

(a) Microstructural Evolution Tool
(Written in Python)

R1 ($\bar{\eta}$, μ , σ), R2 ($\bar{\eta}$, μ , σ), R3 ($\bar{\eta}$, μ , σ)
 R1 ($\bar{\eta}$, λ , σ), R2 ($\bar{\eta}$, λ , σ), R3 ($\bar{\eta}$, λ , σ)
 R1 (η , r , σ)

Large Data (≈ 10 TB)
 (Data compressed to hdf5 format)

1. ϵ_a , ϵ_v
2. $(x_j, y_j, z_j) - (x_i, y_i, z_i) \rightarrow \Delta$
3. \bar{C}

Generating Interpolated Data and Statistical Operations

1. Defining interpolation functions
2. Calculating instantaneous displacement
3. Obtaining microstructure evolution parameters

Plotting Functions

1. Plotting instantaneous displacement
2. Plotting mean number of contacts
3. Plotting zero or non-zero contacts

(b) Microstructure Evolution Parameters
(For Interpolated Data)

Parameters (\bar{C} , $\bar{C}(\sigma)$, $A_{ij}(\bar{C}(\sigma)$, c_n , \hat{C} , $\bar{n}(u)$)

- (1) \bar{C} or $\bar{C}(\sigma)$ or $A_{ij}(\bar{C}(\sigma) \rightarrow$ Based on mean number of contacts per particle
- (2) $c_n \rightarrow$ Number of particles with n contacts
- (3) \hat{C} or $\hat{C}(\sigma) \rightarrow$ Based on normalized standard deviation of \bar{C} over entire ϵ_a
- (4) $\bar{n}(u) \rightarrow$ Average number of particles with $\Delta > u$

- (1)-(2) Measure extent of similarity of microstructures
- (3)-(4) Measure extent of particle participation

Four Types of Plots

1. \bar{C} , $\bar{C}(\sigma)$, $A_{ij}(\bar{C}(\sigma)$ vs. ϵ_a
2. c_n vs. ϵ_a
3. \hat{C} , $\hat{C}(\sigma)$ vs. ϵ_a
4. $\bar{n}(u)$ vs. u

Various plots

