquid and gas phases. Verifying this visually is good, but using the radial distribution function is a great method to mathematically verify your visual observation. RDFs are pair correlation functions that look at the probability of find a particle at a given distance from another tagged particle. Each phase is unique in what the RDF looks like. Below shows what each phases looks like:



Each of these curves look like this because of how the particles orient themselves. For example:

Solid – Each taller peak is indicative of an aligned area of the crystal structure. we see the that the solid decays to zero because the particles are ordered and there should be nothing in between the ordered rows

Liquid - We see a large bump because that is within a droplet of liquid. The function decays because it will often have a gap before getting to another drop. This results in a wave-like plot because we are oscillating between a higher probability of finding a cluster.

Gas – Since these are normalized to 1, these pretty quickly decay to 1 because they should not have any particles nearby.