Internship Final Report

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List of Parameters

The liggghts input script performs monodisperse particle packing through successive growth of particle radius. The script incrementally increases the particle size, reaching a desired target volume fraction.

The script dumps the snapshots of packings formed at intermediate volume fractions anging from 0.1 to 0.8, at a step of 0.1.

1. Simulation Settings

atom_style	granular	Use of granular particles - specifies the use of specific properties to the particles
boundary	p p p	Periodic boundary conditions in all directions - particles escaping from one end enter from opposite side
newton	off	Interactions calculated per-atom (Recommended for granular particles)
units	si	All quantities are SI Units

2. Packing & Growth Parameters

alphastart	1e-4	Initial Volume Fraction
alphatarget	0.8	Final Volume Fraction
{m1, m2, ..., m8}	{0.1, 0.2, ..., 0.8}	Intermediate volume fractions
growts	50000	Total Timesteps
growevery	variable {10,.. 100}	Frequency of radius adaptation
timestep	1e-7	Timestep size
n	1000	Number of particles
r	2E-6	Initial particle radius
Rgrowrate	$\left(\frac{alphatarget}{alphastart}\right)^{\frac{growevery}{3 \times growts}}$	Growth Multiplier per stage The radius at ith stage is calculated as - $R_i = R_o \times (Rgrowrate)^i$

3. Material Parameters

Young's Modulus	5e6 Pa
Poisson's Ratio	0.45

Density	2500 kg/m³
Coefficient of restitution	Elastic = 1 Inelastic (variable) = {0.1, 0.3, 0.5, 0.7}
Cohesion energy density	3e5 J/m³ (For cohesion in sJKR)
pair_style	`model hertz tangential off` `model hertz tangential off cohesion sjkr`

Governing Equations for Particle Interactions

The main interactions between particles are either **Pure Hertz** & **Simplified-JKR (sJKR)**. The force acts on the particles only when the two are in contact with each other and there are no long range contacts.

1. Pure Hertz

The liggghts command used is -
`pair_style gran model hertz tangential off`

The Hertz Force is given as -
F = Normal Force + Tangential Force
Each force has two components (Overlap + Relative Velocity). Here, no tangential components will be considered but only the normal force interactions which is given as -

$$F = k_n \times \delta n_{ij} - \gamma_n \times vn_{ij}$$

$k_n = \frac{4}{3} Y^* \cdot \sqrt{R^* \cdot \delta_n}$

$\gamma_n = -2\sqrt{\frac{5}{6}} \cdot \beta \sqrt{S_n \cdot m^*}$ where $\beta = \frac{ln(e)}{\sqrt{\{ln(e^2) + \pi^2}}$ where e = coefficient of restitution

Y^* = Effective Young's Modulus
R^* = Effective Particle Radius
δ_n = Overlap $(R_i + R_j - dist)$
vn_{ij} = Normal Component of Relative Velocity
From the expression, we can understand that for elastic collisions, $e = 1$, the velocity term will reduce to 0 and only the normal component will exist

2. sJKR Cohesion Model

The liggghts command used is -
`pair_style gran model hertz tangential off cohesion sjkr`
As installation of Liggghts - JKR failed, we are using the simplified version which adds an additional normal force when particles are in contact, tending to maintain the contact.
The force is defined as where k is an additional material property that was defined in the script -

$$F = k \cdot A$$

k = Cohesion Energy Density
A = Area of Contact
There are two models sJKR & sJKR2 where there is a difference in calculation of area of contact.

sJKR -

$$A = \frac{\pi}{4} \cdot \frac{((d-r_i-r_j)\cdot(d+r_i-r_j)\cdot(d-r_i+r_j)\cdot(d+r_i+r_j)}{d^2}$$

The contact radius is calculated geometrically giving the above area. Link to derivation

sJKR2 -
More simplified area of contact is used here

$$A = 2 \cdot \pi \cdot \delta_n (2 \cdot R^*)$$

Where δ_n is the overlap and R^* is the effective radius

1. Motion of Particles

Once the net force on a particle is calculated, the motion of the particle is governed by Newton's Second Law of Motion.

$$F_{net} = m \cdot a$$

$$F_{net} = m \cdot \frac{d^2x}{dt^2}$$

m = mass of particle
a = acceleration of particle
As no tangential forces are present, there is no rotation as applied torque is zero.

The parameters used with the new packing generated

The packing are generated for the following set parameters -

- Number of Particles = 1000
- Initial Volume Fraction = 1e-4
- Initial Radius = 2e-6
- Final Volume Fraction = 0.8

The radius growth takes place at an interval of 0.1 volume fraction after which the particle snapshot is dumped. So while generating the packings for 0.8, we get the packings for intermediate fractions as well

- Time Step Size = 1e-7
- Total Time Steps = 50000

Starting with keeping the cohesion elastic (No Normal force due to relative velocity). The simulations are performed by varying the coefficient of restitution as {0.1, 0.3, 0.5, 0.7}.

Grow Every	Number of Operations	RGrowRate	% Growth at every step
10	5000	1.000599326	0.05993259788
25	2000	1.001498988	0.1498988499
40	1250	1.00239946	0.2399459926
50	1000	1.003000224	0.3000223964
80	625	1.004804677	0.480467726
100	500	1.006009449	0.6009449271

The packings can be generated for the desired % growth at every step that have specific frequency of growth rate given by growevery

How the parameters RDF & Q6 are calculated and variations in the packings

1. Radial Distribution Function

The RDF, g(r) helps quantify variation of number of particles with distance in the packing which is calculated as -

$$g(r) = \frac{dn_r}{4 \cdot \pi \cdot r^2 \cdot dr \cdot \rho}$$

dn_r = Number of Particles in the shell

r = Distance

dr = Shell Thickness

ρ = Bulk Density (Number of particles over volume)

The pairwise distance between particles is calculated and binned into radial shells using histogram which gives us the number of particles present at the particular distance. The expected number is calculated using the bulk density.

```
counts, _ = np.histogram(distances, bins=r_bins)
```

```
shell_volumes = 4 * np.pi * r_centers**2 * dr ideal_counts = density *
shell_volumes * num_particles / 2
g_r = counts / ideal_counts
```

After obtaining the RDF g(r), we can calculate the Coordination Number as -

$$CN = 4 \cdot \pi \cdot \int_0^{r_c} r^2 \cdot g(r)\, dr$$

Other parameter obtained from the RDF plot are

- Maximum g(r) Peak
- r/d at the peak
- Minimum g(r)
- r/d at the peak

2. Q6

The bond orientation parameter Q6 is a measure that quantifies the symmetry in the arrangement of neighboring particles around a central particle. It helps distinguish between random and ordered (crystalline) structure.
Spherical Harmonics are used to understand this symmetry. The spherical harmonic function is Y_{6m} of degree 6 & the order m varies from -6 to +6. So, 13 q_{6m} are calculated.

For i^{th} central particle having j surrounding particles,

$$q6_m(i) = \frac{1}{N_b(i)} \sum_{j=1}^{N_b(i)} Y_{6m}(\theta_{ij}, \phi_{ij})$$

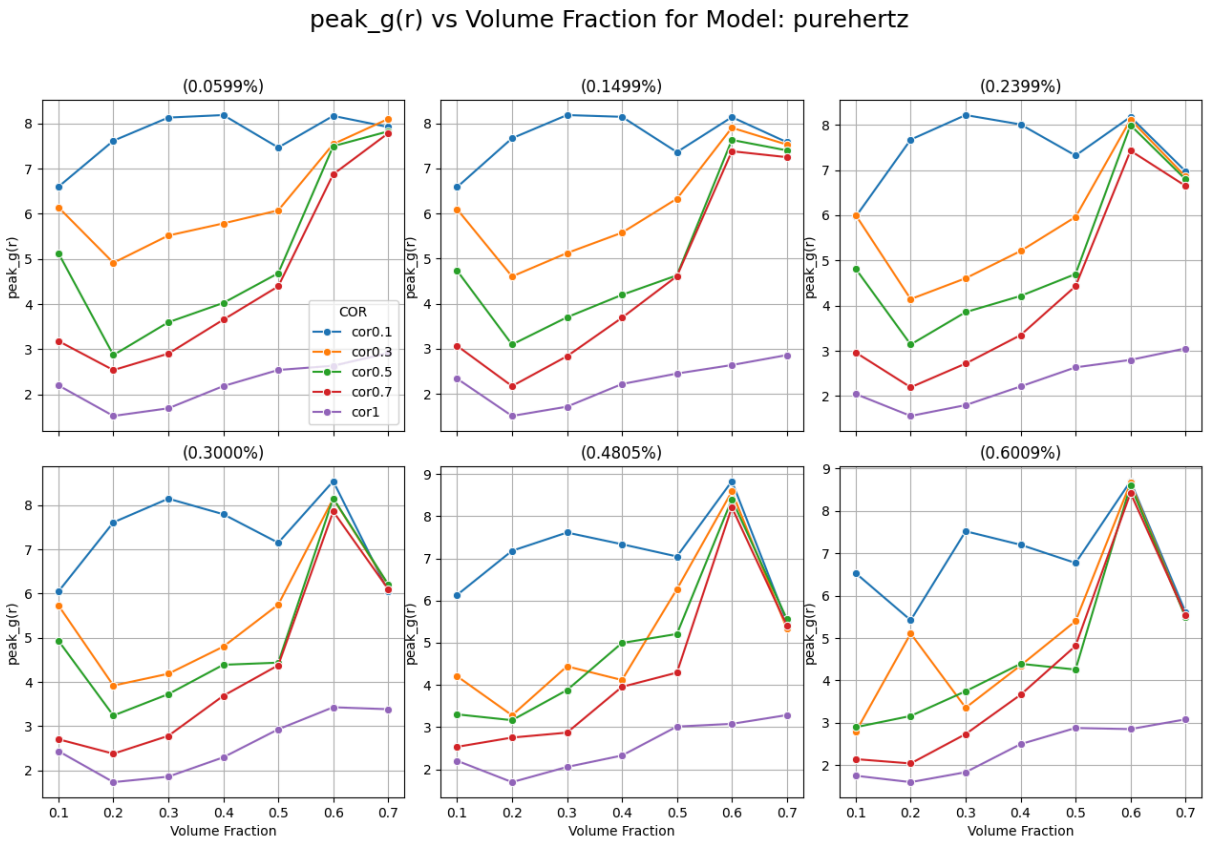
$$Q_6(i) = \sqrt{\frac{4 \cdot \pi}{3} \sum_{m=-6}^{m=+6} |q_{6m}(i)|^2}$$

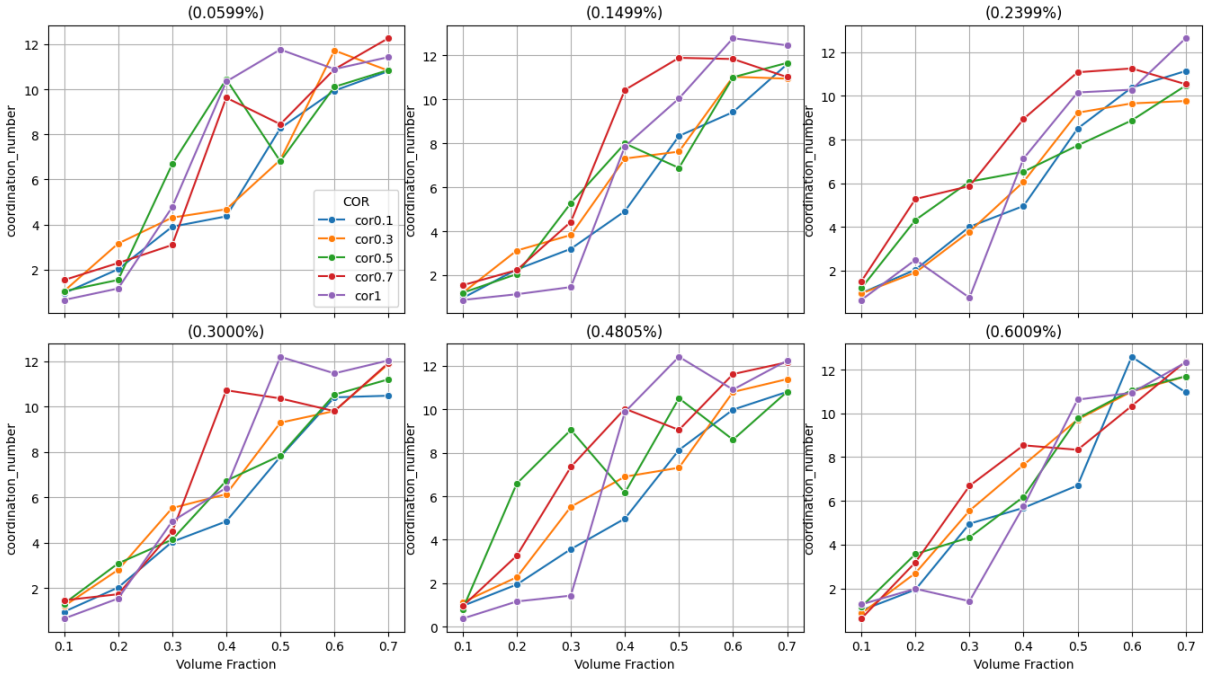
FCC (Crystalline Structure)	0.574
Random Packing	0 to 0.2
Partly Ordered	In between

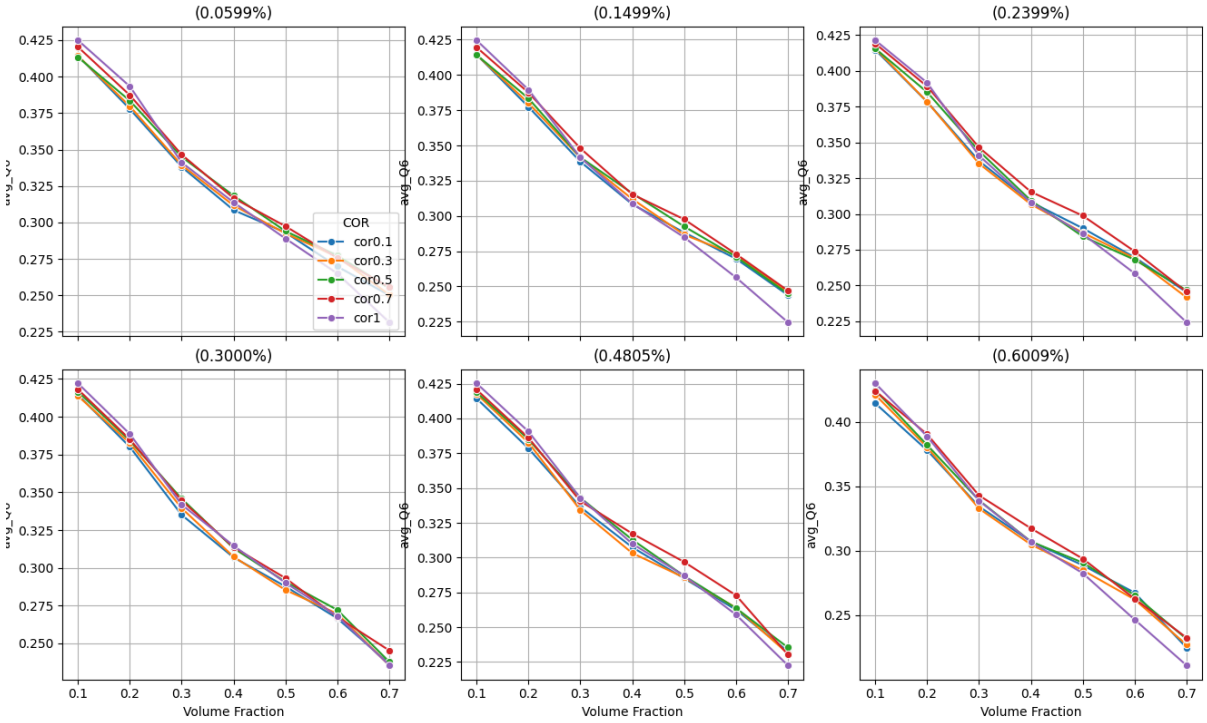
In the post processing, the spherical harmonic library in python is used -

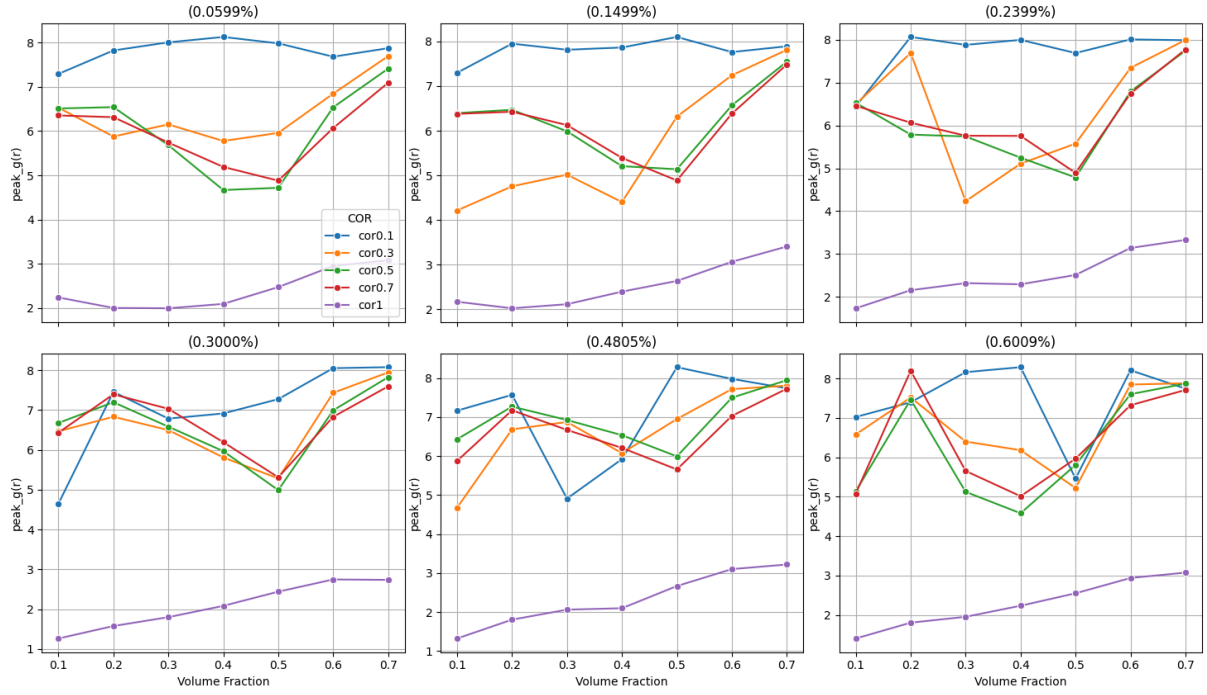
```
from scipy.special import sph_harm
```

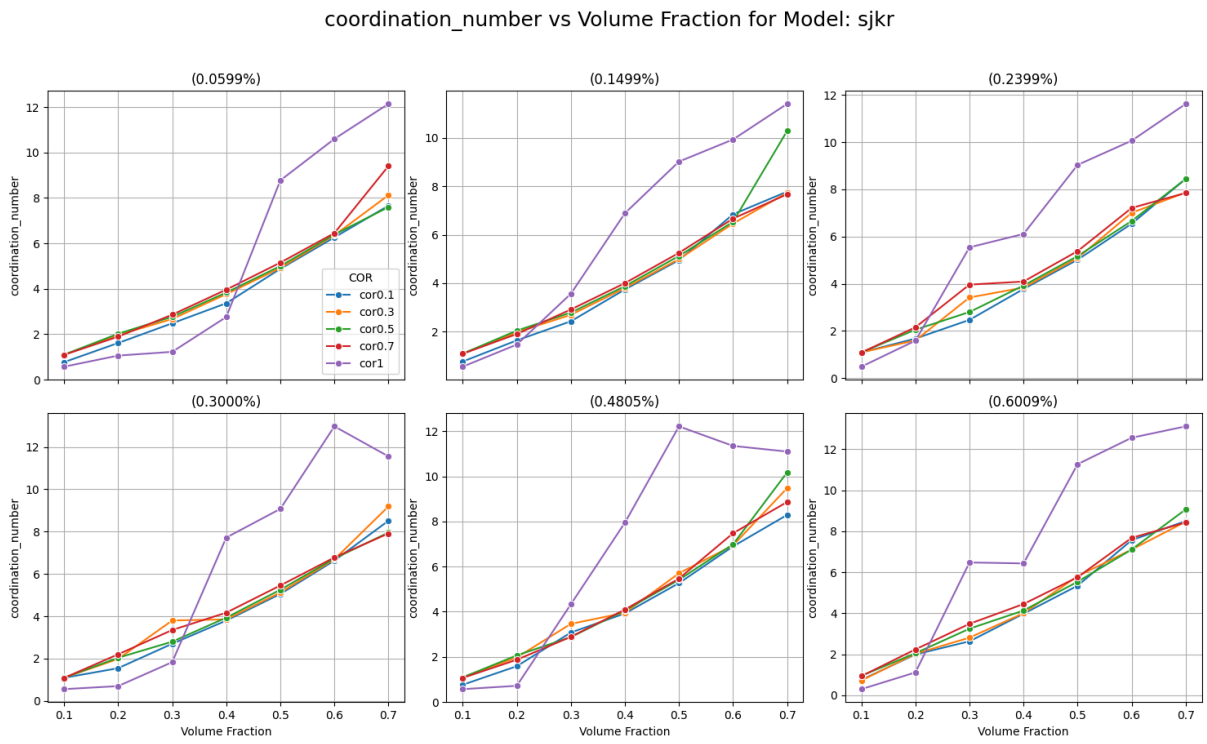
3. Plots

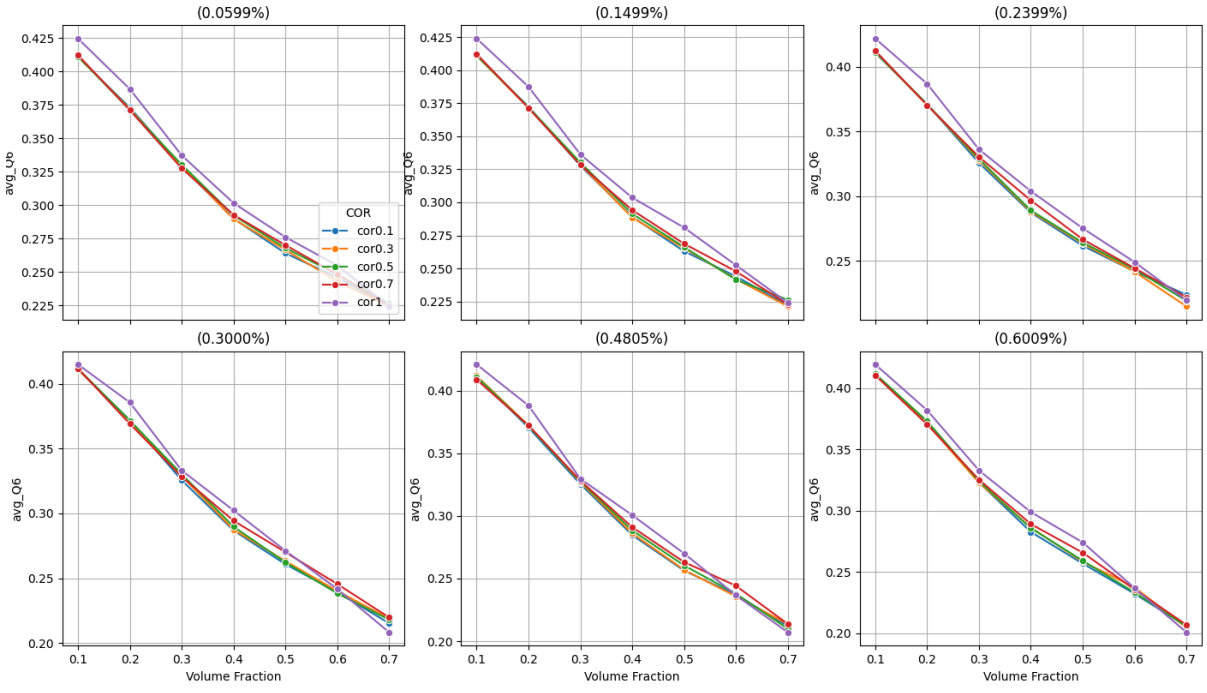

peak_g(r) vs Volume Fraction for Model: purehertz
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
peak_g(r)
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1


coordination_number vs Volume Fraction for Model: purehertz
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
coordination_number
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1


avg_Q6 vs Volume Fraction for Model: purehertz
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
avg_Q6
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1


peak_g(r) vs Volume Fraction for Model: sjkr
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
peak_g(r)
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1


coordination_number vs Volume Fraction for Model: sjkr
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
coordination_number
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1


avg_Q6 vs Volume Fraction for Model: sjkr
(0.0599%)
(0.1499%)
(0.2399%)
(0.3000%)
(0.4805%)
(0.6009%)
avg_Q6
Volume Fraction
COR
cor0.1
cor0.3
cor0.5
cor0.7
cor1

Important Links

1. Link to the SpreadSheet having the Parameter Data
2. LIGGGHTS Script for Pure Hertz Model
3. LIGGGHTS Script for sJKR model
4. Python Post Processing Code Scripts