Impact of Particle Roughness on Packing

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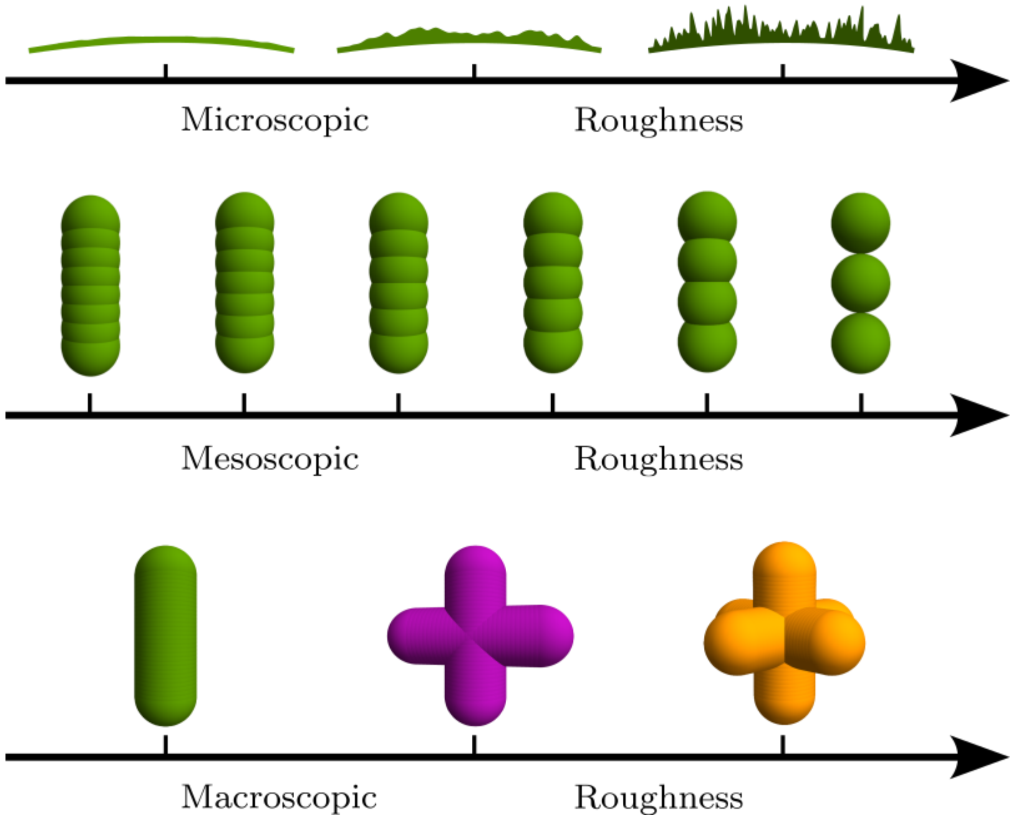
10 March 2026, DPG Dresden 2026



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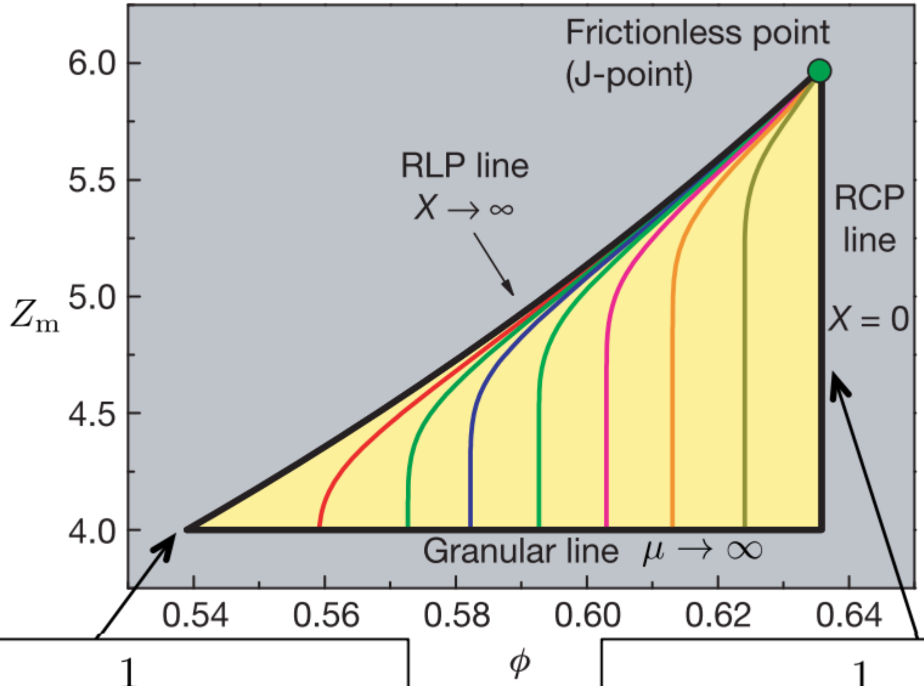
Historical context

- Z_m: Number of contacts
- X : Compactivity (large X ~ loose configuration)
- μ : Friction coefficient



$$\phi_{rlp} = \frac{1}{1+\sqrt{3}/2} \approx 0.536$$

$$\phi_{rcp} = \frac{1}{1+\sqrt{3}/3} \approx 0.634$$

Baule, A. et al. (2018). Edwards statistical mechanics for jammed granular matter. Reviews of Modern Physics

- Friction affects packing fraction
  - RLP : high friction
  - RCP : low friction

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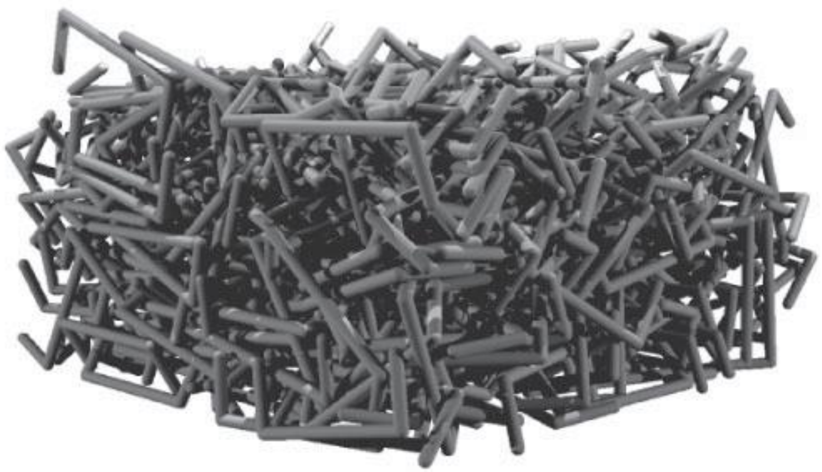
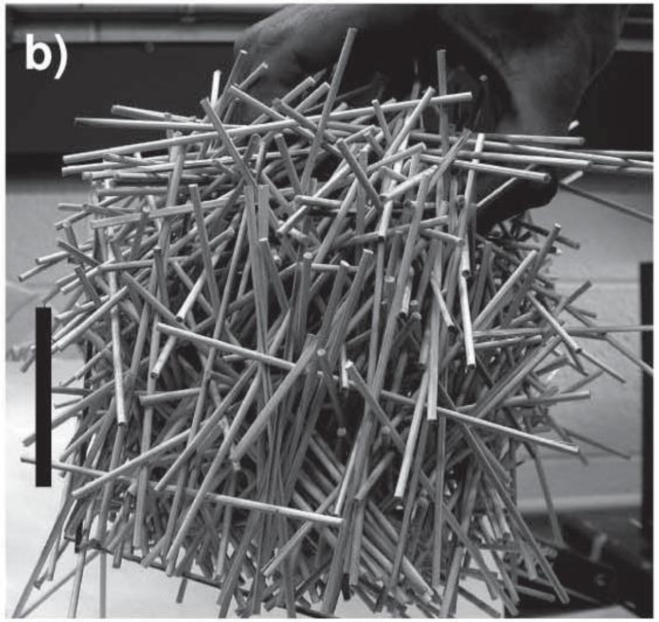
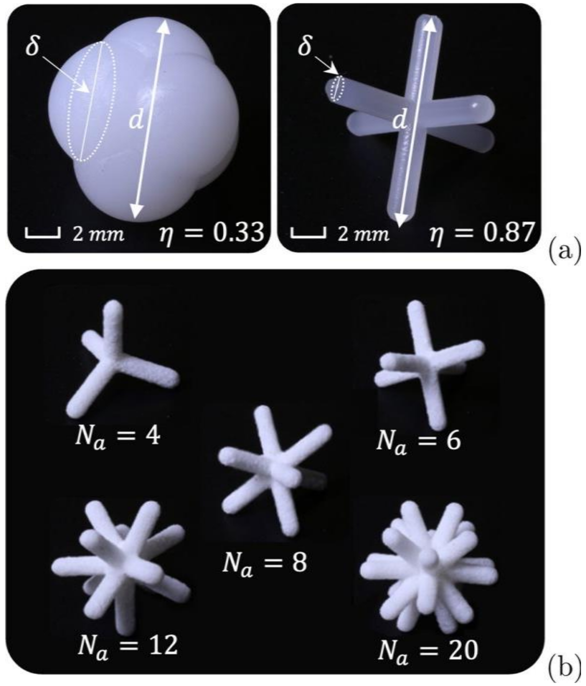
Historical context



Gravish, N. et al. (2012). Entangled Granular Media. Physical Review Letters



Blouwolff, J. et al. (2006). The coordination number of granular cylinders. Europhysics Letters



Aponte, D. et al. (2025). Experimental exploration of geometric cohesion and solid fraction in columns of highly non-convex Platonic polypods. Granular Matter

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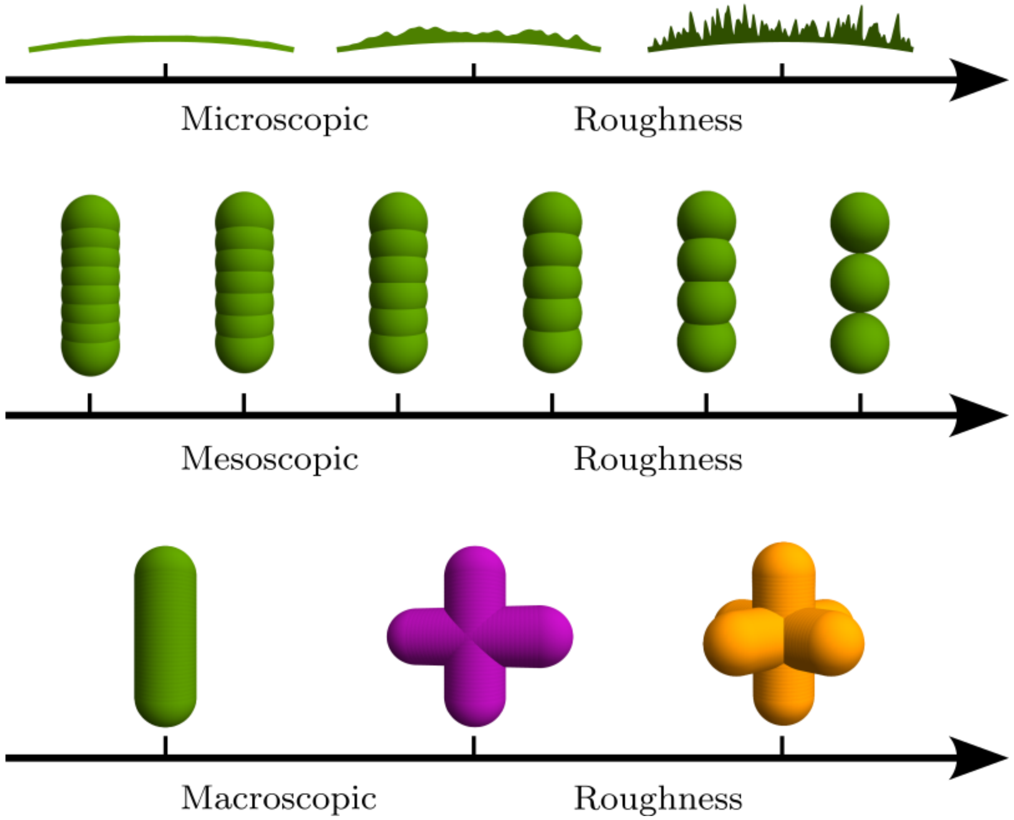
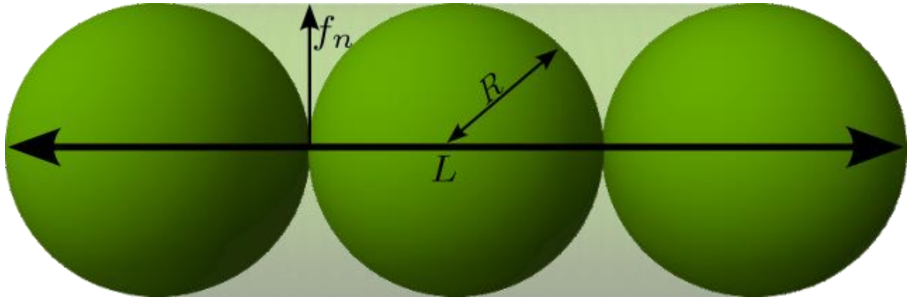
Roughness



Simple parameter

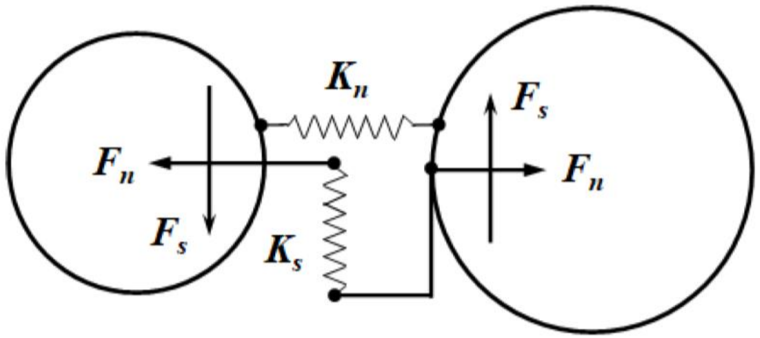


$$\mu_{\mathrm{meso}} = 1 - \frac{f_n}{R}$$

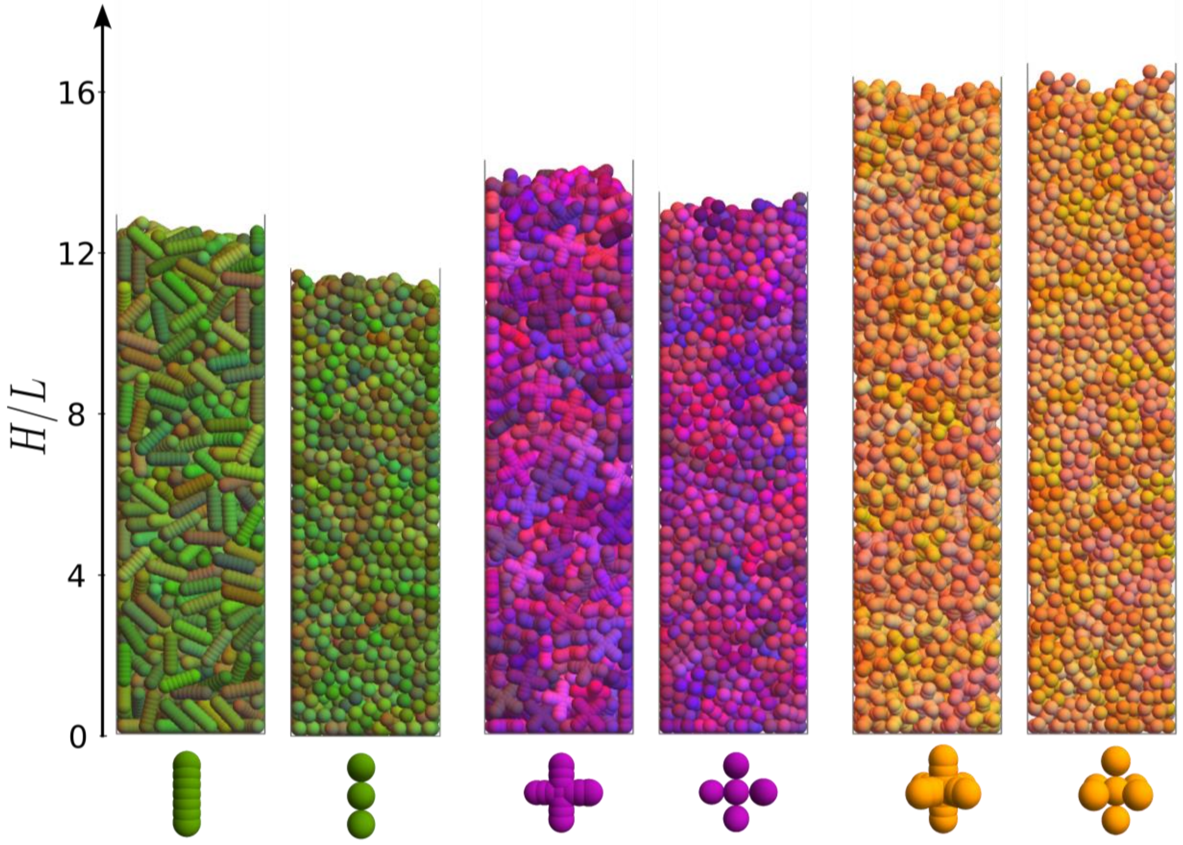
Discrete Element Modeling

- Random placing
- Gravity deposition
- Hertzian contact

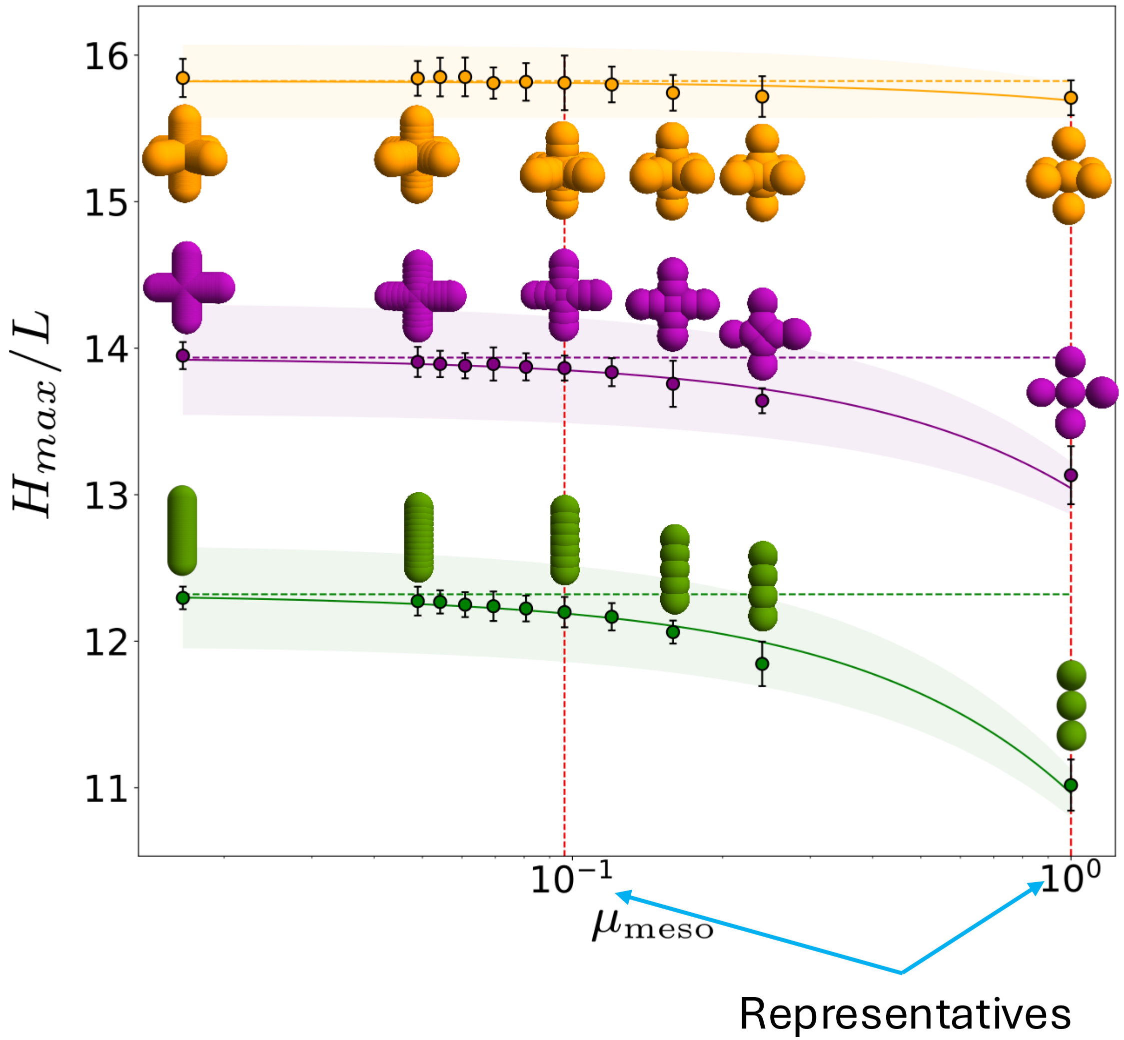
Contact Model



Zhu, R., Gao, H., Zhan, Y., & Wu, Z.-X. (2022). Construction of Discrete Element Constitutive Relationship and Simulation of Fracture Performance of Quasi-Brittle Materials. Materials



Maximum Height



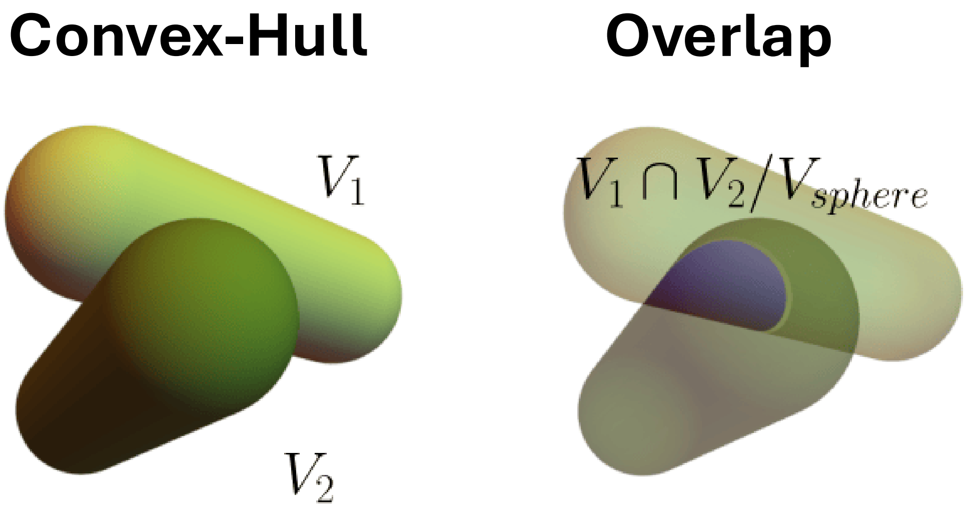
Model

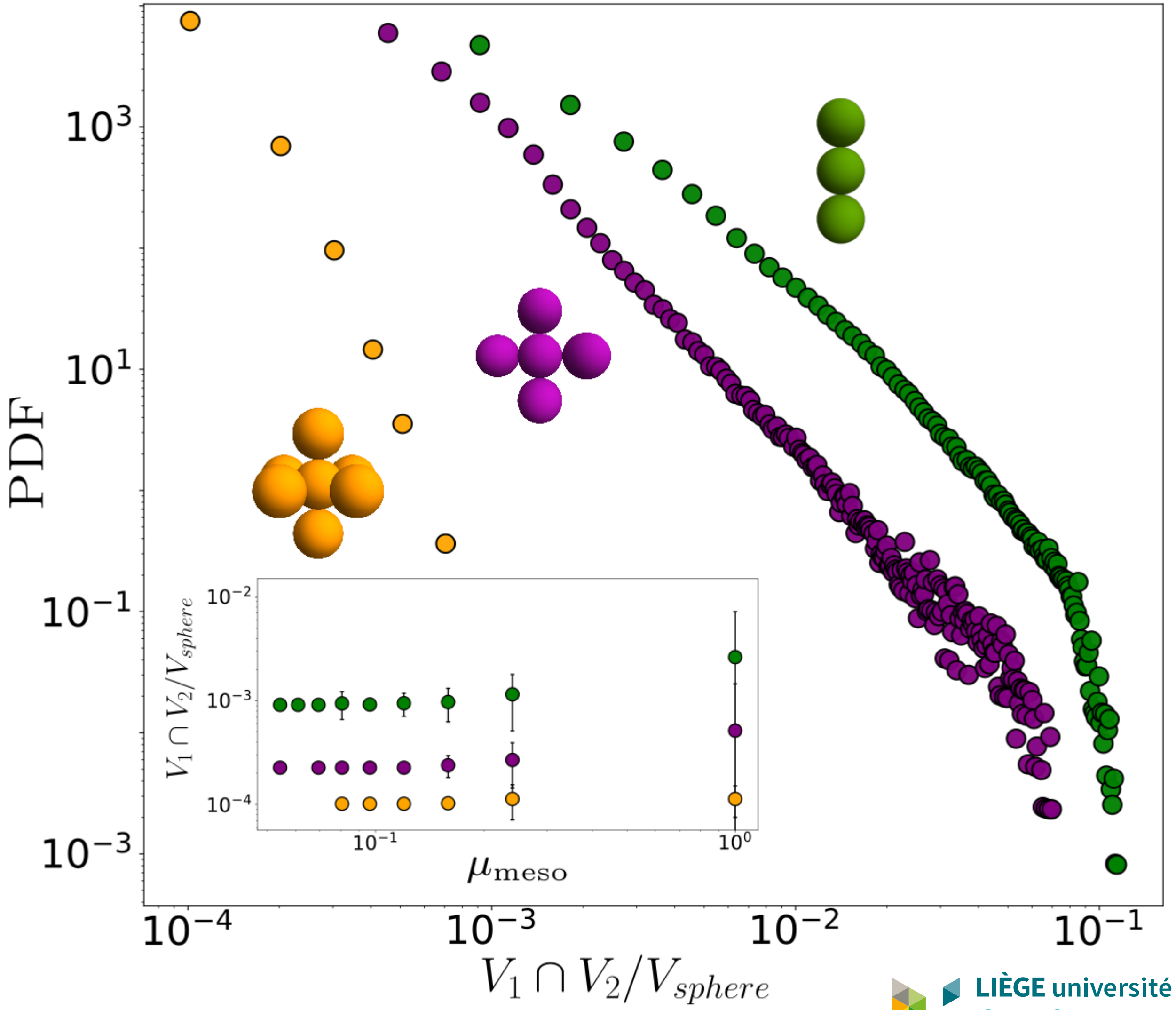
$$H_{max}(n) = H_1 + H_\Delta(1 - \mu_{meso})$$

New parameter

$$\mu_{macro} = 1 - \frac{H_\Delta}{H_1}$$

Convex-Hull Overlap





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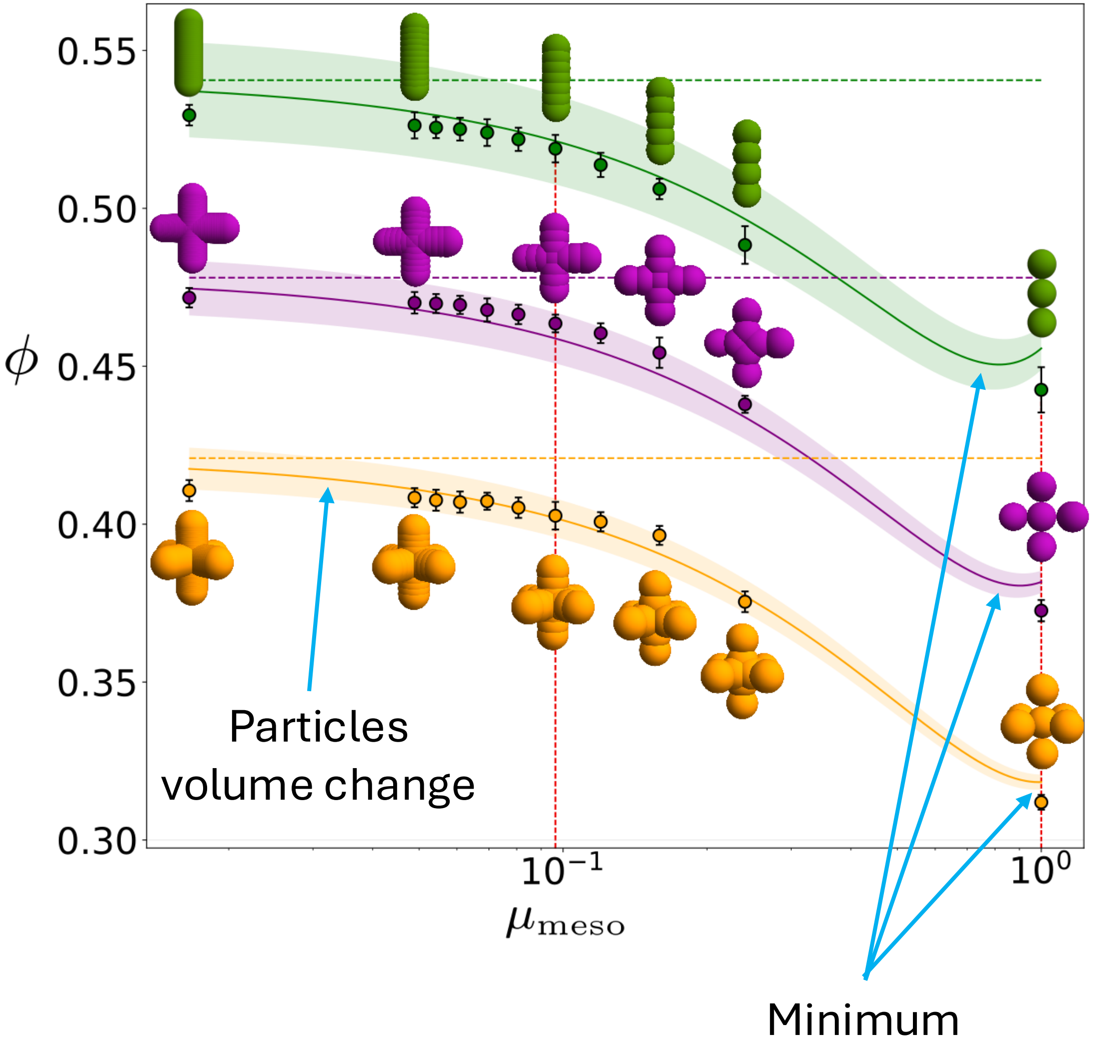
Packing fraction



Semi-empirical Model

$$\phi(\mu, \mu_{\mathrm{meso}}, \mu_{\mathrm{macro}}) \approx \frac{N v_n}{V_{max}}$$

$$= \phi_1 \frac{(1-\mu_{\mathrm{meso}})^2 + 3}{3(1-\mu_{\mathrm{macro}})(1-\mu_{\mathrm{meso}}) + 3}$$

Linear modulation

Minimum ?

$$\mu_{\mathrm{meso}} = \frac{2 - \mu_{\mathrm{macro}} - \sqrt{1 + 3(1-\mu_{\mathrm{macro}})^2}}{1 - \mu_{\mathrm{macro}}}$$

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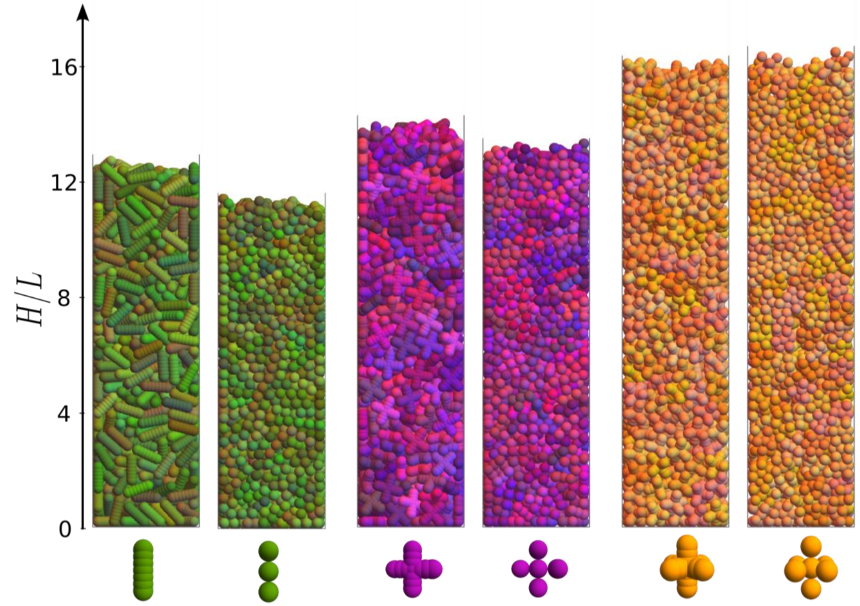
Take-home message

- Bumpiness of particles μ_{meso} impact:

  - Packing fraction through interlocking



  - Effect modulated linearly by the shapes of particles μ_{macro}

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Perspectives

Extent this study to a wide range of macroscopic roughness

Study other observables (e.g. Angle of repose)

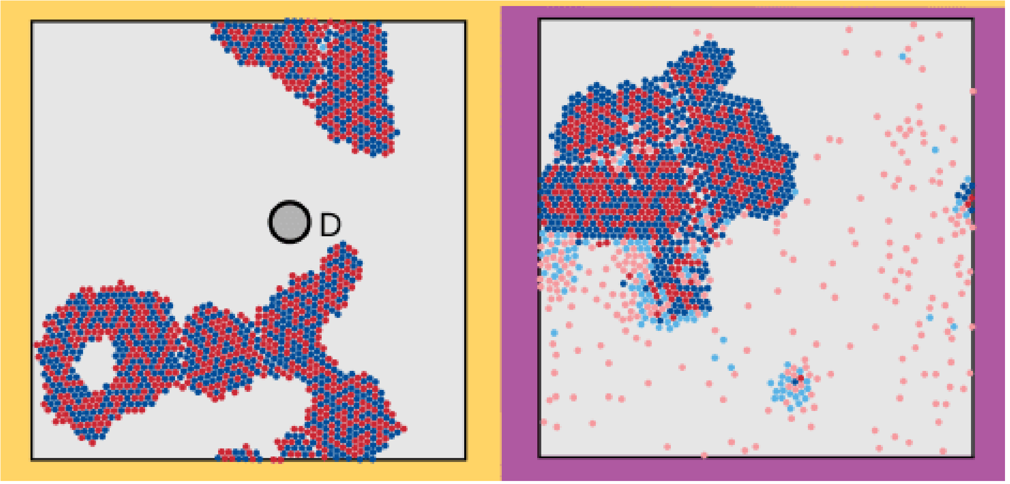
Use Edwards theory to check our semi-empirical modelling

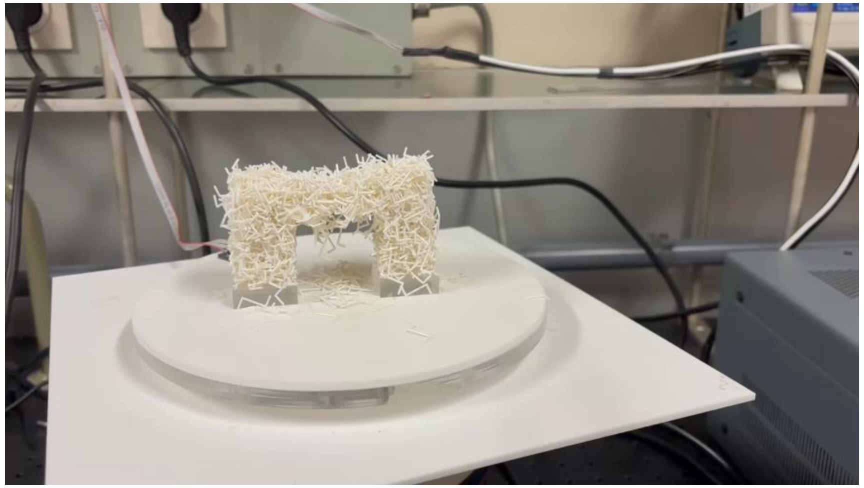
Shape manufacturing with less materials

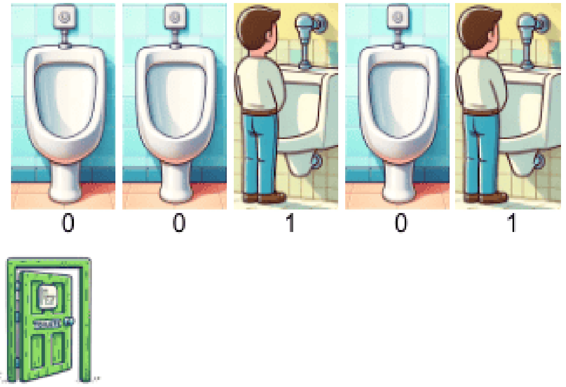
Model through DEM with less spheres

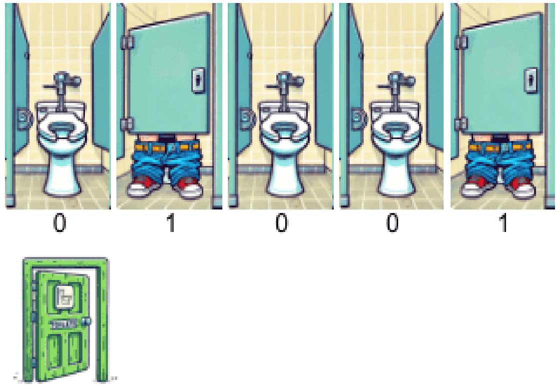
Question

Others

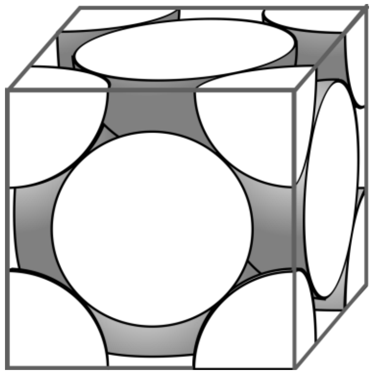








Historical context



$$\phi = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

1611 Kepler Conjecture: Maximal close packing for spheres

1831 Gauss proof in case of lattice arrangement

1900 Included as part of the 23 unsolved problem of Hilbert

2017 Formal proof by Thomas Hales et al.

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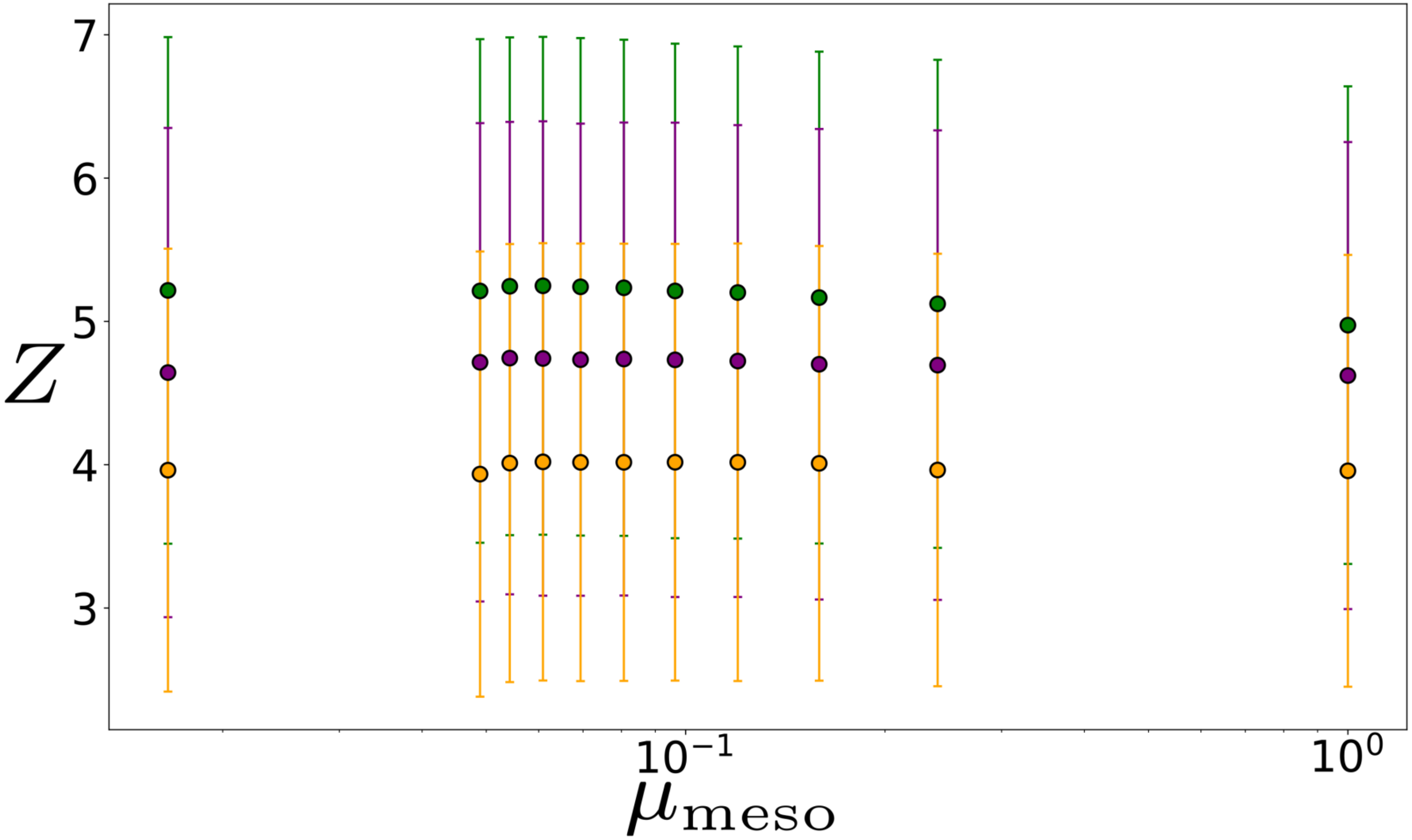
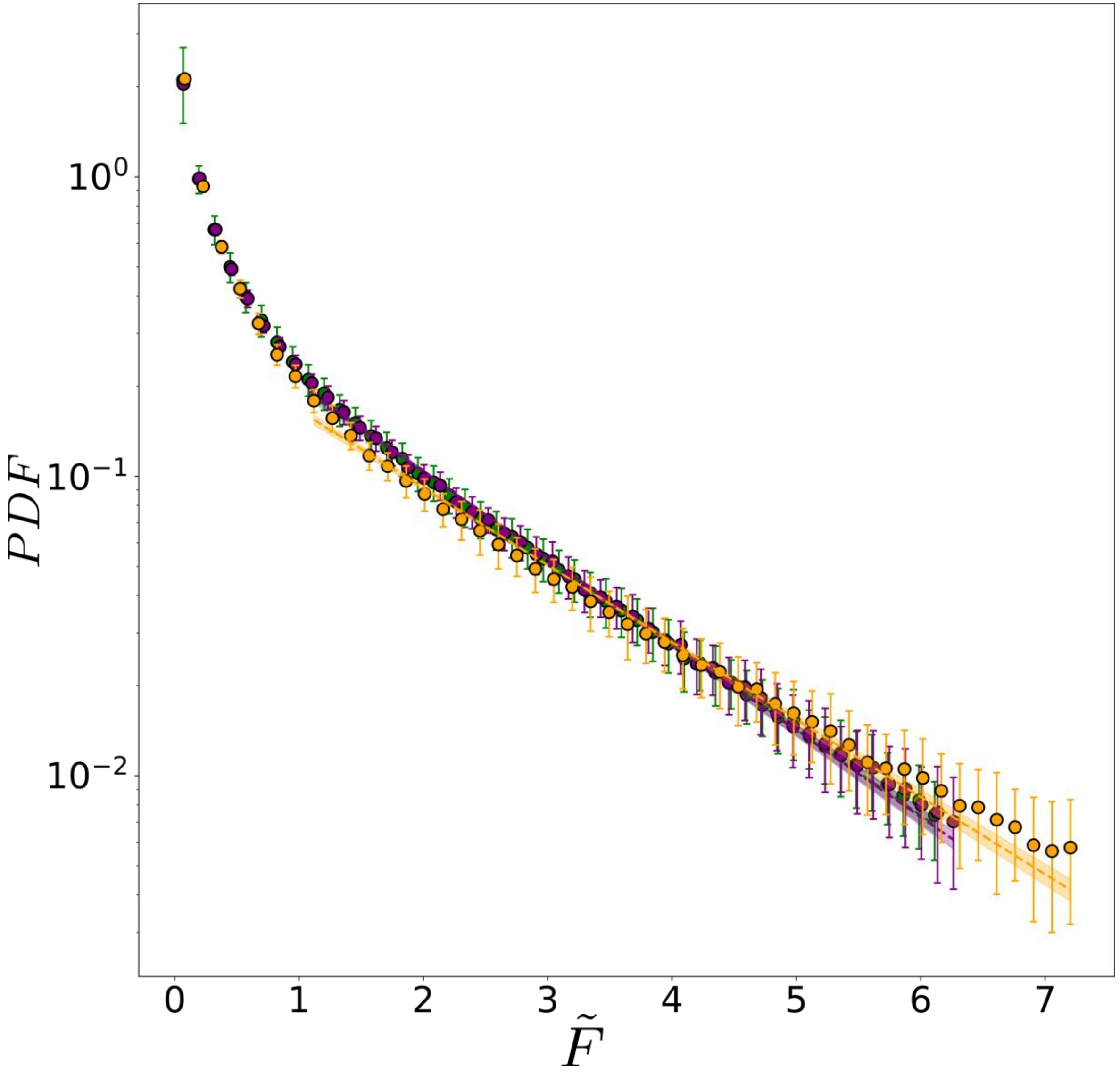
Coordination number



Constant with meso

Vary with macro

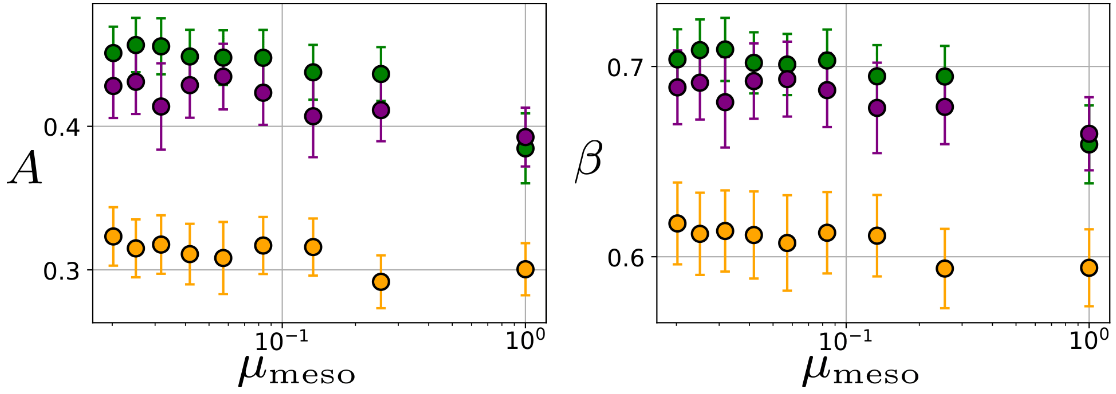
Forces distribution



Model

$$A \exp\left(-\beta \tilde{F}\right) \text{ for } \tilde{F} > 1$$

Fitting parameters



Constant with meso **Vary with macro**

Slide DEM

$$\mathbf{F} = m\mathbf{a} \qquad \mathbf{I}\dot{\omega} + \omega \times (\mathbf{I}\omega) = M$$

$$F_n = K_n \delta_n^{3/2} + \eta_n v_n \qquad F_t = K_t \delta_t^{3/2} + \eta_t v_t$$

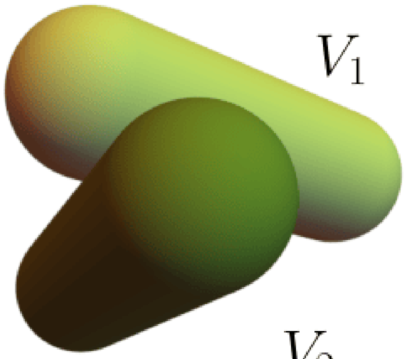
$$\mu_{\text{macro}} \approx \{0.88, 0.94, 0.99\}$$

Table 1 Simulation parameters

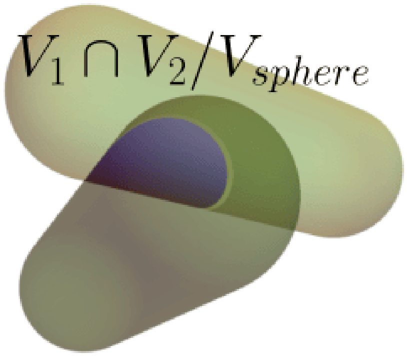
Property	**Ranges of values**
Density, ρ	1.2×10^3 kg m^{-3}
Young's Modulus, E	2.5 GPa
Poisson's Ratio, ν	0.35
Coefficient of Restitution, e	0.3
Coefficient of Friction, μ	0.4
Box Dimension, $l_x \times l_y \times l_z$	$0.1 \times 0.1 \times 0.5$ m^3
Maximum Simulation Time, t_{max}	15 s
Time Step, dt	1×10^{-6} s
Shapes	Rod,Cross,Star
Number of Particles, N	3780,2268,1620
Mass, m	0.3139,0.5277,0.7301 g
Moment of inertia along x, I_{xx}	5.2, 5.8, 10.7 µg m^2
Moment of inertia along y, I_{yy}	5.2, 10.1, 10.7 µg m^2
Moment of inertia along z, I_{zz}	5.2, 5.8, 10.7 µg m^2
Sphere radius, R	2.5 mm
Rod Length, L	$6R$
Gravity, g	9.81 kg m s^{-2}

Slide Remove overlap

Convex-Hull



Overlap



$$F_n = mg$$

$$\hat{\delta}_n = \left(\frac{16 m_{\text{star}} g}{K_n} \right)^{\frac{2}{3}} \approx 5.10^{-4} R$$

$$10 \hat{\delta}_n^2 R / R^3 \approx 10^{-6}$$

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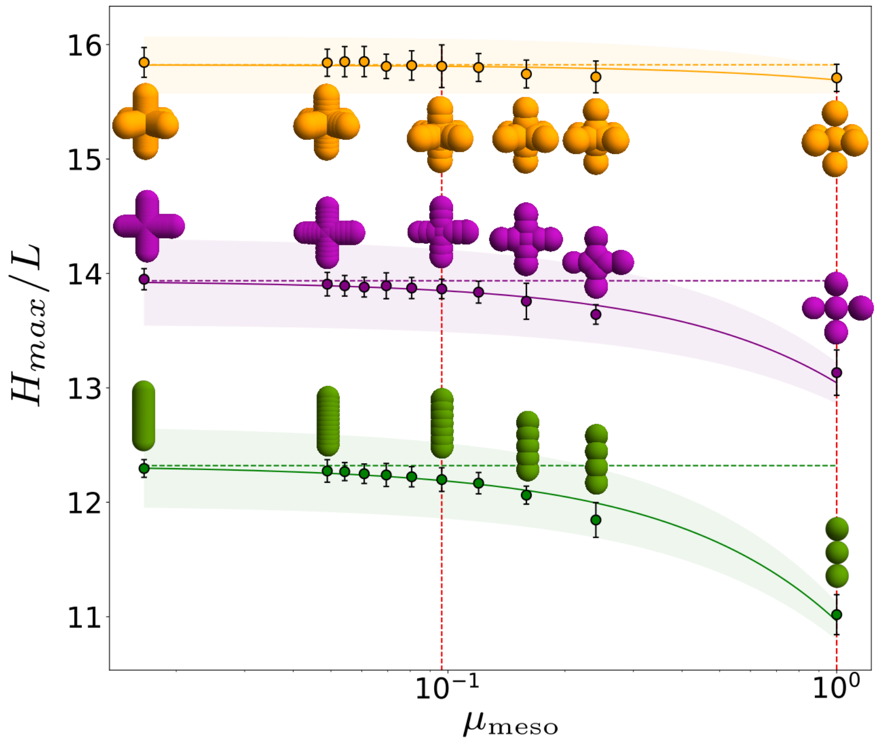
Slide Model packing fraction

$$\phi(\mu_{\text{meso}}, \mu_{\text{macro}}) \approx \frac{Nv_n}{V_{max}} = \frac{N}{l_x l_y}\frac{v_n}{H_{max}}$$

$$= \frac{Nv_\infty}{4 l_x l_y}\frac{(1-\mu_{\text{meso}})^2+3}{H_\Delta(1-\mu_{\text{meso}})+H_1}$$

$$= \phi_1 \frac{(1-\mu_{\text{meso}})^2+3}{3(1-\mu_{\text{macro}})(1-\mu_{\text{meso}})+3}$$

$$v_n = \frac{(1-\mu_{\text{meso}})^2+3}{4} v_\infty$$



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Edwards thermodynamics

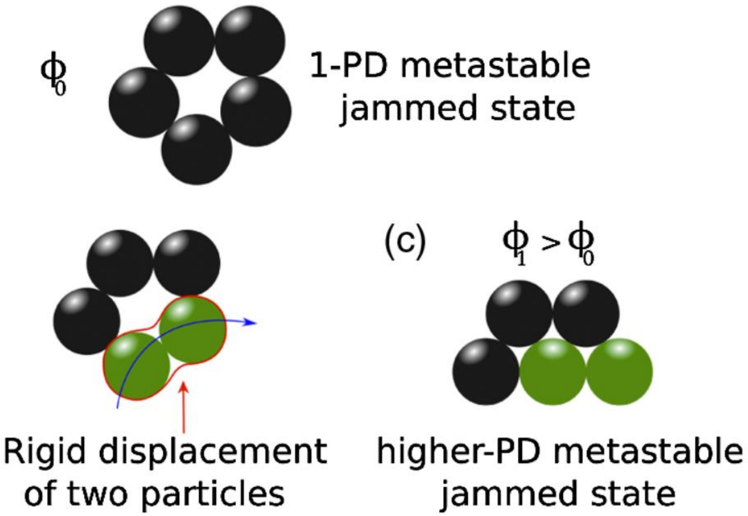
- A.K.A granular statistical mechanics
- Key idea 1989-1994:
  - State variable = Volume $\mathcal{W}(\{\mathbf{r}_i, \hat{\mathbf{t}}_i\})$
  - Proper definition for *jammed* configurations
  - Ergodicity & Equiprobability of micro-states

Usual statistical mechanics	Edwards statistical mechanics
Energy (conserved)	Volume (variable)
Metastable state	*Jammed* state
Temperature	Compactivity
Hamiltonian	Stress-moment

Edwards, S. F., & Oakeshott, R. B. S. (1989). Theory of powders. Physica A: Statistical Mechanics and Its Applications, 157(3), 1080–1090. https://doi.org/10.1016/0378-4371(89)90034-4
Baule, A., Morone, F., Herrmann, H. J., & Makse, H. A. (2018). Edwards statistical mechanics for jammed granular matter. Reviews of Modern Physics, 90(1). https://doi.org/10.1103/revmodphys.90.015006

Jamming

- *Jamming*: Metastability w.r.t. Displacements
  - Packing Fraction do not increase
  - k-Particle-Displacement (k-PD), other fixed
  - Ground state for $k \to \infty$
  - Ground state allows for 2-5% of particle displacement



Concept	Typical case
Excluded Volume Constraints	No Overlap
Mechanicals Constraints	Forces & Torques balance

Baule, A., Morone, F., Herrmann, H. J., & Makse, H. A. (2018). Edwards statistical mechanics for jammed granular matter. Reviews of Modern Physics, 90(1). https://doi.org/10.1103/revmodphys.90.015006

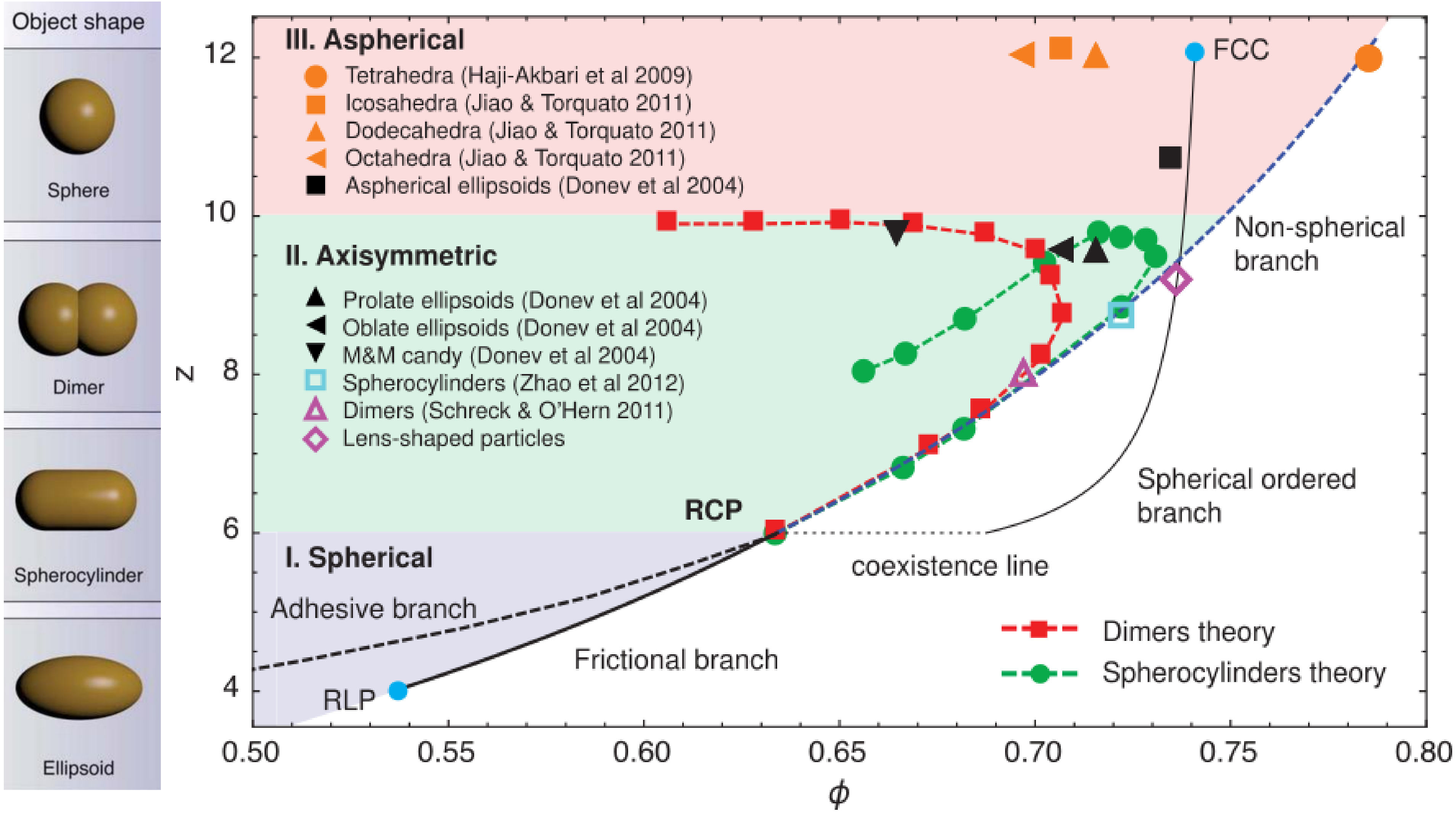
Typical Observable

$$S(V) = \lambda \log \Omega(V) \qquad \Omega(V) = \int d\mathbf{q}\,\delta(V - \mathcal{W}(\mathbf{q}))\Theta_{\text{jam}} \qquad X^{-1} = \frac{\partial S(V)}{\partial V}$$

- Compactivity X
- Granular material undergoing vertical tapping
- Application to spherical shapes
- Application to nonspherical shapes

Baule, A., Morone, F., Herrmann, H. J., & Makse, H. A. (2018). Edwards statistical mechanics for jammed granular matter. Reviews of Modern Physics, 90(1). https://doi.org/10.1103/revmodphys.90.015006

Shape modeling



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