Colloidal Fluids: Monte Carlo Simulations of Hard Spheres

Thomas Matheickal

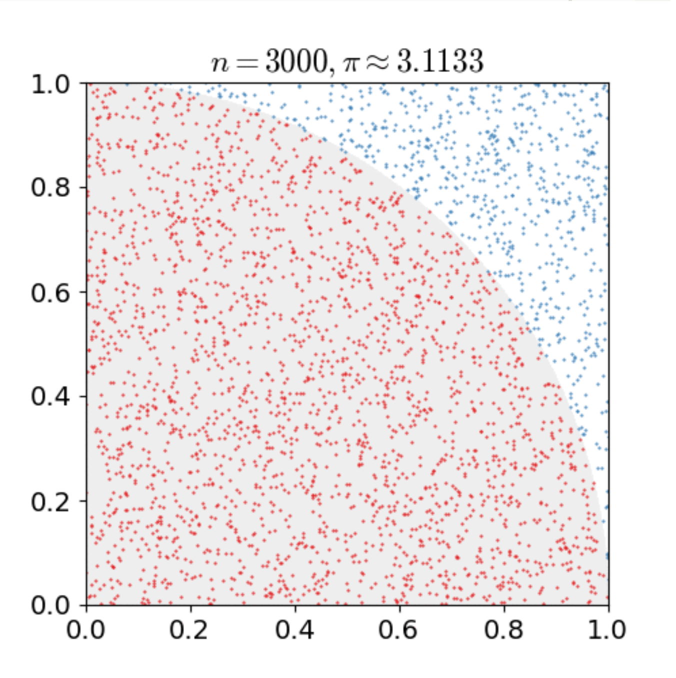
Durham University

Introduction

- Hard spheres act as a useful model for both classical and colloidal fluids
- Model the elastic bouncing atoms exhibit at short ranges
- In 1957, Alder and Wainwright simulated elastic collisions between hard spheres using Monte Carlo Simulation
- Uses repeated sampling and random numbers from probability functions to obtain numerical results

$$V(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} 0 & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| \geq \sigma \\ \infty & \text{if} \quad |\mathbf{r}_1 - \mathbf{r}_2| < \sigma \end{cases}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the two particles.

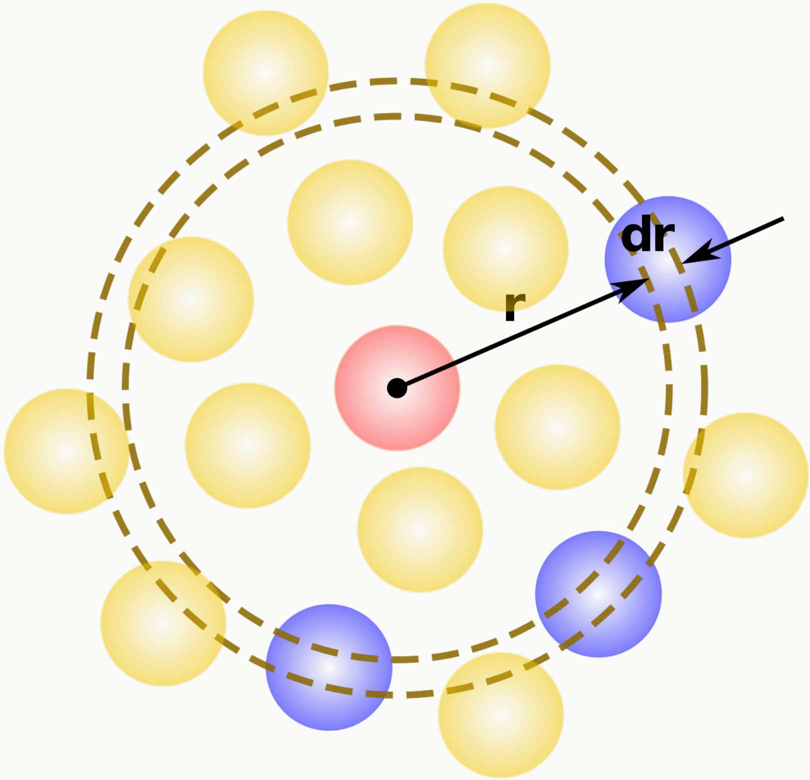


https://en.wikipedia.org/wiki/Monte_Carlo_method

Objectives

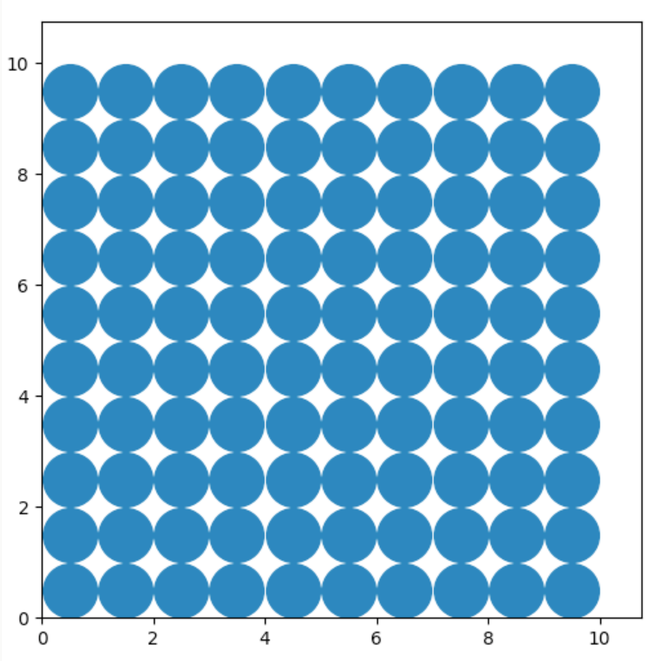
- Want to determine the structural significance of the fluid-solid transition using Monte Carlo simulation
- The Pair Distribution Function, g(**r**) describes how density varies as a function of distance from a reference particle.
- It is the measure of the probability of finding a particle at a distance **r** away from a reference particle, relative to that of an ideal gas
- The ensemble average of the pair distribution function is plotted against values of **r**

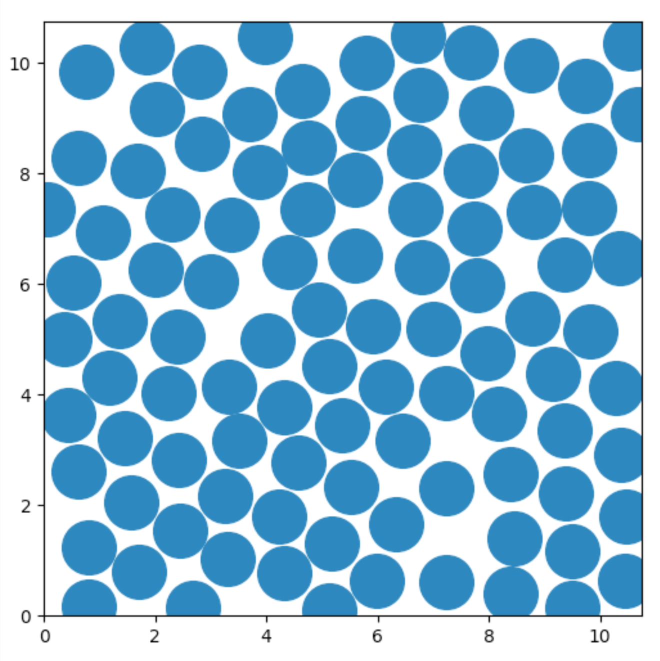
$$g(r) = \frac{n(r)}{n_{\text{ideal}}(r)}$$

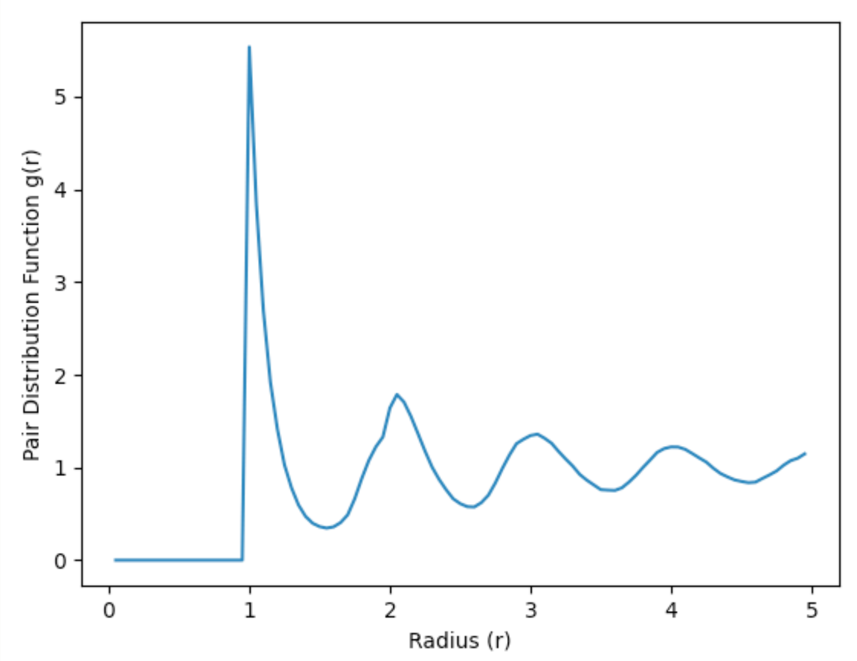


https://en.wikipedia.org/wiki/Radial_distribution_function

Results







Area Fraction = 0.68
N = 100
Radius = 0.5

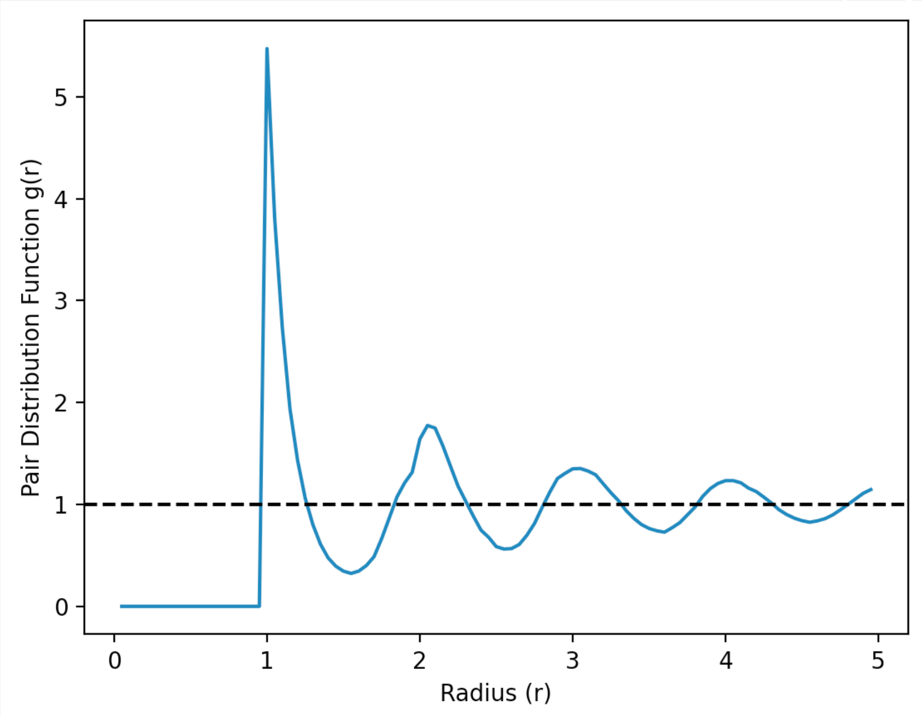
Equilibrated to a new configuration after 100,000 steps

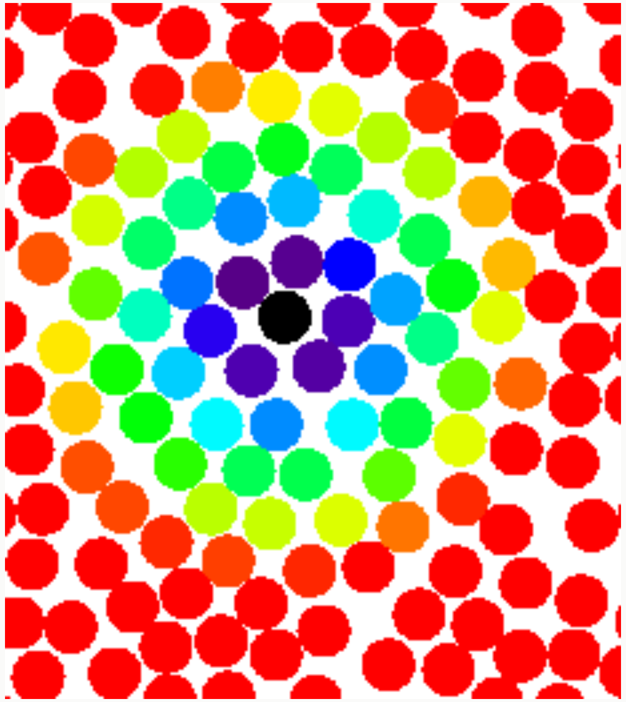
g(r) = 0 before r = 1

Sharp Peak at radius = 1

Sinusoidal dampened wave converging to g(r) = 1

PDF Convergence

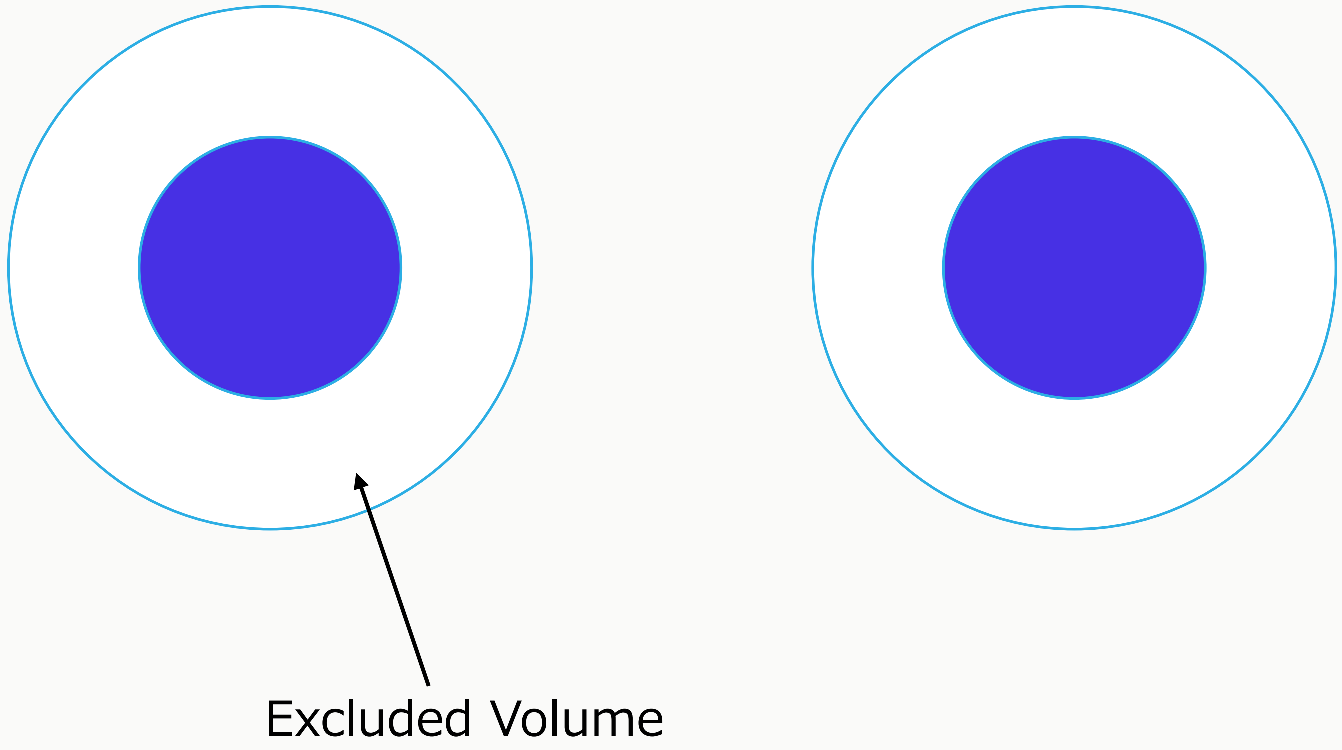




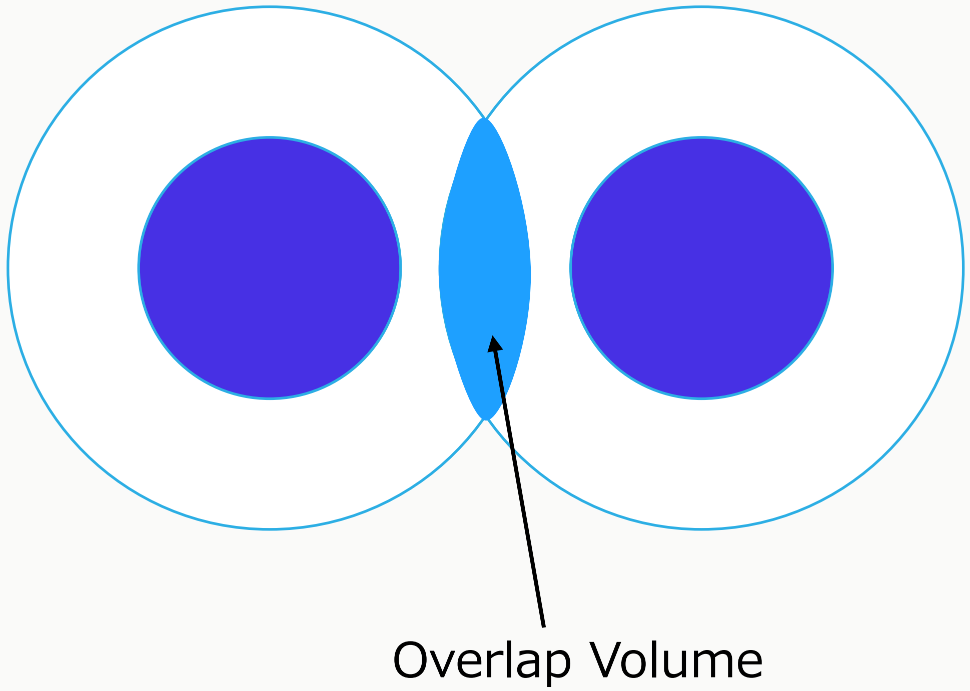
http://www.physics.emory.edu/faculty/weeks/idl/gofr.html

$$g(r) = \frac{\rho(r)}{\rho_0}$$

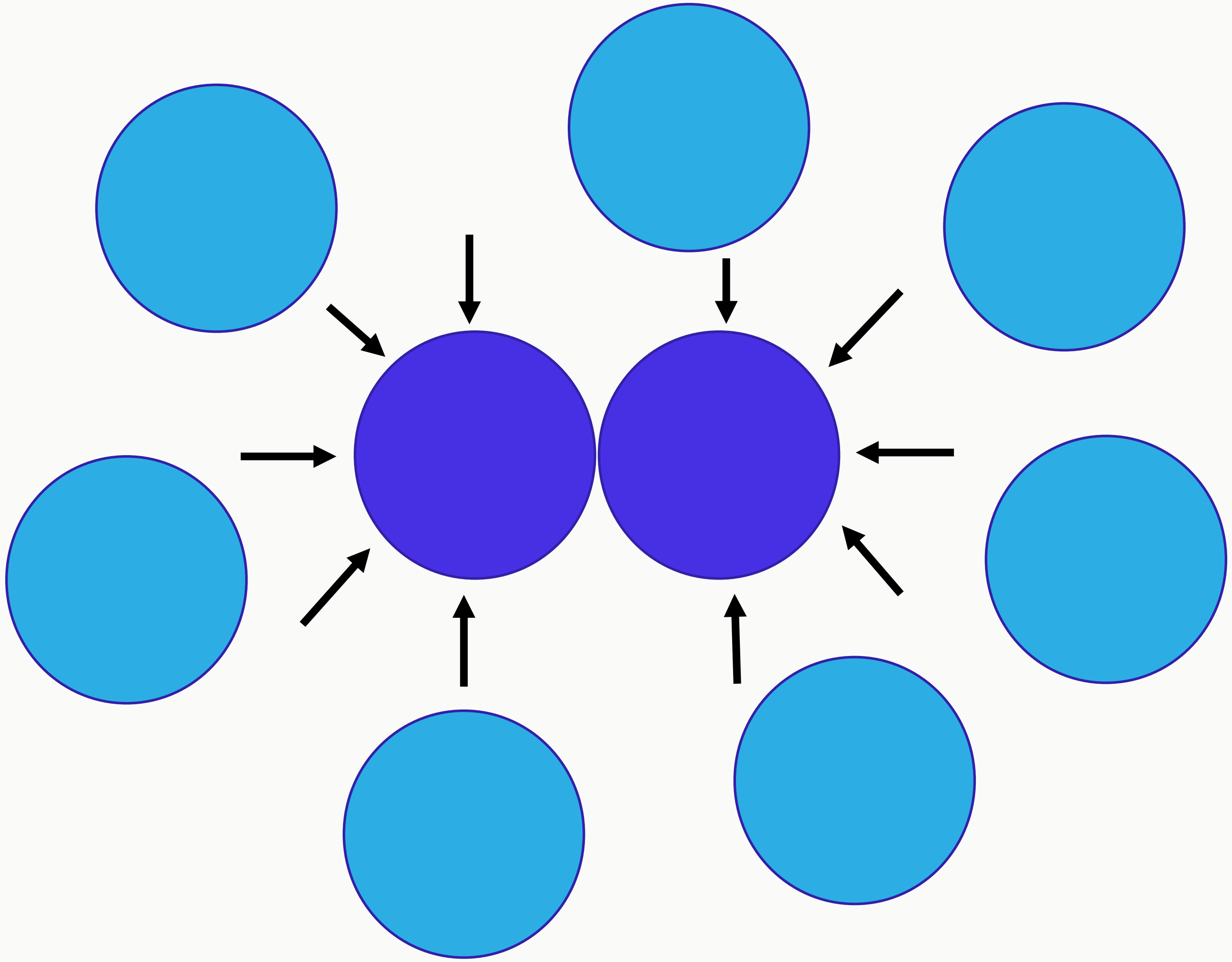
Depletion Force



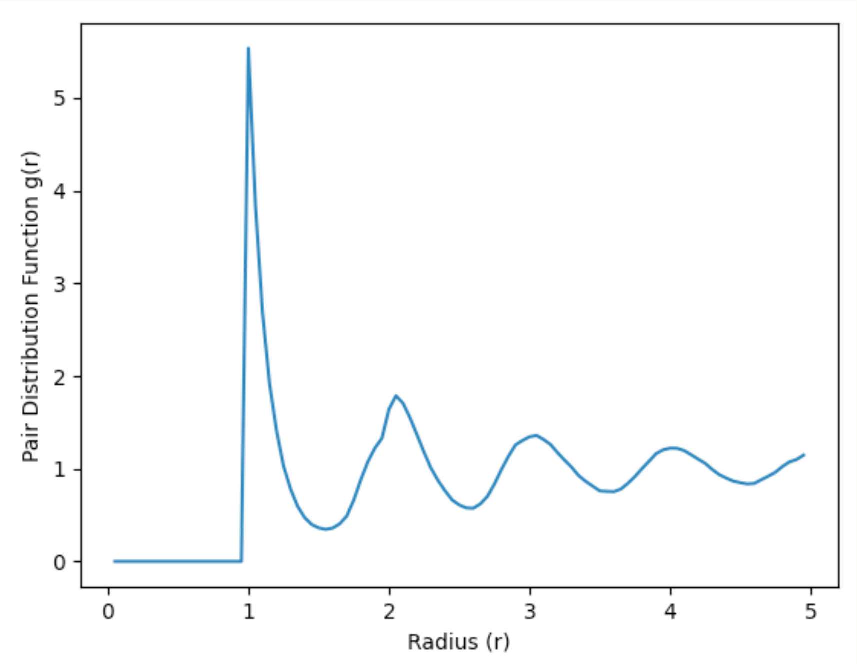
Depletion Force

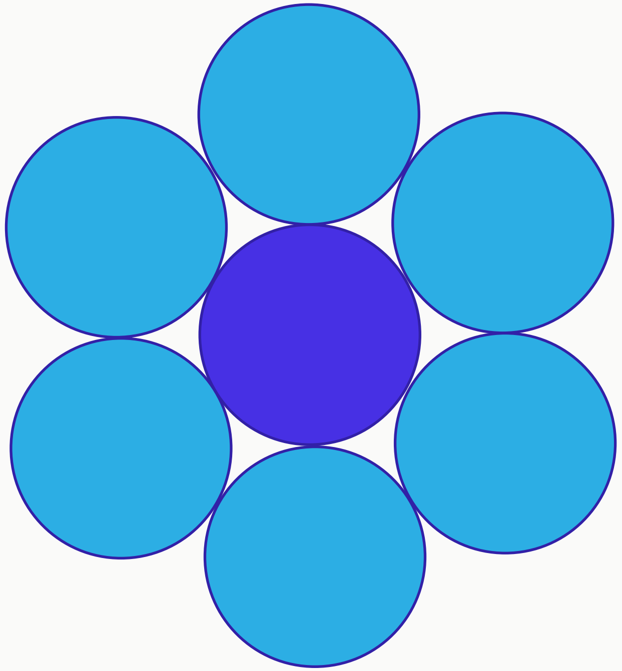


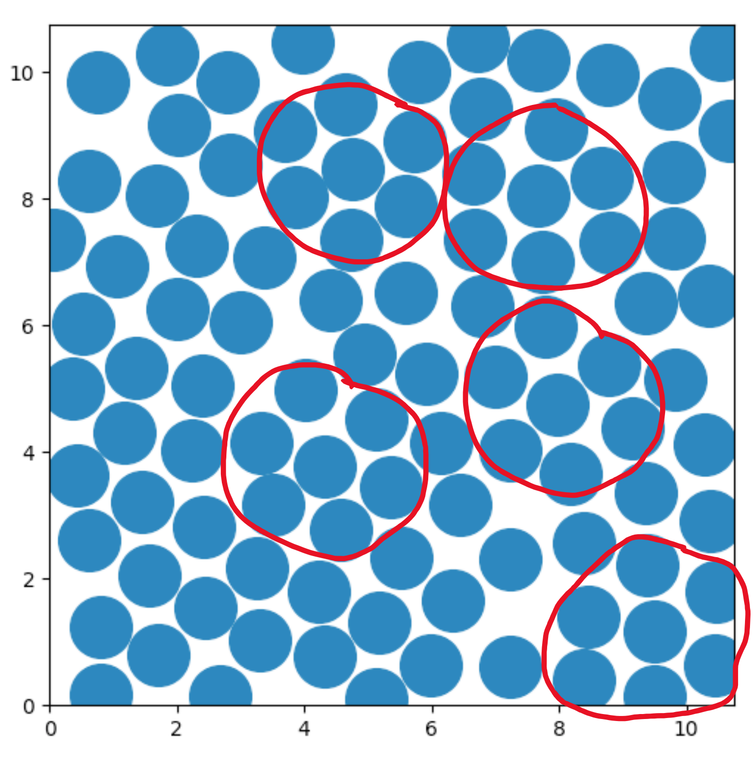
Depletion Force



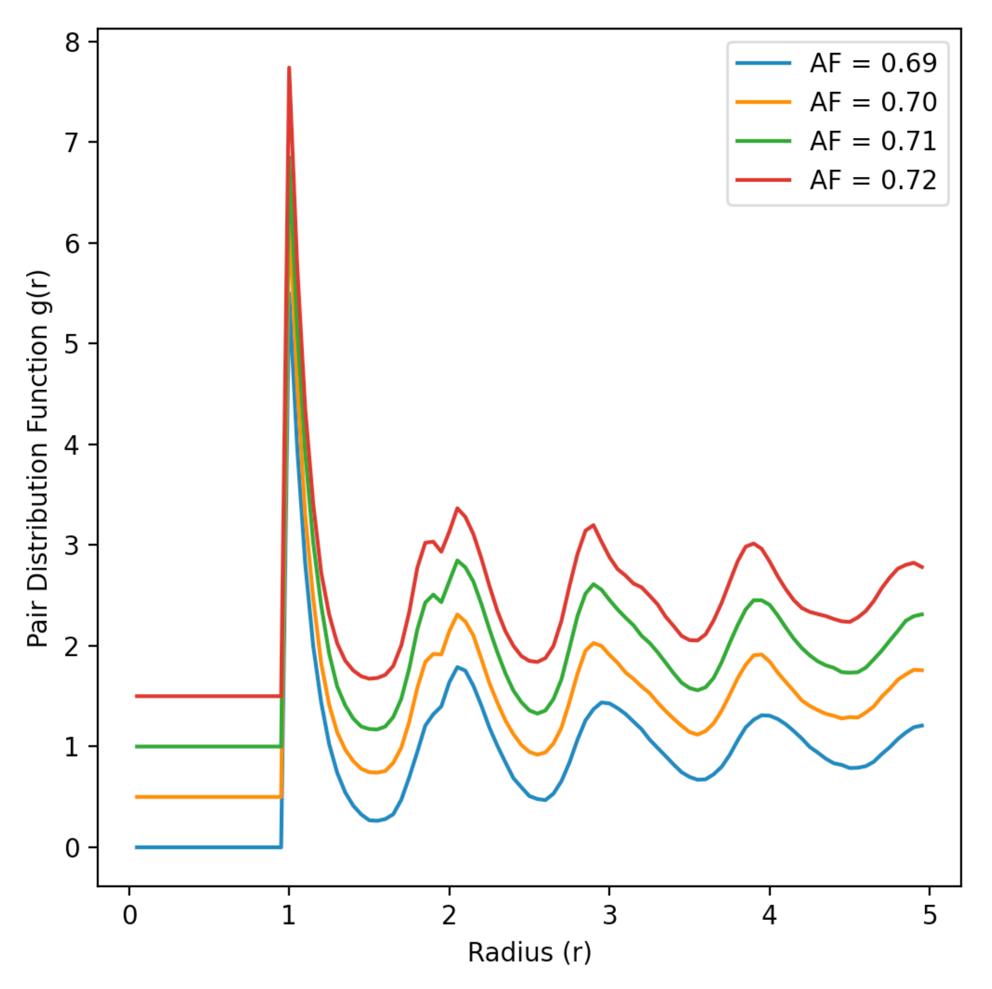
Depletion Force



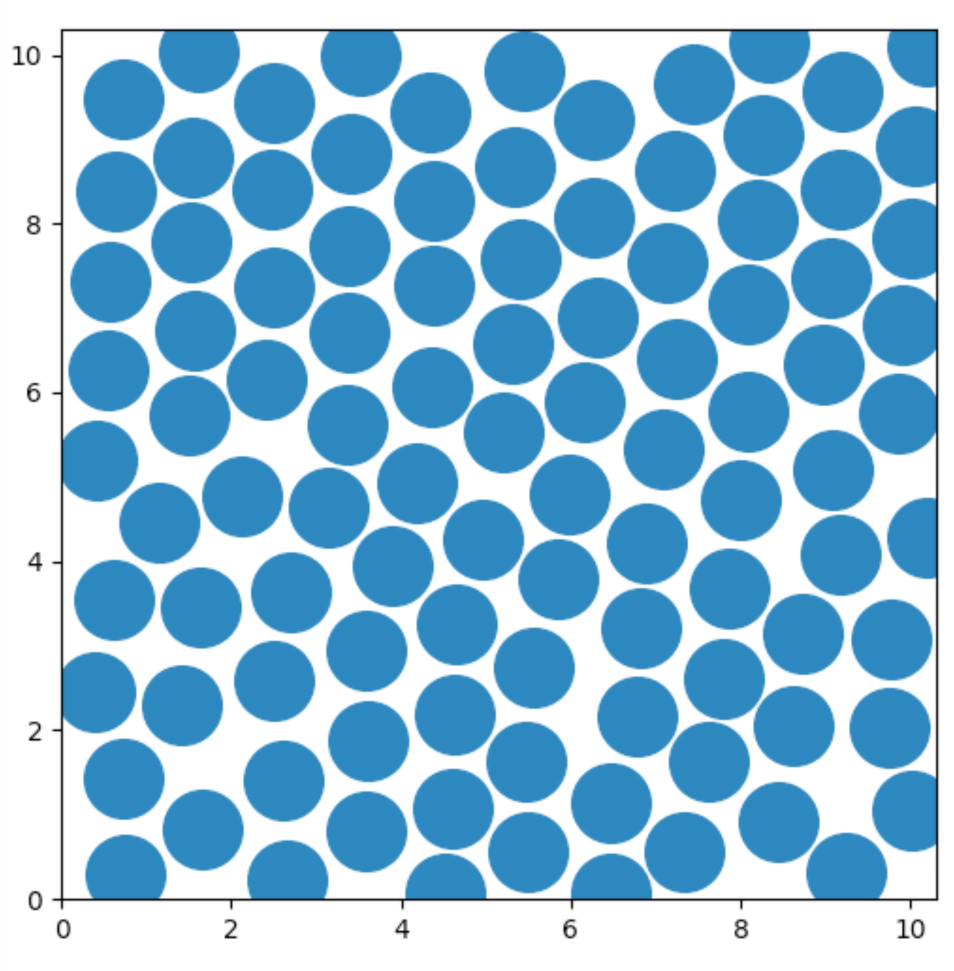




New Peak



AF = 0.69
AF = 0.70
AF = 0.71
AF = 0.72
Pair Distribution Function g(r)
Radius (r)
0
1
2
3
4
5
6
7
8



0
2
4
6
8
10