Protein Simulation in Lammps

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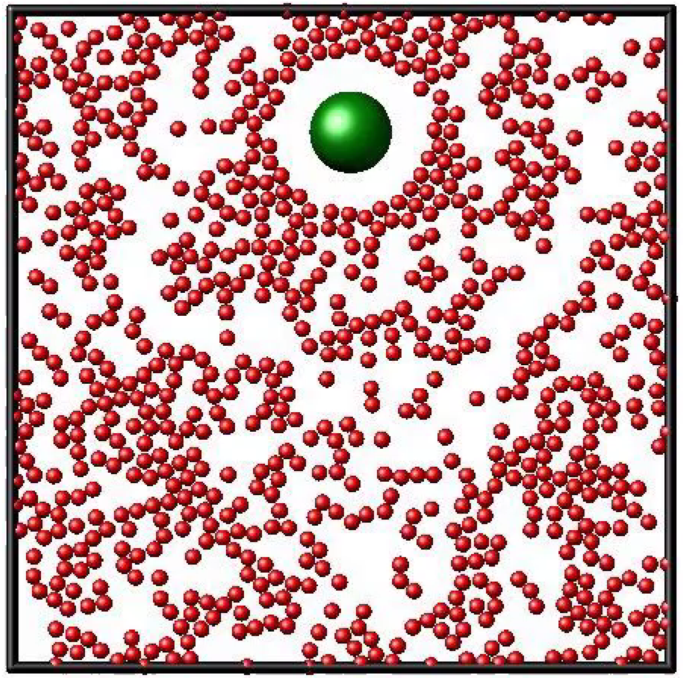
Phys 230 – Spring 2021

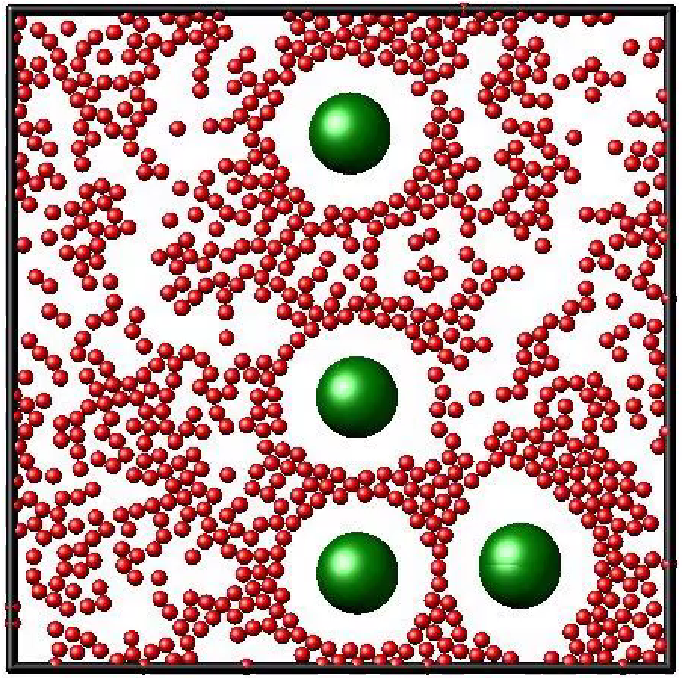
Part 1: Modeling the system as a large particle (A) surrounded by the solvent (B)

Particles – Brownian Motion

Original



Add 5 Particles



Changing the Interaction types

Original

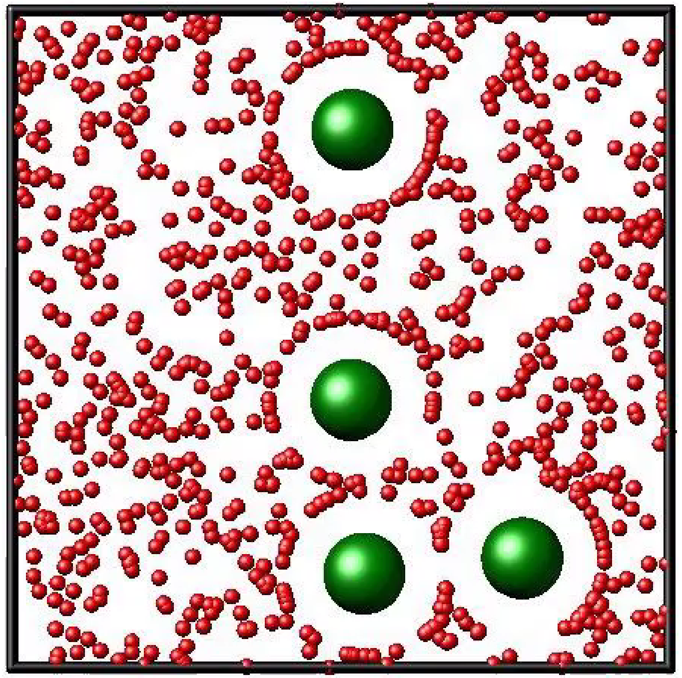
#Soft pair interaction between all particles

pair_style soft   1.0

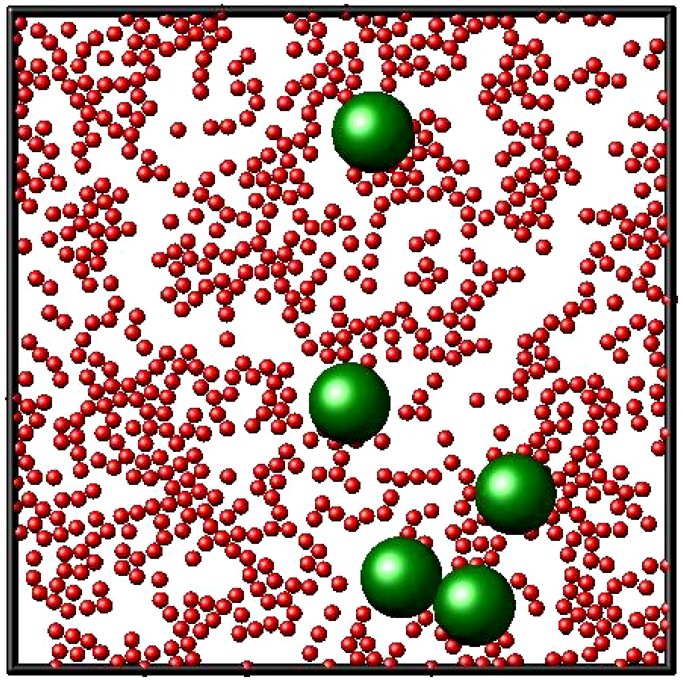
pair_coeff 1 1 10.0 1.0

pair_coeff 1 2 10.0 5.0

pair_coeff 2 2 10.0 5.0



Changing the Interaction types



“3 interaction types”

pair_style hybrid lj/cut 1.0 soft 5.0 yukawa 0.5 1.0

pair_coeff 1 1 lj/cut 10.0 1.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 yukawa 0.50 1.0

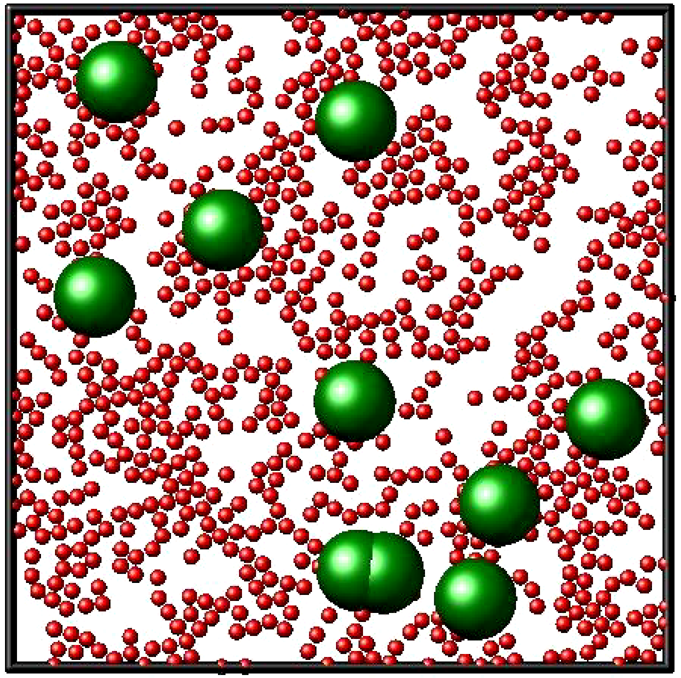
- Moving way too fast.
- Large particles are all over the place.
- Try changing the velocity

Changing a bunch of things

Changes:

- 10 large particles
- Mass of large particles 500 instead of 50
- Change global cutoff for soft interaction to 5.0
- Change yukawa interaction to 0.50 and 1.0 (instead of 10.0 and 5.0)

Did something useful, but still all over the place



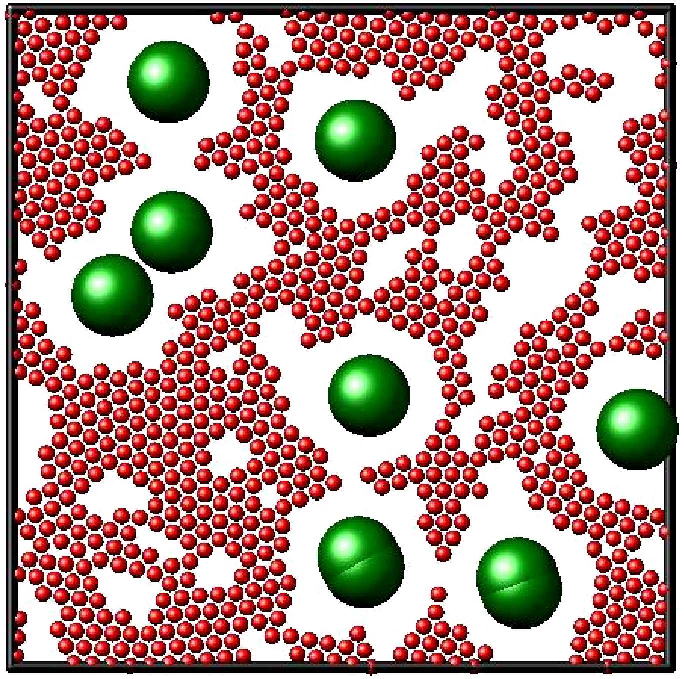
Changing velocity

Changing velocity corresponding to temp

"Velocity all create 2.0 dist gaussian (temp of 2.0)"

- Changed velocity to 1.0
- changed **yukawa** screening length to 3.5,
- cutoff to 4.0 and
- energy to 5.0

Getting closer!

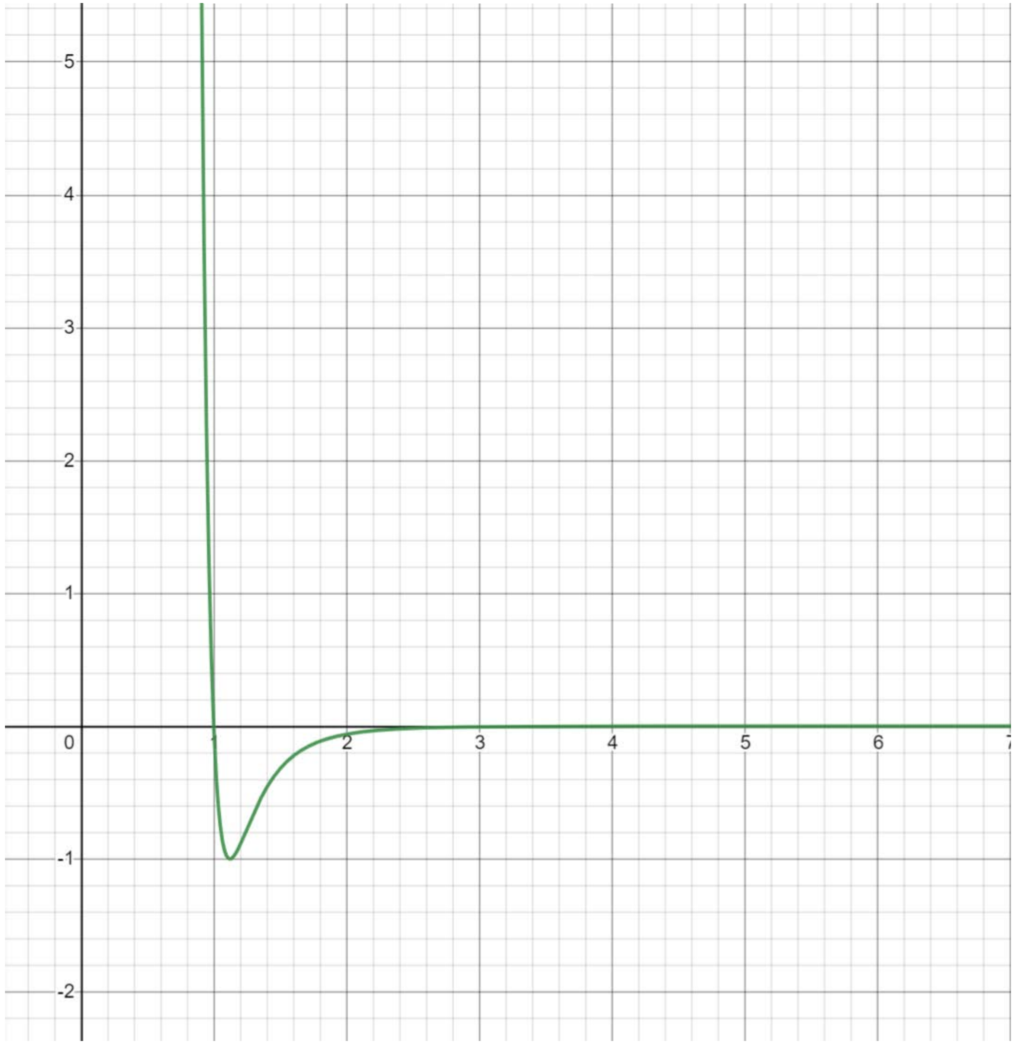


Consider the Interactions

pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0
pair_coeff 1 1 lj/cut 1.0 1.0

Lennard-Jones

$$y = 4(1)\left(\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6}\right)$$



pair_style lj/cut

LJ - Interaction

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c$$ *

Pair_coeff

Definition of coefficients

*

ϵ (energy units)

σ (distance units)

LJ cutoff (distance units)

*From the LAMMPS manual https://lammps.sandia.gov/doc/pair_style.html

https://www.desmos.com/calculator

```
pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0
pair_coeff 1 2 soft 10.0 5.0
```

$$y = 10 \cdot \left[1 + \cos\left(\frac{\pi r}{(5)}\right)\right]$$

Soft Repulsion

Pair_style soft

Soft repulsion

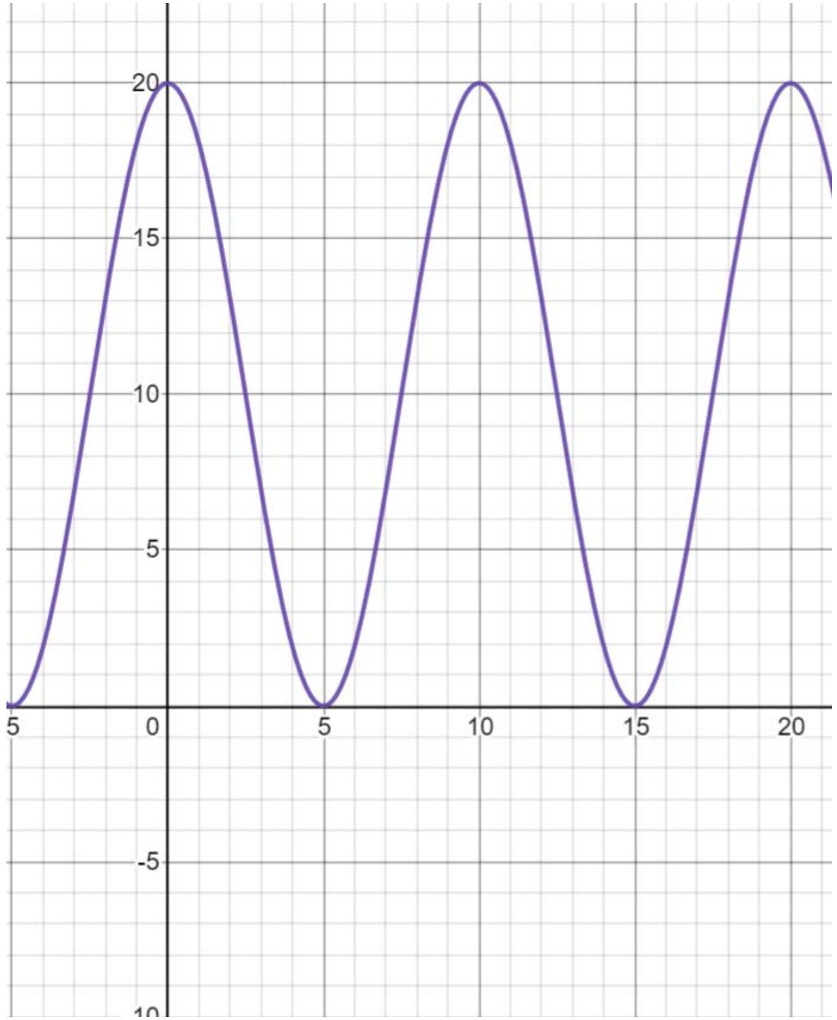
$$E = A\left[1 + \cos\left(\frac{\pi r}{r_c}\right)\right] \qquad r < r_c$$ *

Pair_coeff

Definition of coefficients

A (energy units)

cutoff (distance units) *



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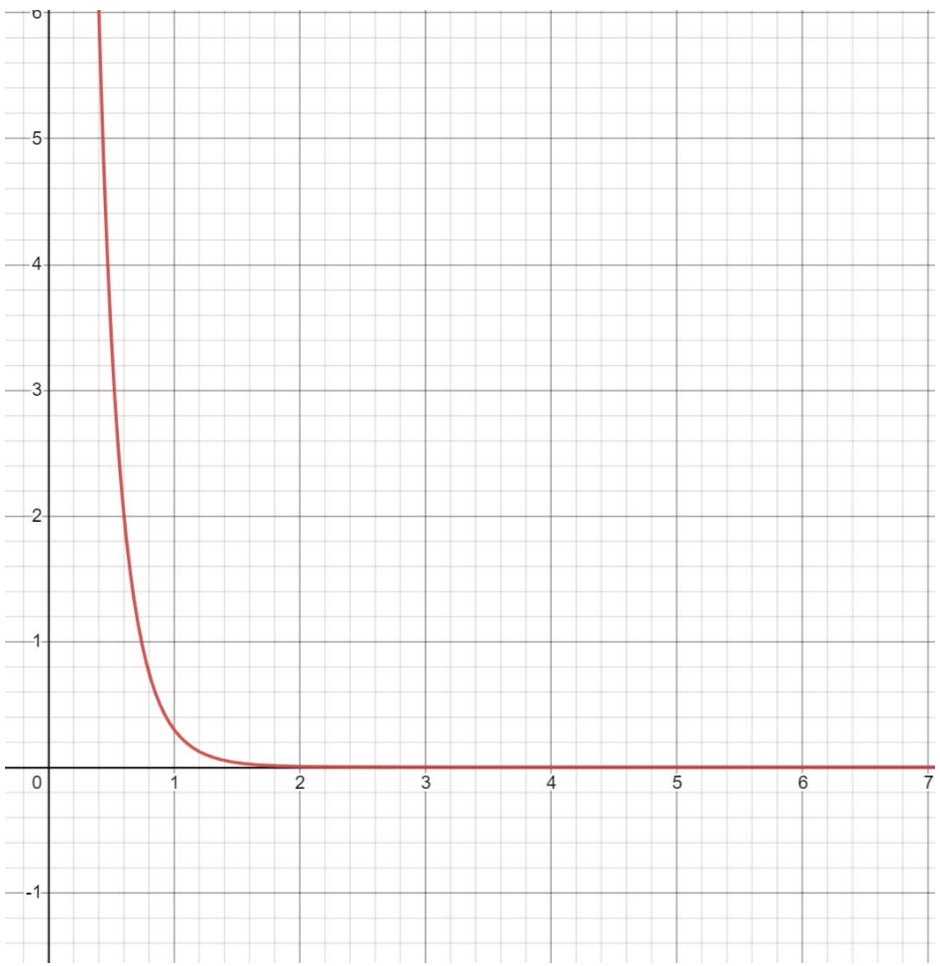
*From the LAMMPS manual
https://lammps.sandia.gov/doc/pair_style.html

pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0

pair_coeff 2 2 yukawa 10.0 5.0

Yukawa

$$y = 10\,\frac{e^{-(3.5)r}}{r}$$



https://www.desmos.com/calculator

Pair_style yukawa

Yukawa Interaction

$$E = A\frac{e^{-\kappa r}}{r} \qquad r < r_c$$ *

```
pair_style yukawa kappa cutoff
```
*

kappa = screening length (inverse distance units)

cutoff = global cutoff for Yukawa interactions (distance units)

Pair_coeff

Definition of coefficients

A (energy*distance units) *

cutoff (distance units)

*From the LAMMPS manual https://lammps.sandia.gov/doc/pair_style.html

All Together

Final Interactions

pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0

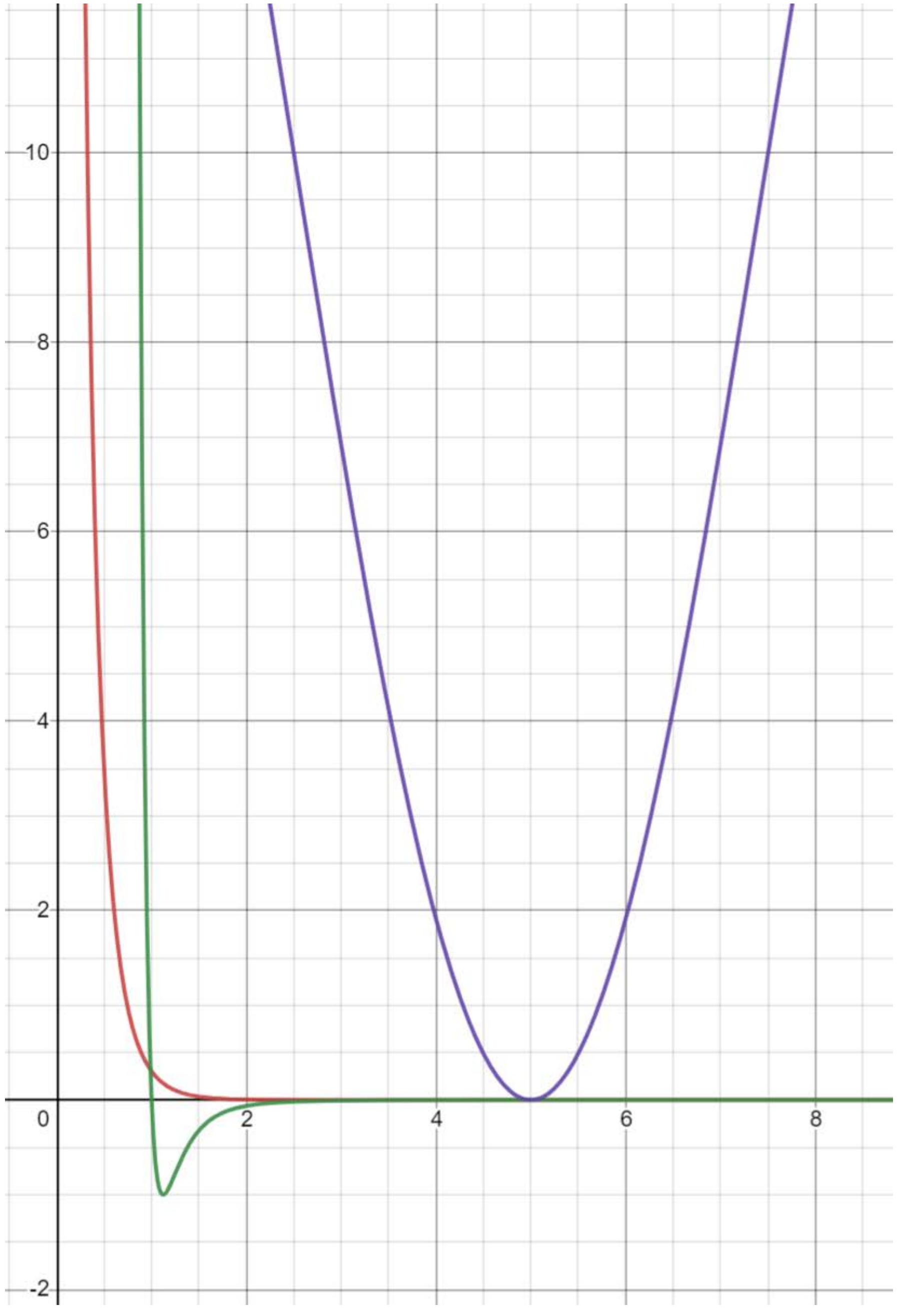
pair_coeff 1 1 lj/cut 1.0 1.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 yukawa 10.0 5.0

Also

- Change velocity back to 1.5
- yukawa cutoff to 5.0 and
- energy to 10 for more dramatic effect



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All Together

Final Interactions

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pair_coeff 1 1 lj/cut 1.0 1.0

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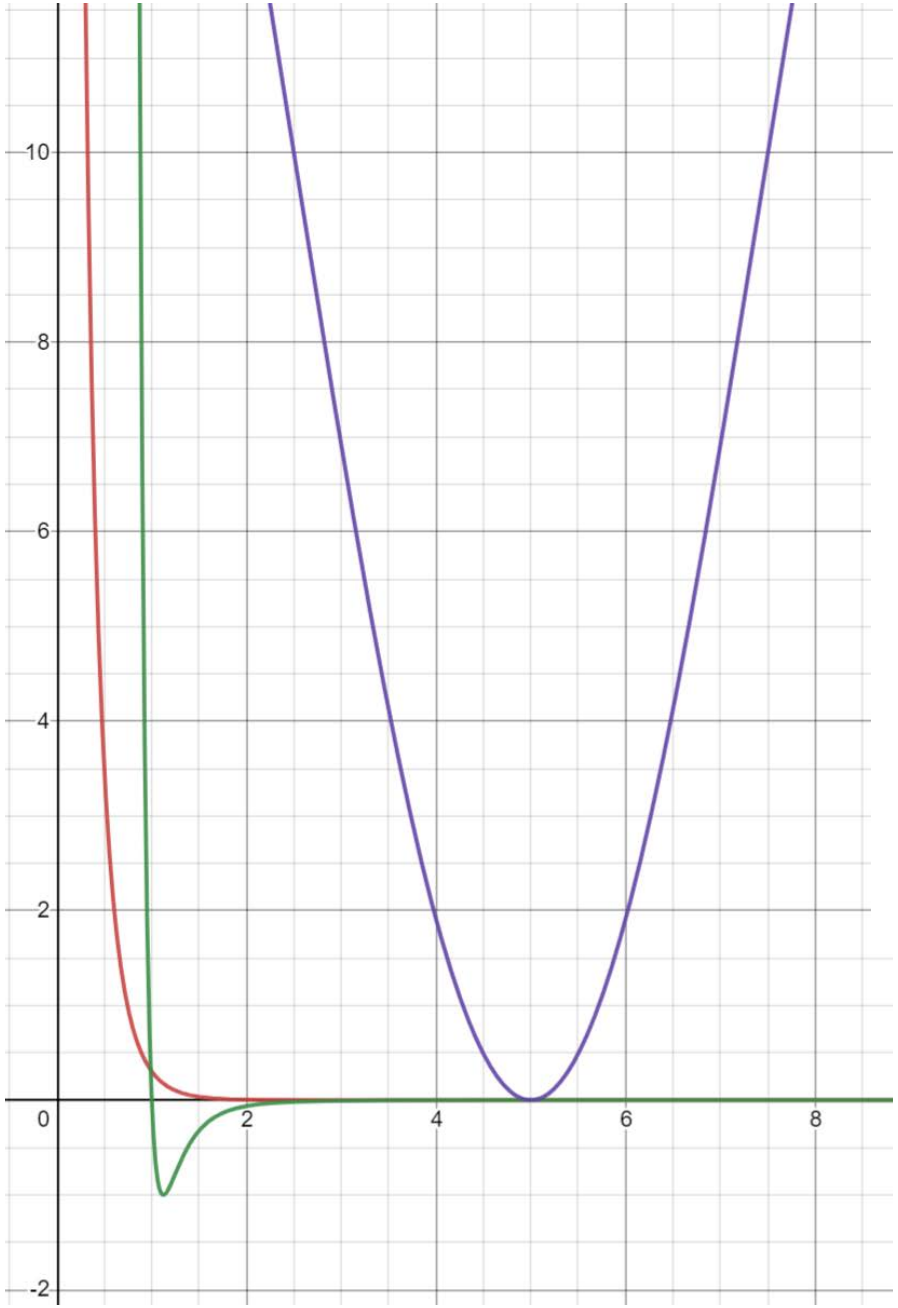
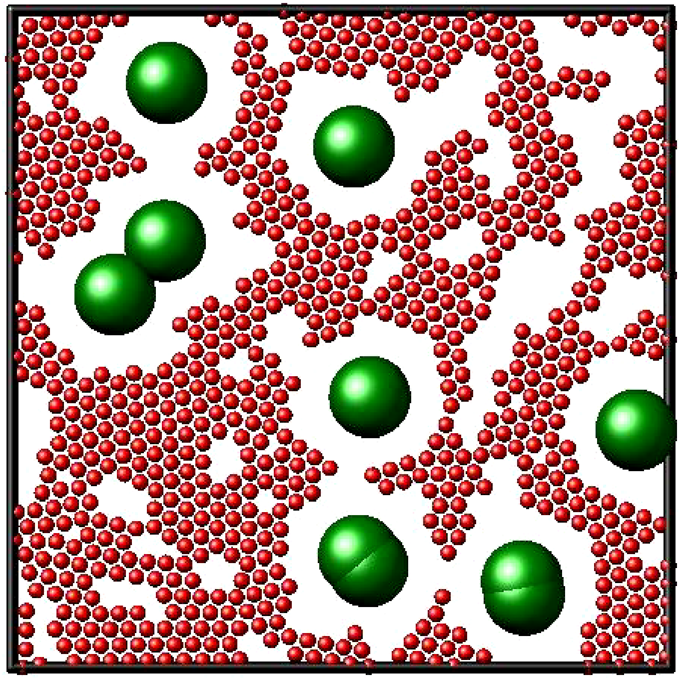


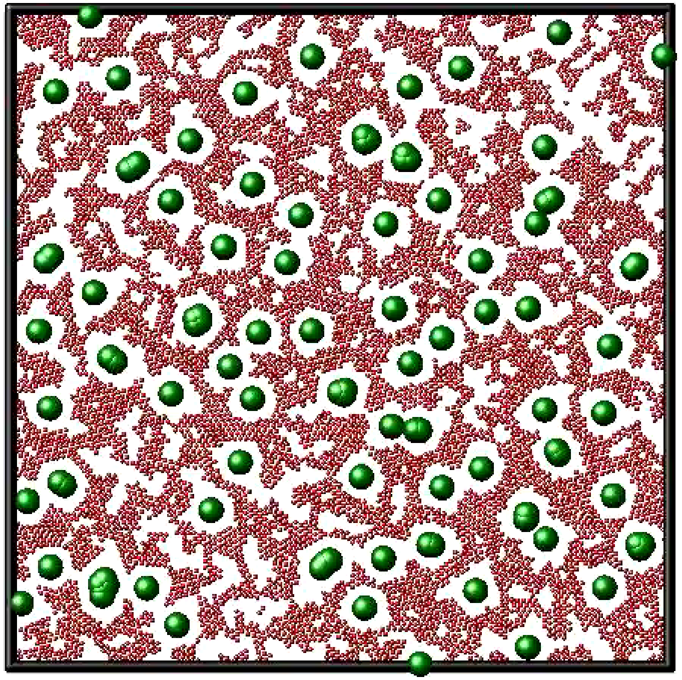
https://www.desmos.com/calculator



Make it Bigger!!!!!

10x particles, 10x area in box,

10x # of steps



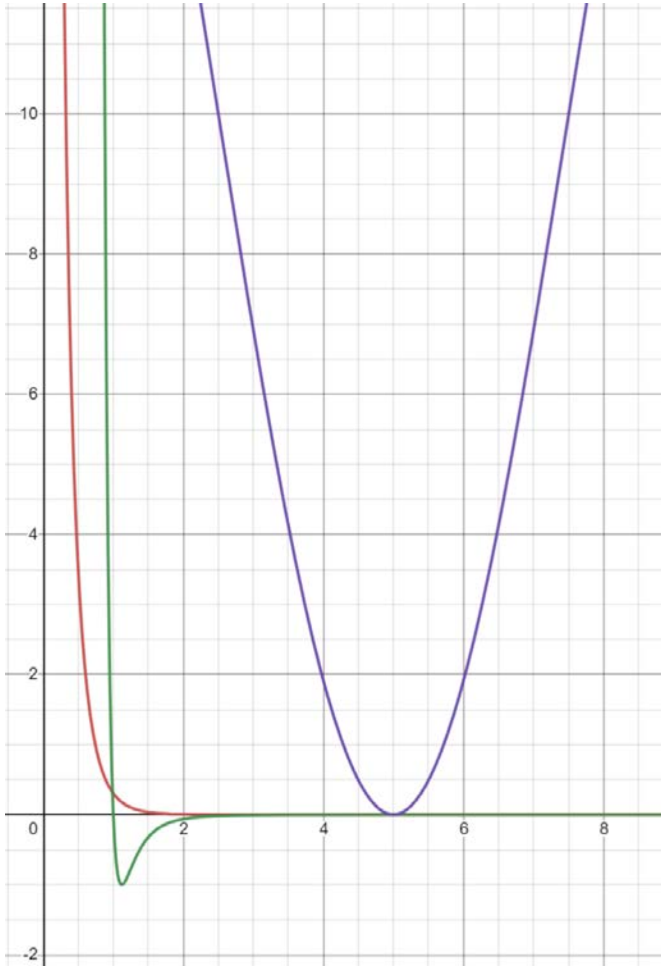
Final Interactions

pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0

pair_coeff 1 1 lj/cut 1.0 1.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 yukawa 10.0 5.0

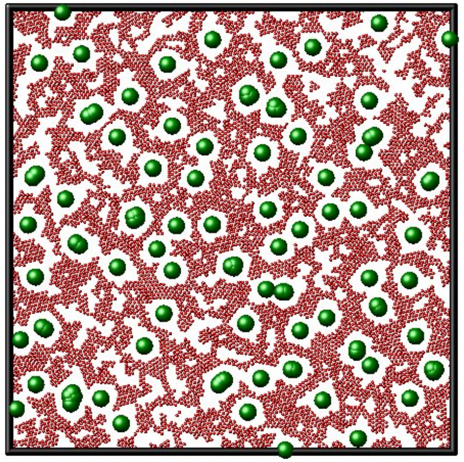


https://www.desmos.com/calculator

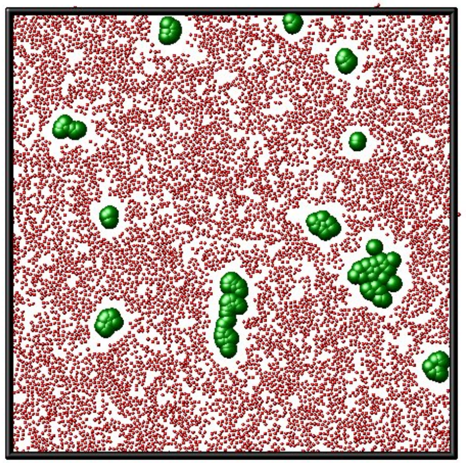
Future Goals:

Time Progression of the Radial Distribution Function :

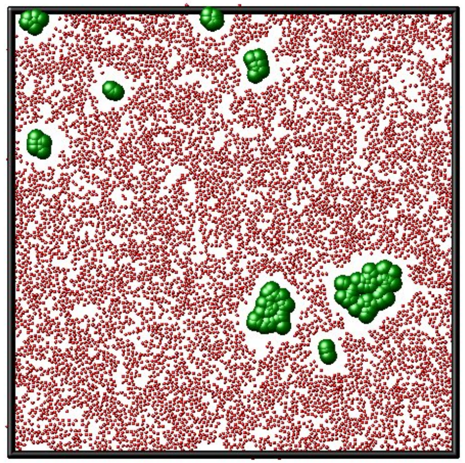
measuring the self-assembly



t=0



t=2,500,000



t=5,000,000

By determining the pair correlation function of the large particles – and how it progresses with time.

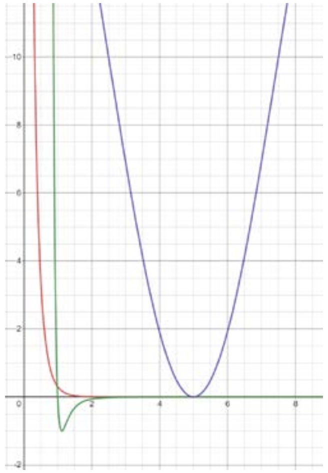
Future Goals: Time Progression of the Radial Distribution Function : measuring the self-assembly

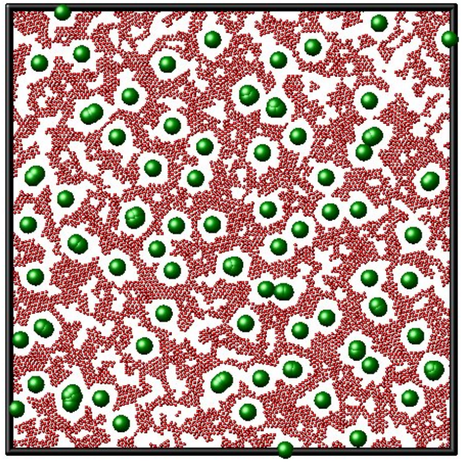
pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 3.5 5.0

pair_coeff 1 1 lj/cut 1.0 1.0

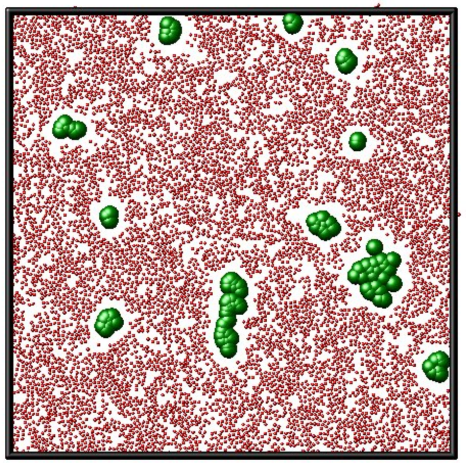
pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 yukawa 10.0 5.0

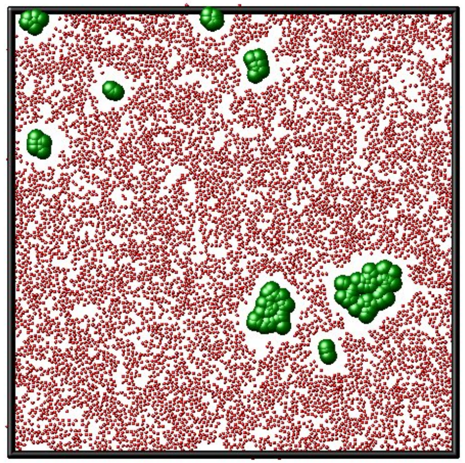




t=0



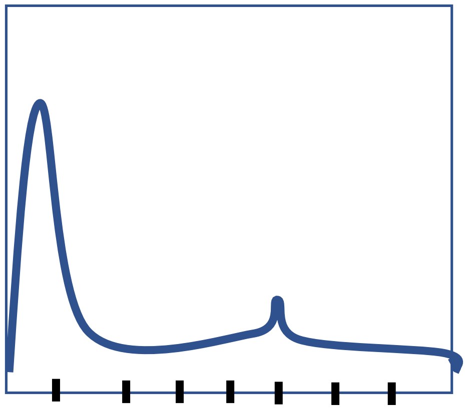
t=2,500,000



t=5,000,000

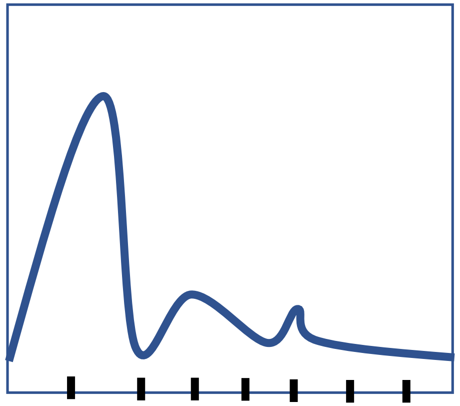
Predictions:

arb. units



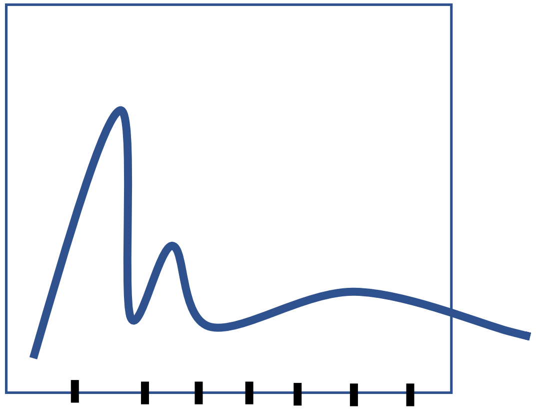
r

arb. units



r

arb. units



r

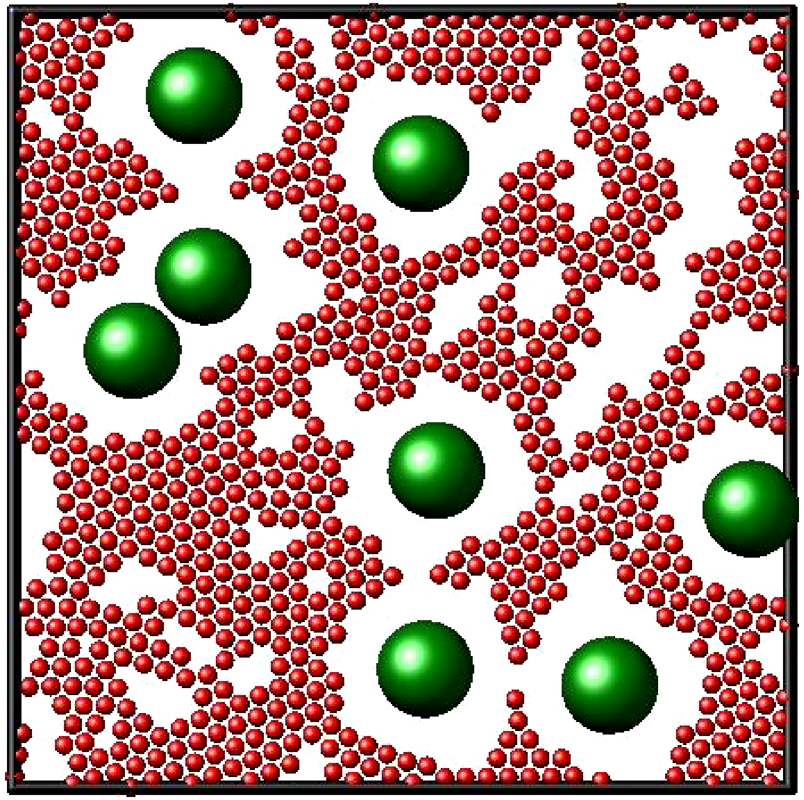
The small particles will always give a peak near 1, so that's not very interesting. Since this is a simulation, we can focus on the distribution of large particles only.

A Question that Came up:

Was whether the yukawa interaction is actually repulsive or attractive?

If the yukawa interaction between two larger green particles is repulsive, and yet they are still assembling due to the soft repulsive interactions they have with the smaller red particles, then it is an interesting result.

Changing the large particles interactions to zero interaction



pair_style hybrid lj/cut 2.0 soft 7.0 zero 5.0

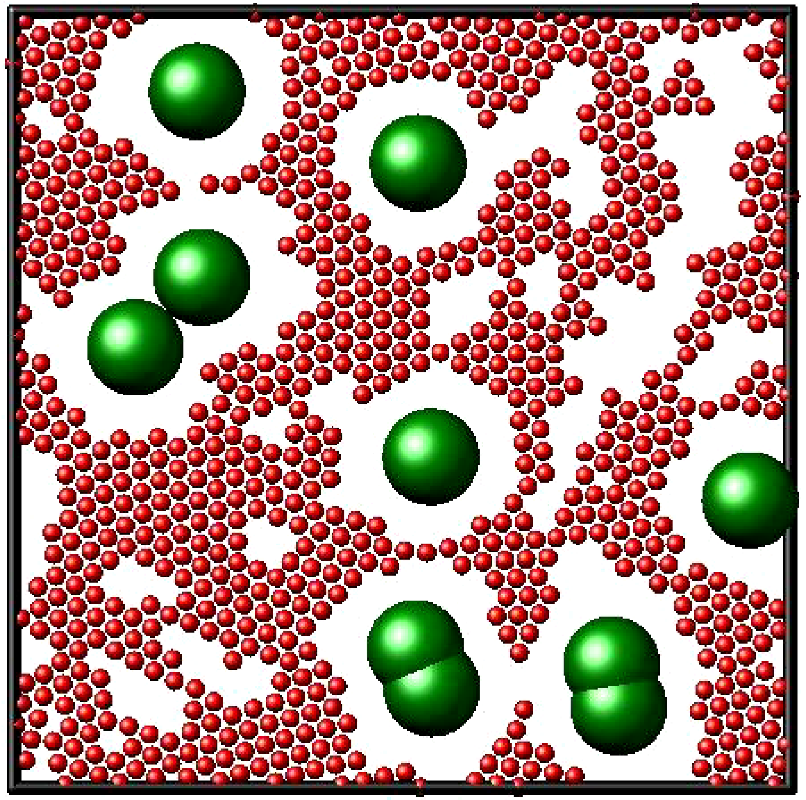
pair_coeff 1 1 lj/cut 1.0 1.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 zero

This showed that the large particles assemble without any attractive force between them.

Changing the large particles interactions to lennard-jones with a deep potential well



pair_style hybrid lj/cut 7.0 soft 7.0

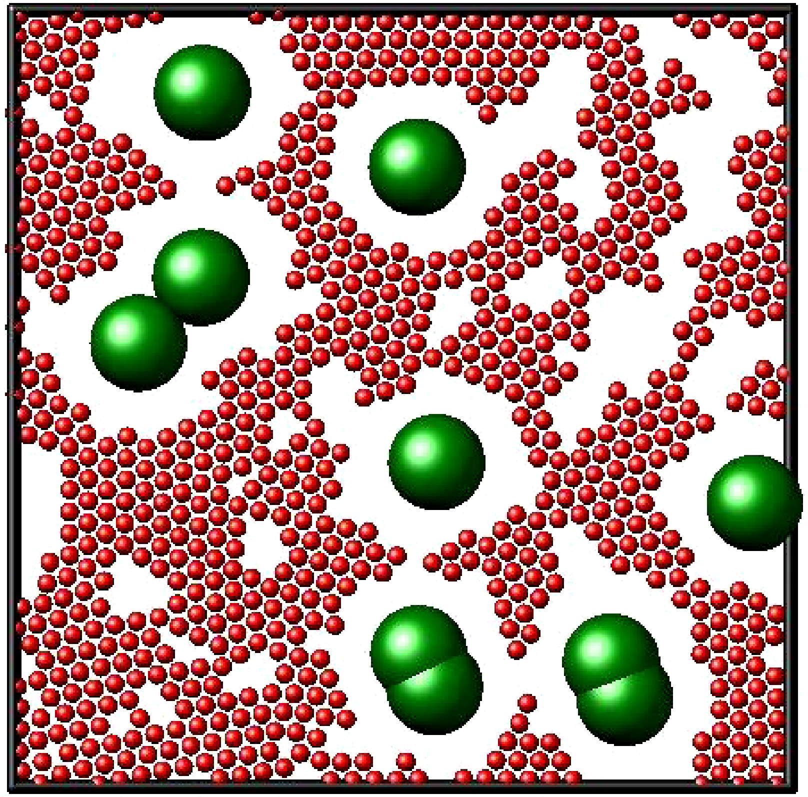
pair_coeff 1 1 lj/cut 1.0 1.0 2.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 lj/cut 20.0 2.0

This showed that the large particles assemble and then arrange into the distance from each other associated with that potential well, but then move together as one entity.

Changing the large particles interactions to a soft repulsive interaction



pair_style hybrid lj/cut 7.0 soft 7.0

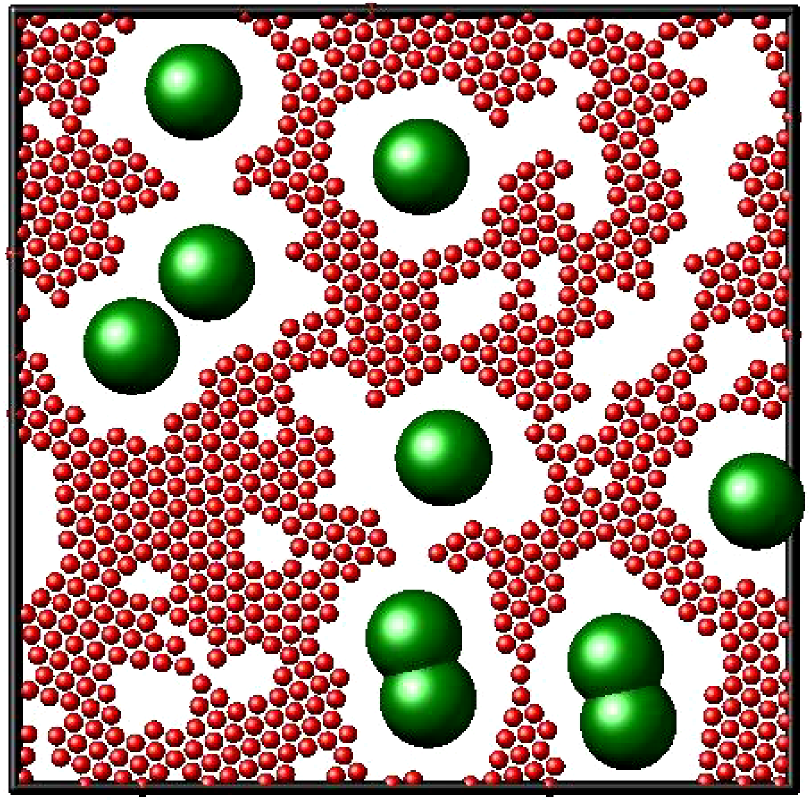
pair_coeff 1 1 lj/cut 1.0 1.0 2.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 soft 20.0 2.0

This showed that the large particles assemble even though they repel each other. They continue to repel each other, but are pushed back together by the interactions with the small particles.

Changing the large particles interactions back to a yukawa interaction with shallow curve, large cut-off distance,low screening length, & high energy



pair_style hybrid lj/cut 2.0 soft 7.0 yukawa 0.3 15.0

pair_coeff 1 1 lj/cut 1.0 1.0

pair_coeff 1 2 soft 10.0 5.0

pair_coeff 2 2 yukawa 100.0 15.0

The settings allow the large particles to interact with each other while still farther away than before, and so they were able to repel each other to a certain distance away, although they are forced to that distance by the interactions with the smaller particles. And they continue to interact with each other from there, instead of as a roiling mass that we had in the earlier yukawa interaction experiments. **So it is a repulsive yukawa interaction!** But the large particles are still forced to assemble due to the interactions with the smaller particles. **An interesting result that occurs in real systems.** (e.g. Depletion forces)