Study of Compressed Emulsions

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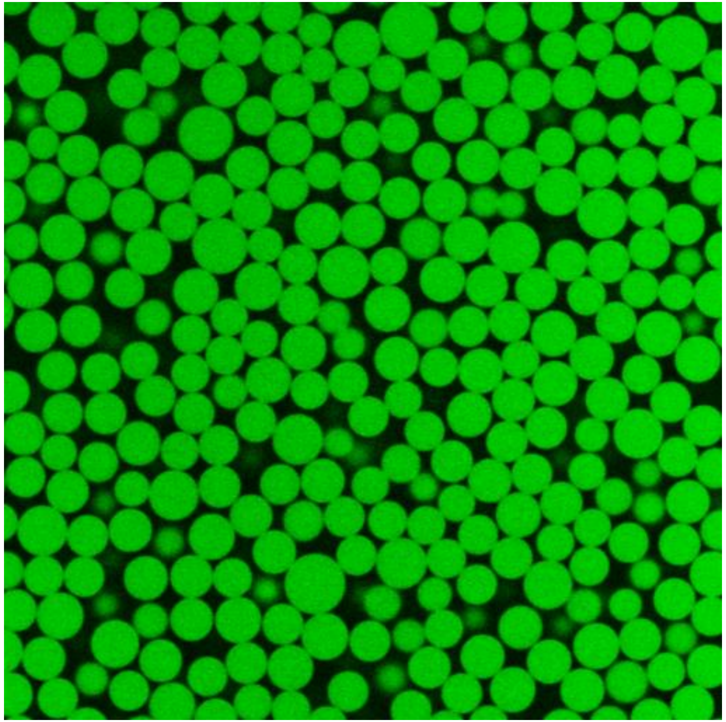
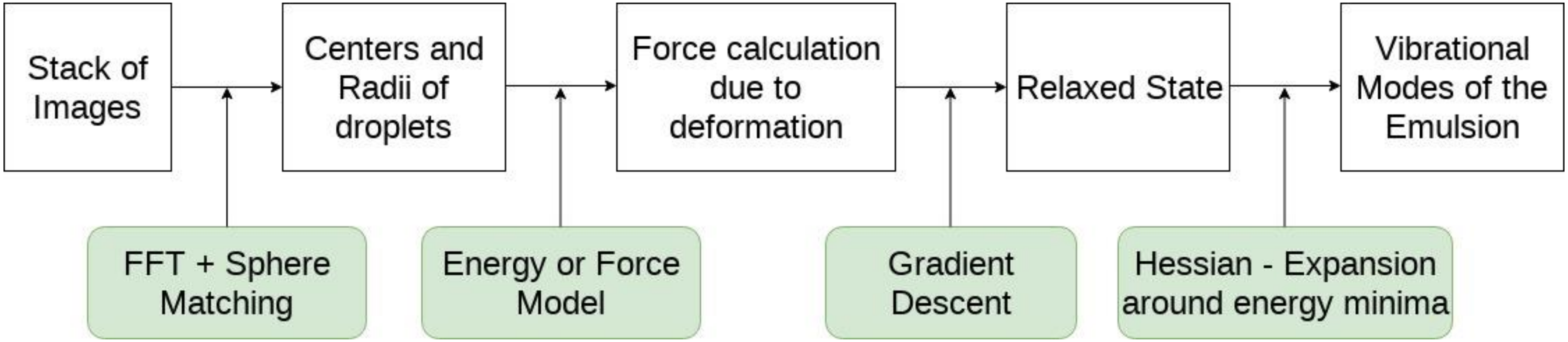
Compressed Emulsions

- Confocal Images (z-stack)
- Deformable spheres (squishy)
- Polydisperse
- Random Close Packing
- Normal force due to compression



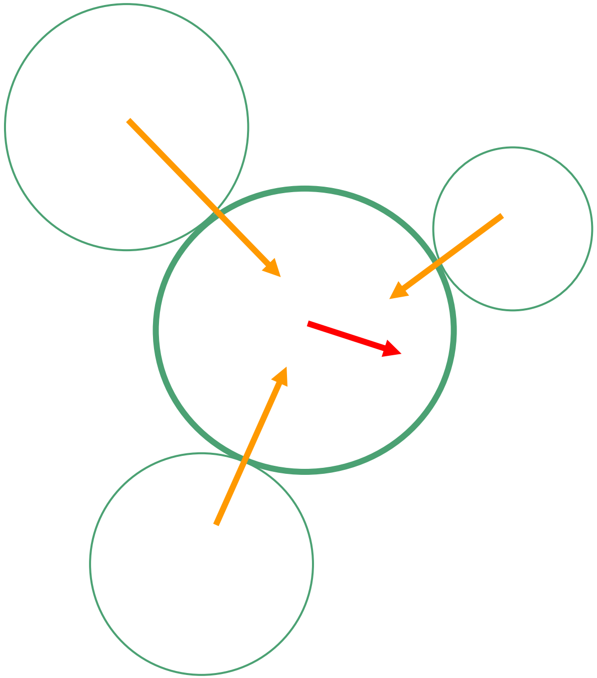
Data from the Brujic Group

Overall Scheme



Objective

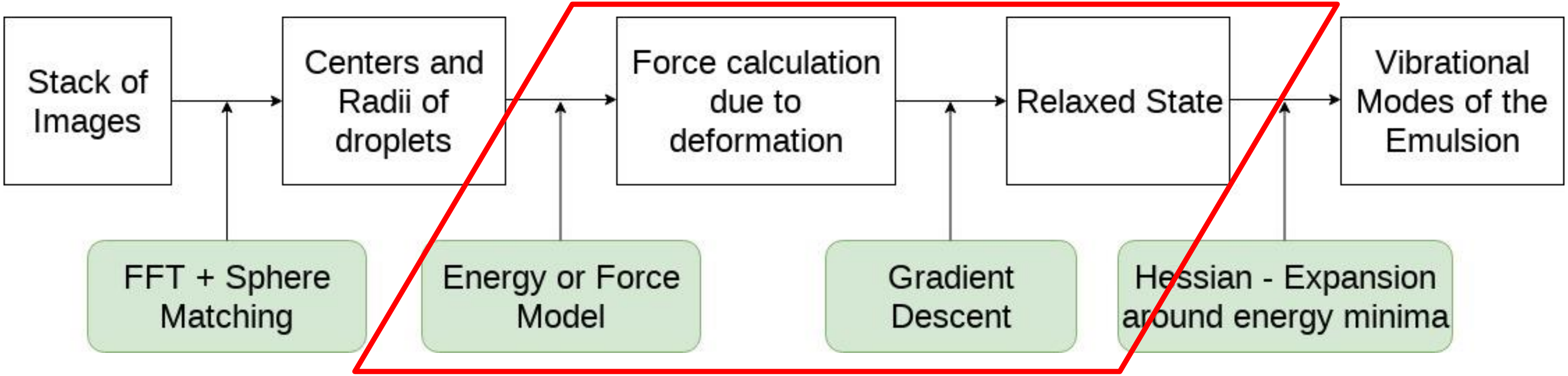
- State 'observed' to be in equilibrium
- Make the force on each droplet equal 0
- Correction by finding new positions / radii



Sources of Error

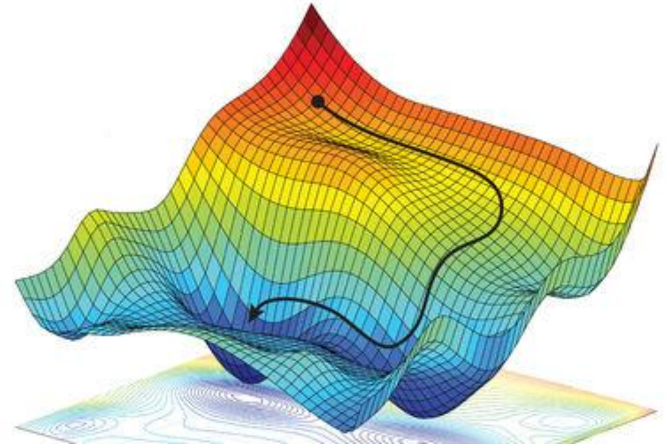
- Experimental
- Calculating center positions and radii
- Force model / Assumptions
- Physical (?)

Overall Scheme



Gradient Descent

- Take steps in the direction of decreasing energy / Force
- Stop at the minimum
- Batch Descent - Simultaneous Update
- Rate $\boldsymbol{\alpha}$



ALEXANDER AMINI, DANIELA RUS. MASSACHUSETTS INSTITUTE OF TECHNOLOGY, ADAPTED BY M. ATAROD/*SCIENCE*

Speeding up the Gradient Descent

Simple Gradient Descent

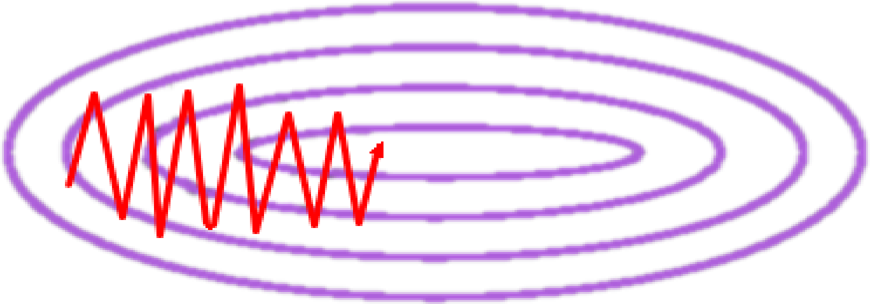
$$\vec{r} = \vec{r} + \alpha \hat{F}$$

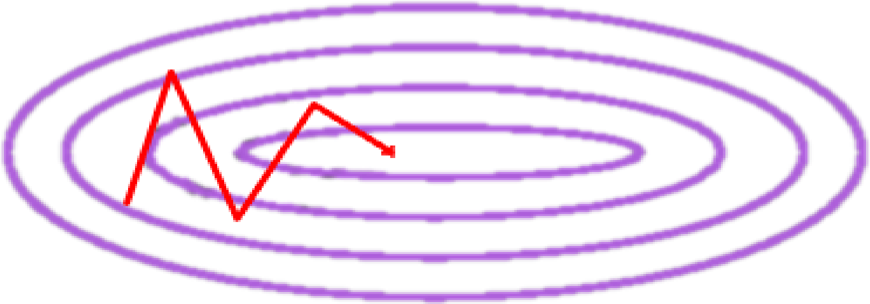
Descent with

Mo

$$\vec{r} = \vec{r} + \alpha \vec{v}$$

$$\vec{v} = \beta \vec{v} + (1 - \beta) \hat{F}$$





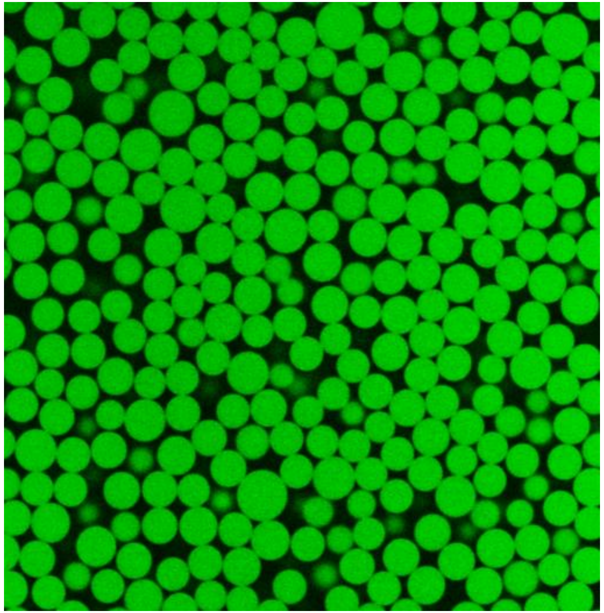
http://dsdeepdive.blogspot.com/2016/03/optimizations-of-gradient-descent.html

Experimental Data

Polydisperse

?

?



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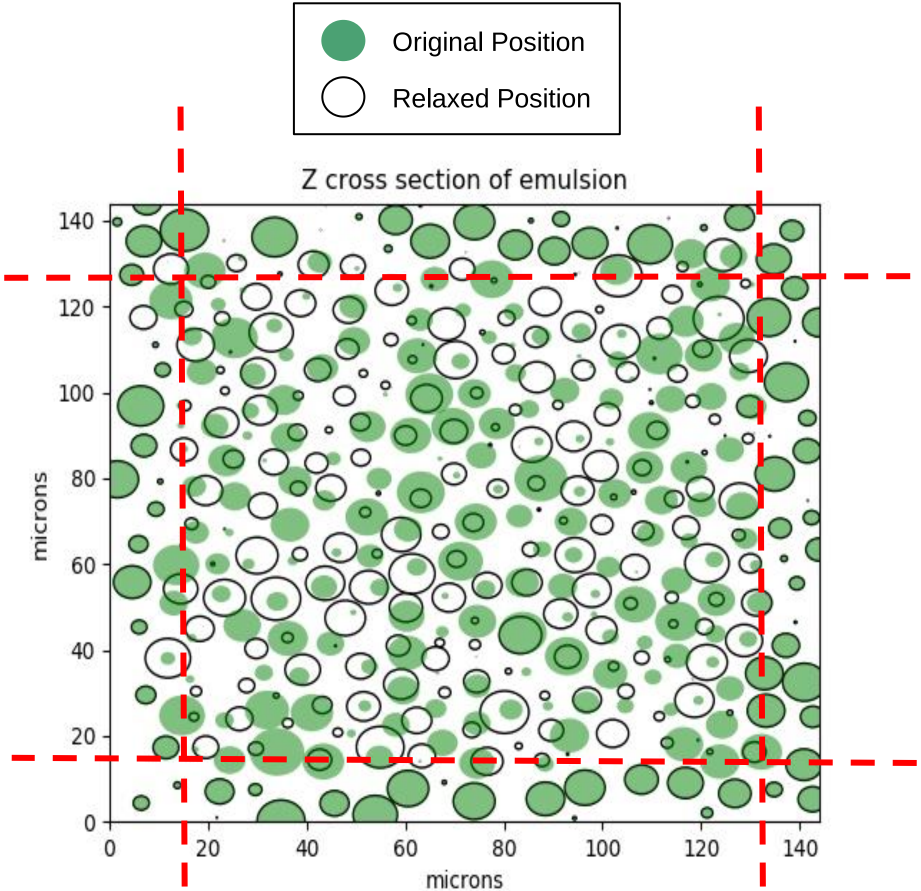
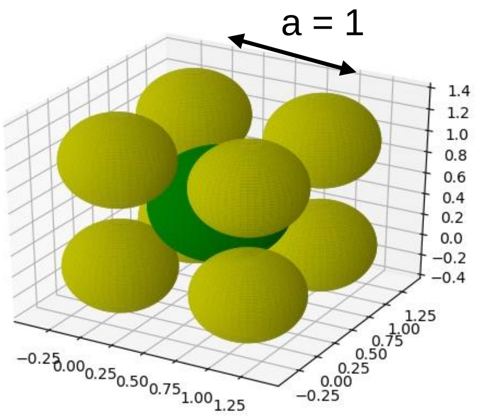


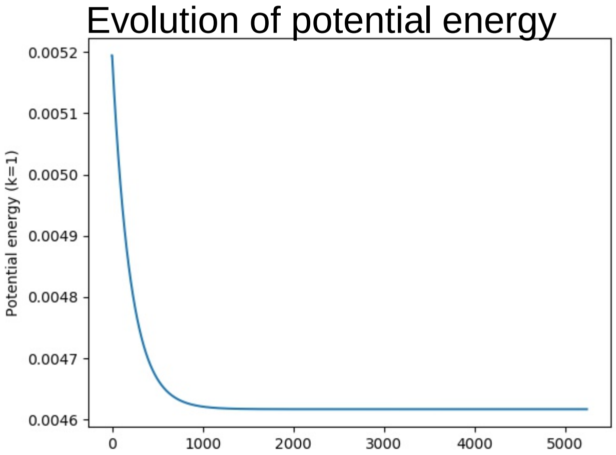
Test Cases / Results

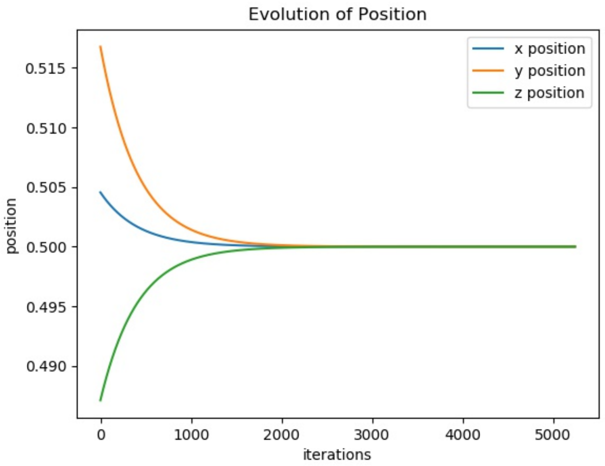
Test 1 : BCC unit cell

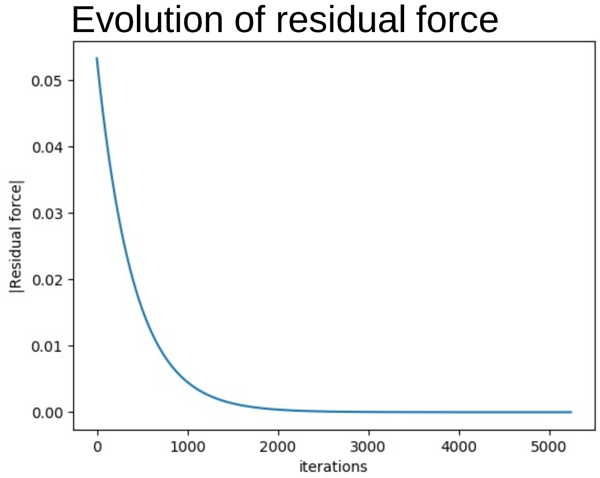
Tested for different radii
Harmonic Potential

Displaced from center
Returns to the center







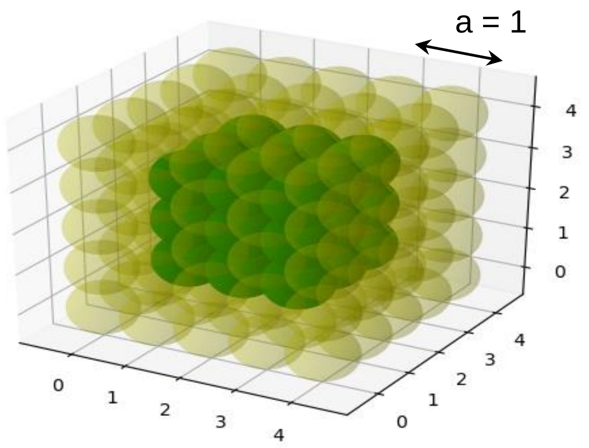


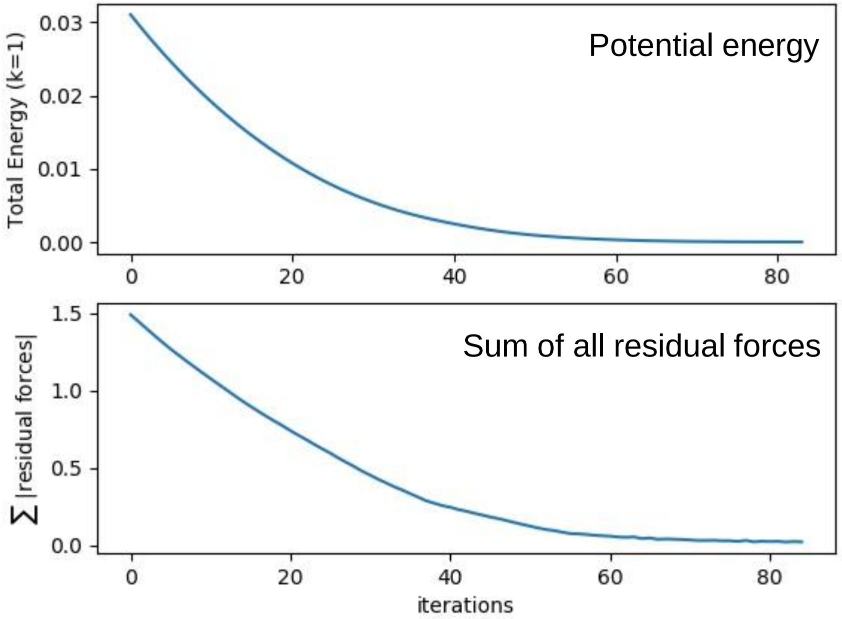
Test 2: 5x5x5 Cubic Lattice

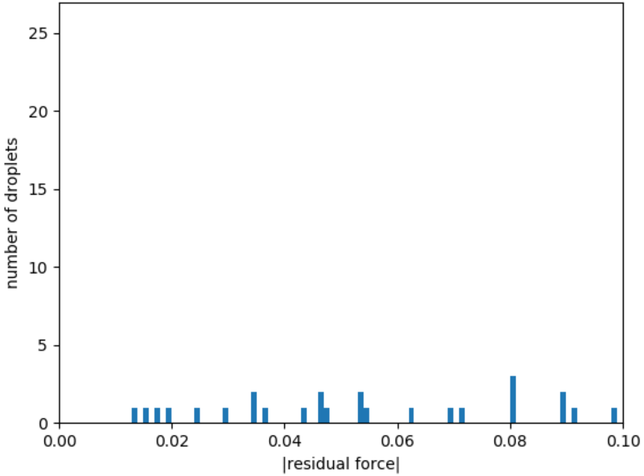
Radii = 0.5*a (just touching)

Harmonic Potential

Displace from lattice points - Relaxation to lattice sites



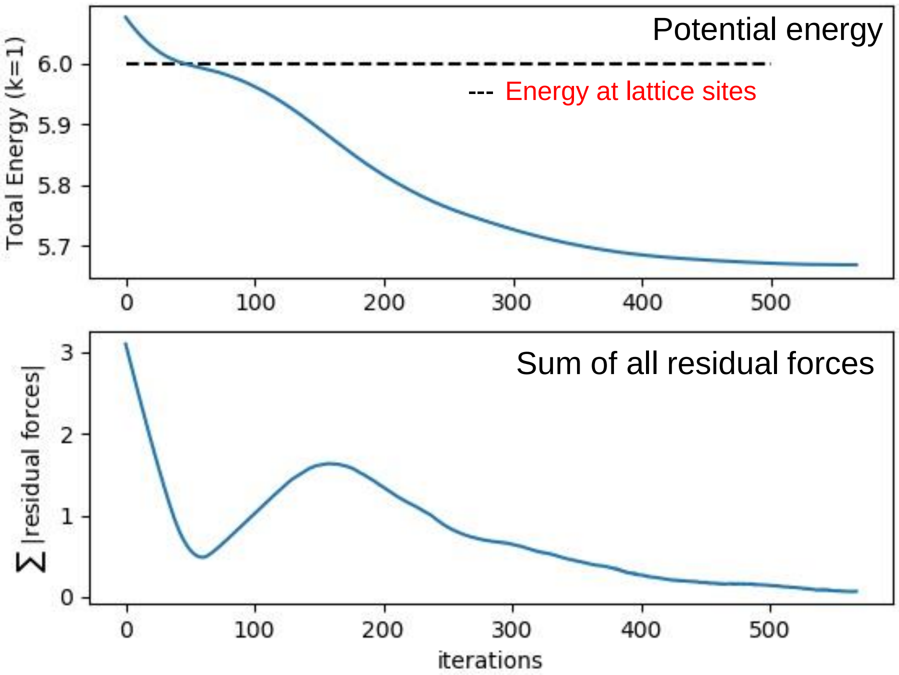


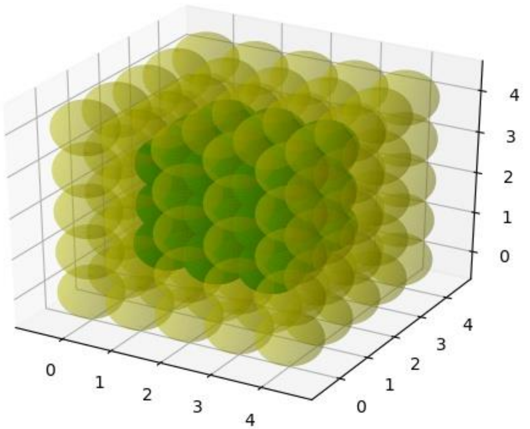


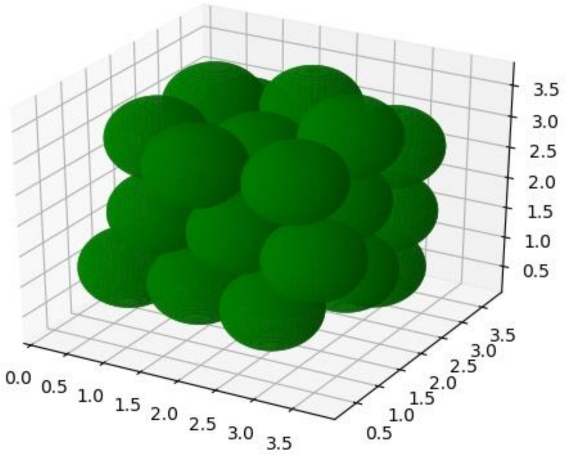
Test 2: 5x5x5 Cubic Lattice

Radii = 0.6*a Harmonic Potential

Start at lattice points - Relaxation NOT to lattice sites!

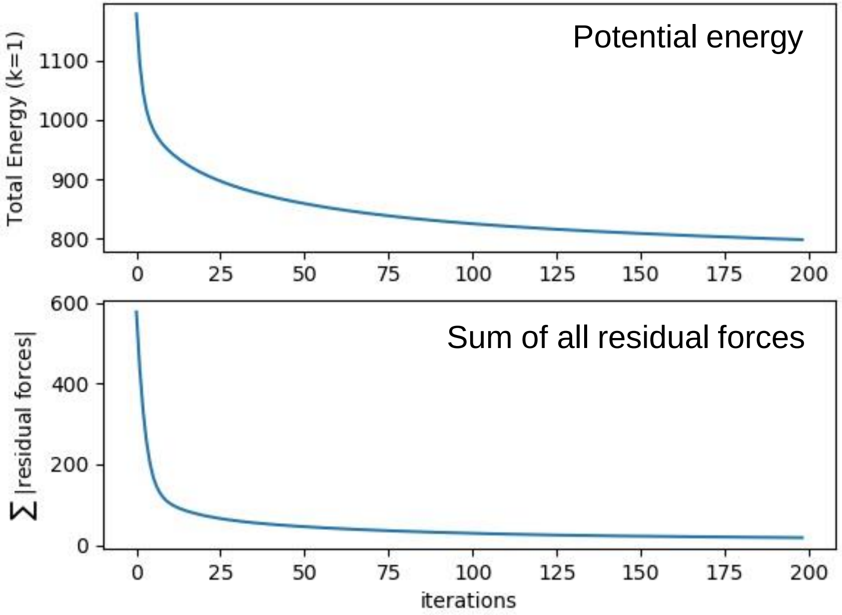


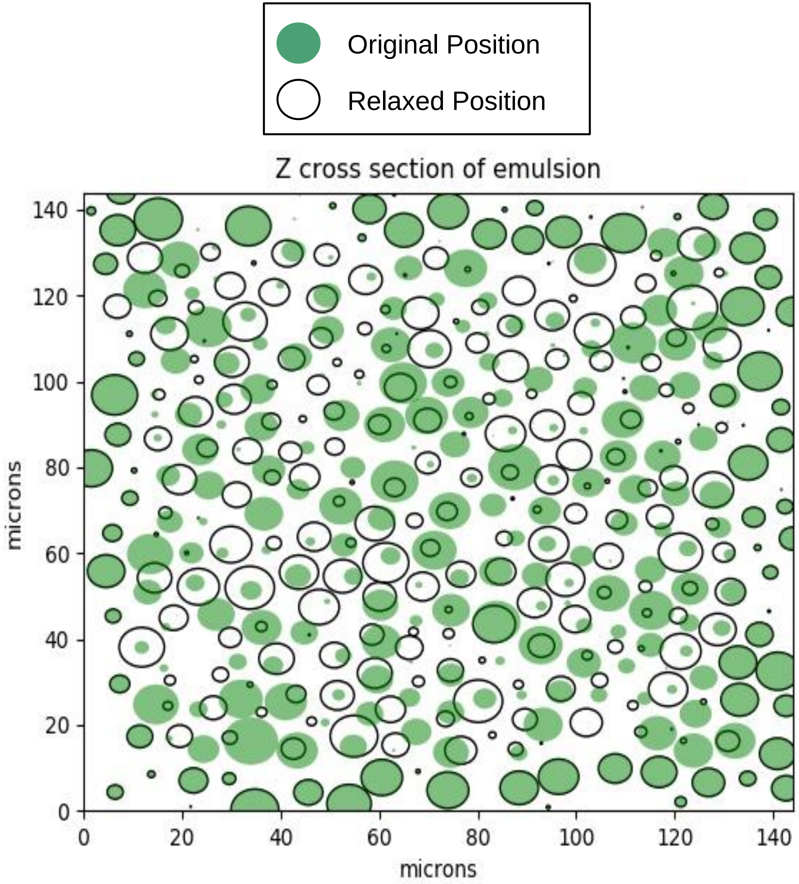




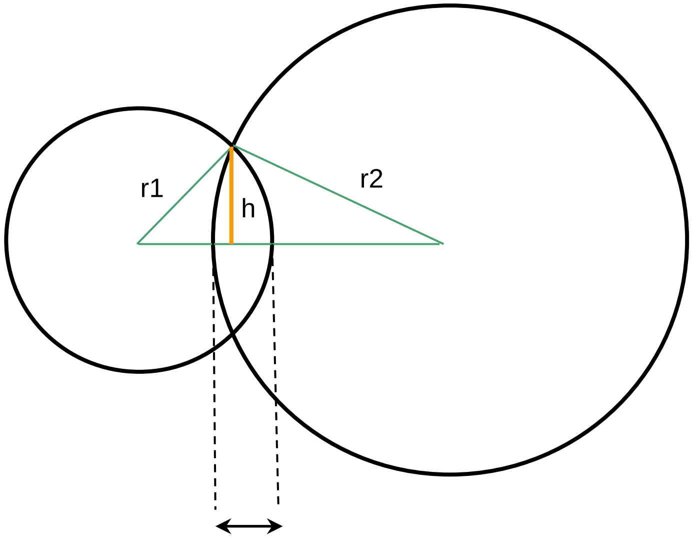
Experimental Data

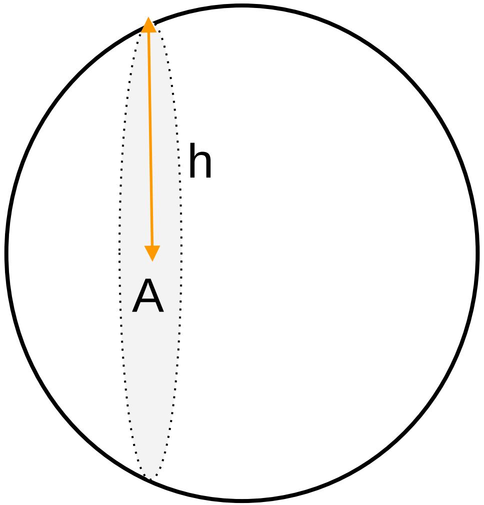
Polydisperse, Harmonic Potential





Area dependent potential: Better approximation



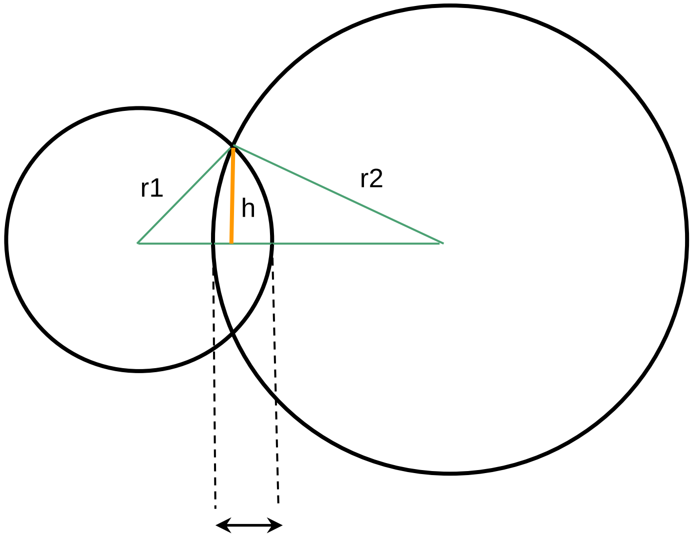


$$f = \frac{\sigma}{\tilde{r}} A$$

$$\tilde{r} = \frac{r_1 r_2}{r_1 + r_2}$$

J. Brujic. Experimental study of stress transmission through particulate matter. Cambridge: University of Cambridge, 2004.

Area dependent potential: Better approximation



$$A = \sqrt{(s)(s-r_1)(s-r_2)(s-(r_1+r_2-x))} = \frac{1}{2}h(r_1+r_2-x)$$

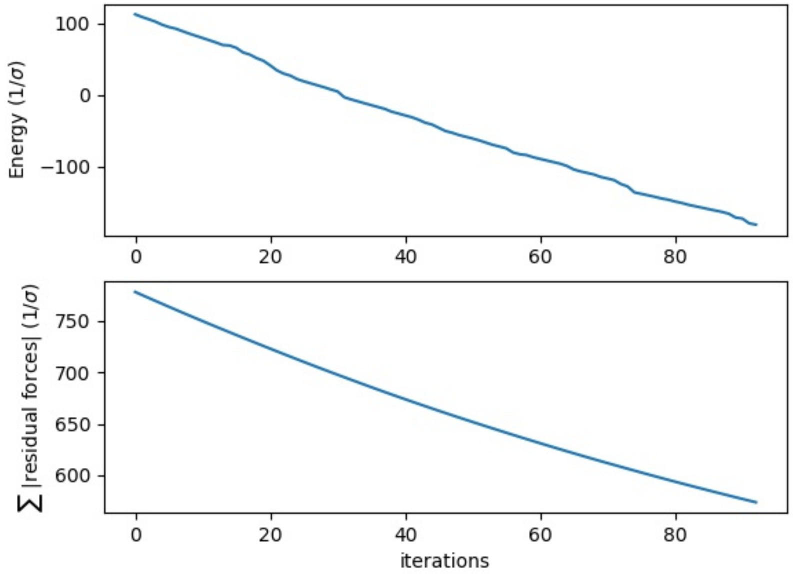
$$\vec{F} = -\frac{\sigma}{\tilde{r}}A\hat{x} = -\sigma\frac{r_1 r_2}{r_1+r_2}\frac{(2(r_1+r_2)-x)(2r_1-x)(2r_2-x)(x)}{4(r_1+r_2-x)^2}$$

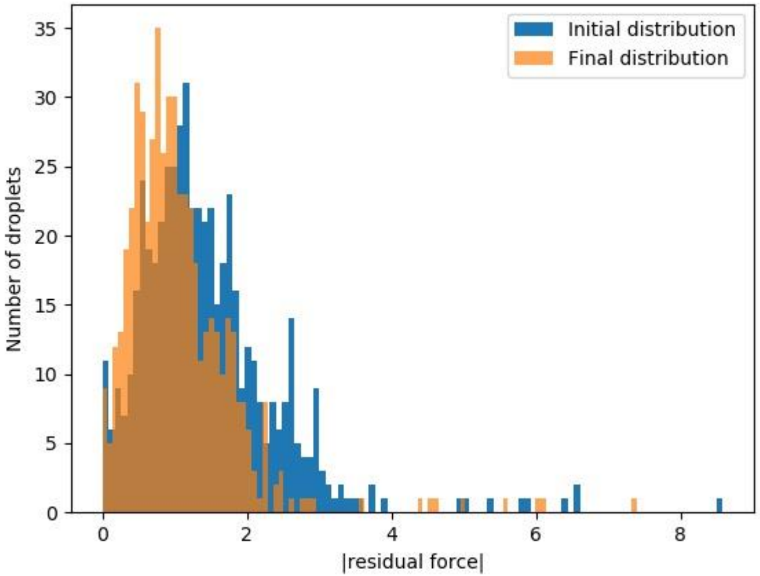
$$U = -\sigma\frac{(r_2+r_1)\left(x^4-4\left(r_2+r_1\right)x^3+12r_1r_2x^2+3\left(r_2-r_1\right)^2\left(r_2+r_1\right)x-3r_2^4+6r_1^2r_2^2-3r_1^4\right)}{12r_1r_2\left(x-r_2-r_1\right)}$$

https://www.integral-calculator.com

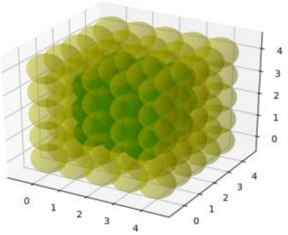
Experimental Data

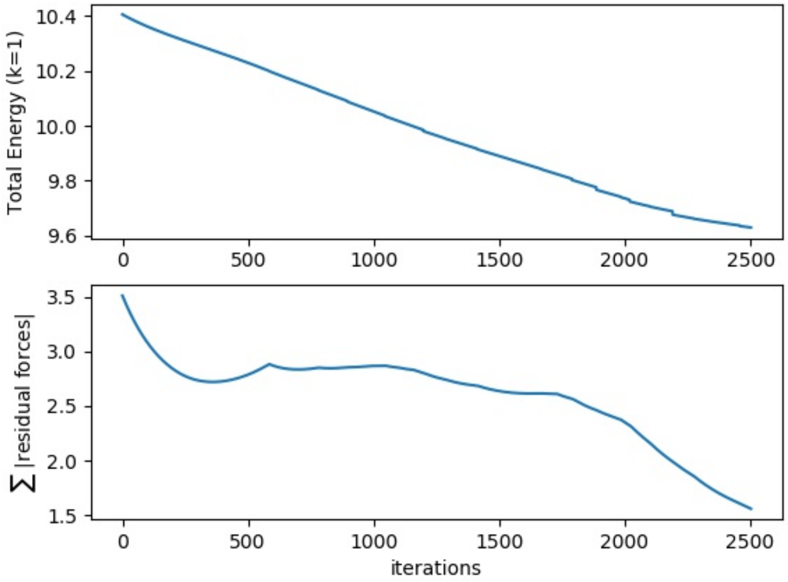
Area dependent potential

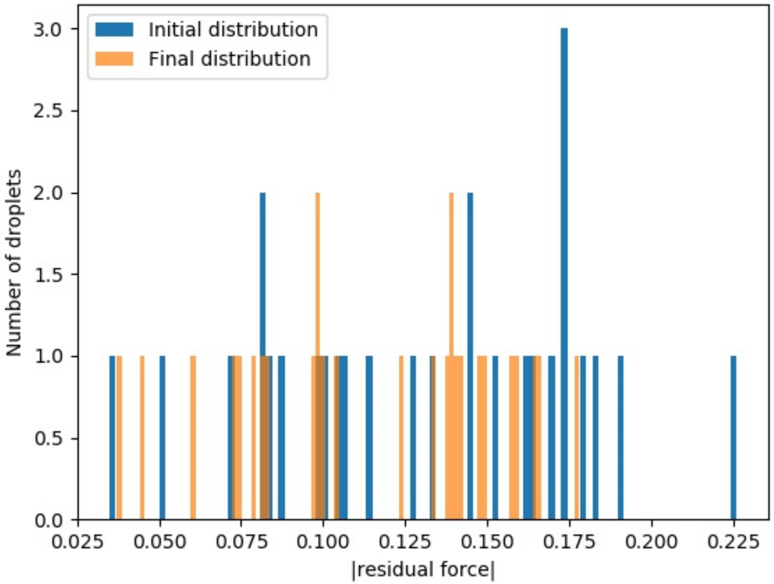




One step simpler: 5x5x5 lattice
Polydisperse, Area dependent potential





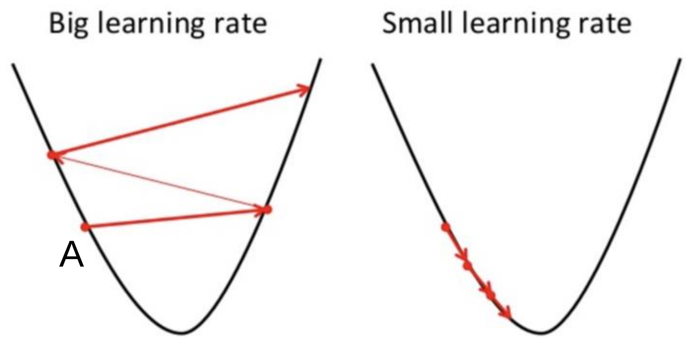


Troubleshooting: Area dependent potential

- Chains of particles, monodisperse✓, polydisperse ✓
- Unit BCC cell, monodisperse✓, polydisperse ✓

- 5x5x5 lattice monodisperse✓
- 5x5x5 lattice polydisperse ✗

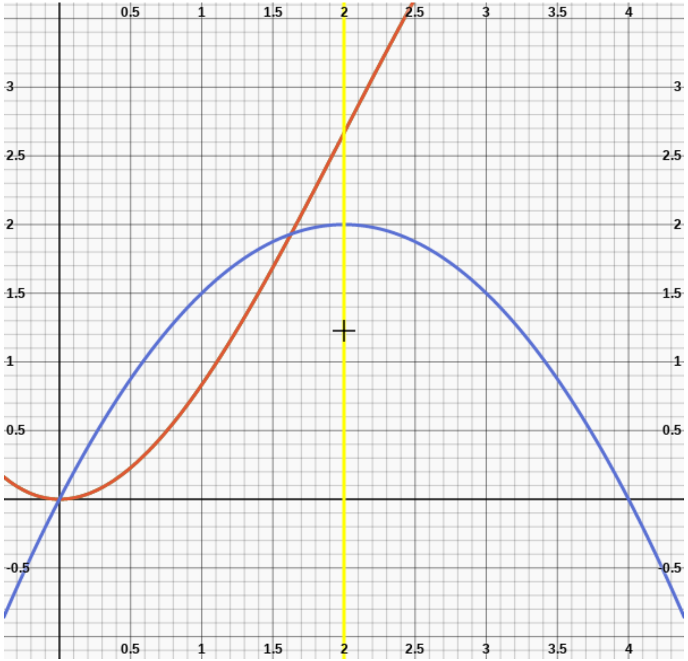
Adaptive Step Size



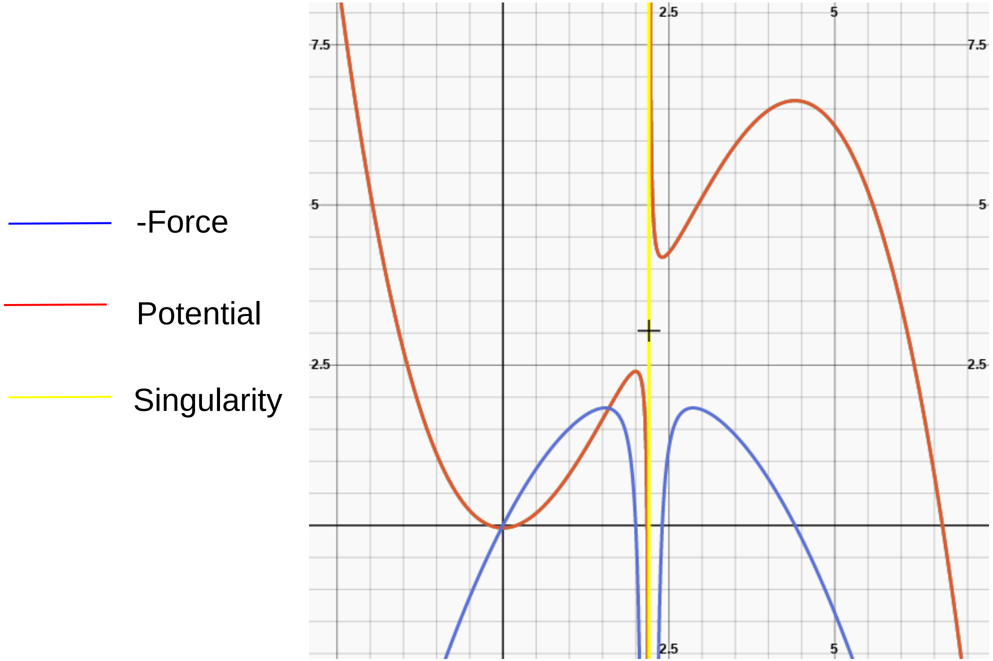
Graph of Potential

$$\vec{F} = -\frac{\sigma}{\tilde{r}} A\hat{x} = -\sigma \frac{r_1 r_2}{r_1 + r_2} \frac{(2(r_1+r_2)-x)(2r_1-x)(2r_2-x)(x)}{4(r_1+r_2-x)^2}$$

$$U = -\sigma \frac{(r_2+r_1)\left(x^4 - 4(r_2+r_1)x^3 + 12r_1r_2x^2 + 3(r_2-r_1)^2(r_2+r_1)x - 3r_2^4 + 6r_1^2r_2^2 - 3r_1^4\right)}{12r_1r_2(x-r_2-r_1)}$$



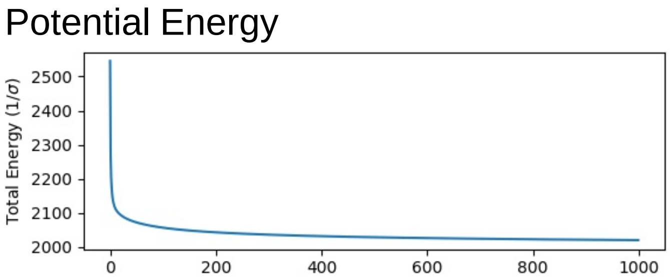
r1 = 1 , r2 = 1, singularity at x= 2



r1 = 1 , r2 = 1.2, singularity at x= 2.2

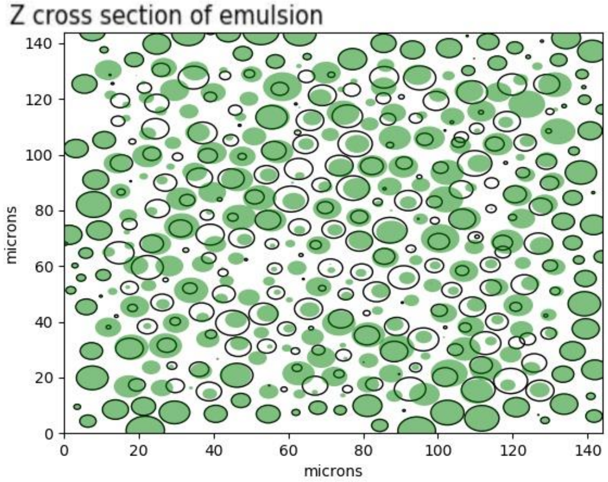
https://www.integral-calculator.com

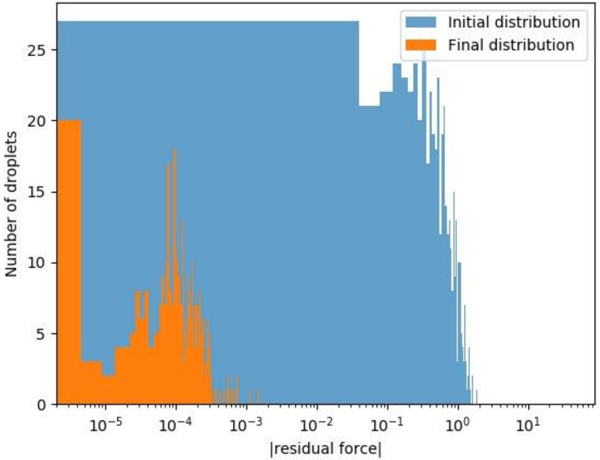
Cubic Potential: Experimental Data



$$U = \frac{1}{3}\sigma x^3$$

$$\vec{F} = -\sigma x^2 \hat{x}$$

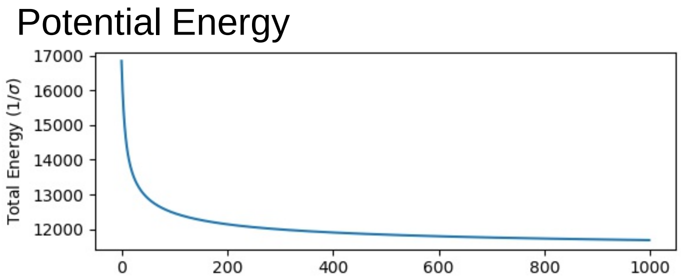




Original Position

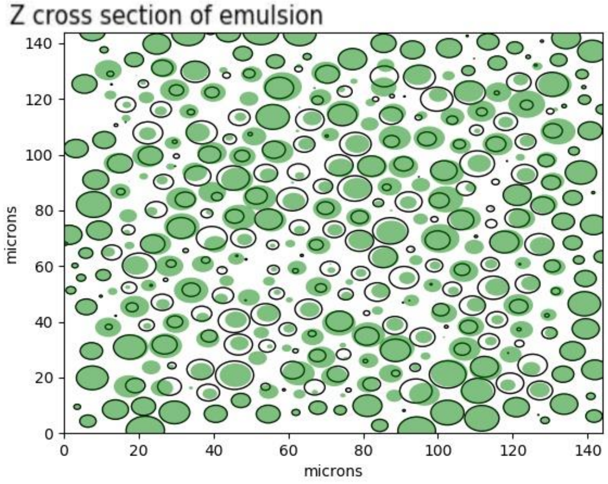
Relaxed Position

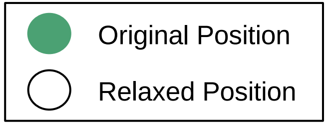
Cubic Potential (Anisotropic): Experimental Data

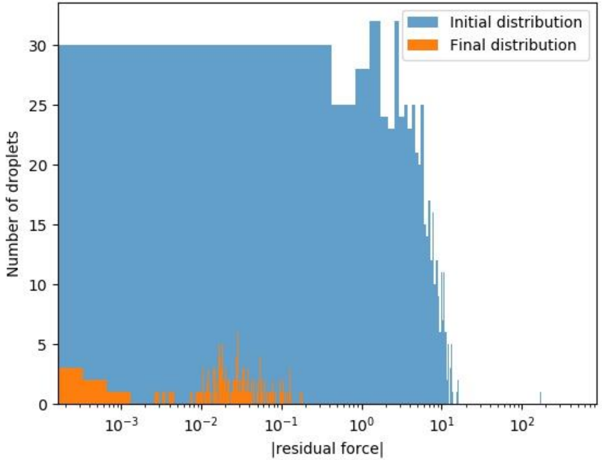


$$U = \frac{1}{3}\sigma \frac{r_1 r_2}{r_1 + r_2} x^3$$

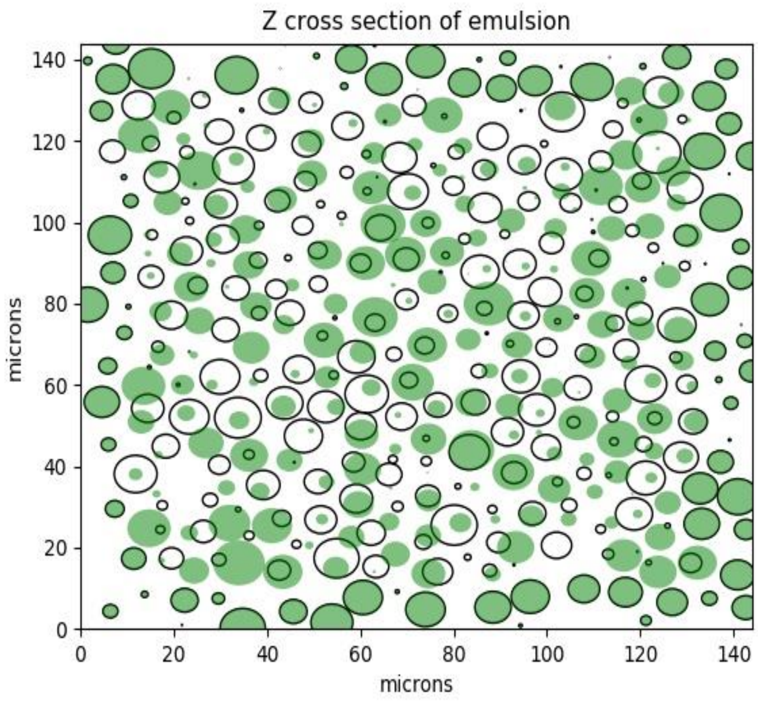
$$F = -\sigma \frac{r_1 r_2}{r_1 + r_2} x^3 \hat{x}$$



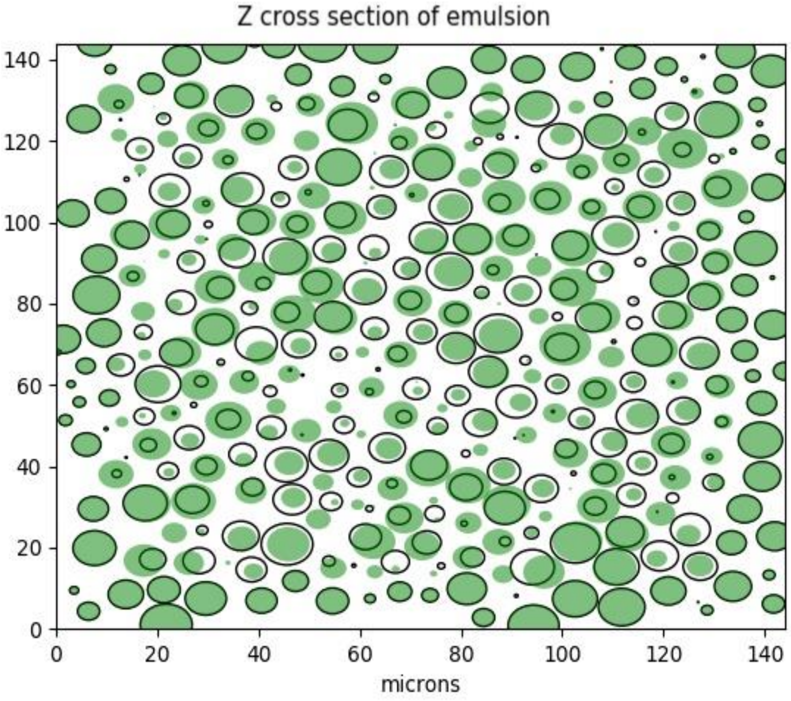




Simple Harmonic Potential



Anisotropic Cubic Potential



Original Position

Relaxed Position

Summary

- Similar potentials work
- Overlaps are small BUT do singularities play a role in the complicated landscape?
- Better Model
- Correcting the radii (simultaneous)

Thank You! Inputs?