Development of a Model for Restructuring of Fractal Soot Aggregates and its Parameterization using AFM Experiments

Egor Demidov*, Ali Hasani, Alexei Khalizov, Gennady Gor

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New Jersey Institute of Technology

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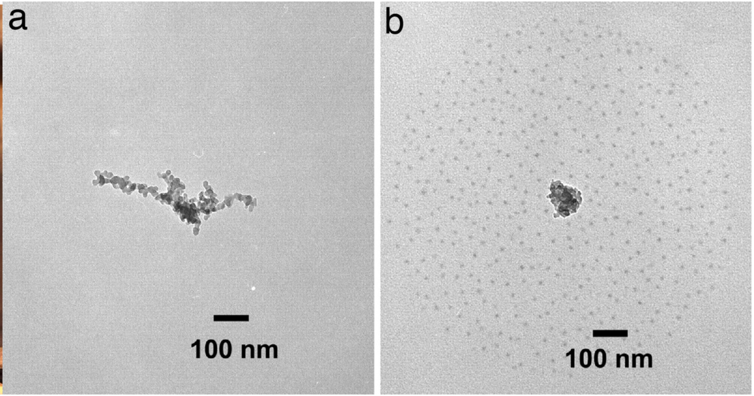
Soot and its morphology

Soot and its morphology



[0] Renyi Zhang et al. "Variability in morphology, hygroscopicity, and optical properties of soot aerosols during atmospheric processing". In: *Proceedings of the National Academy of Sciences* 105.30 (2008), pp. 10291–10296

Soot and its morphology

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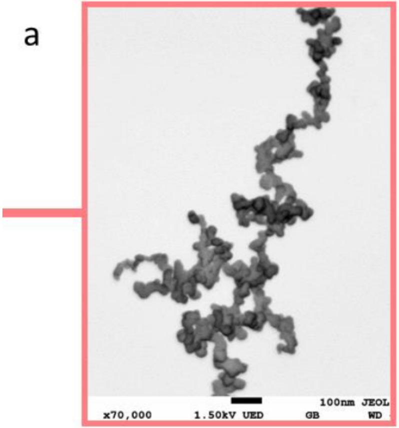
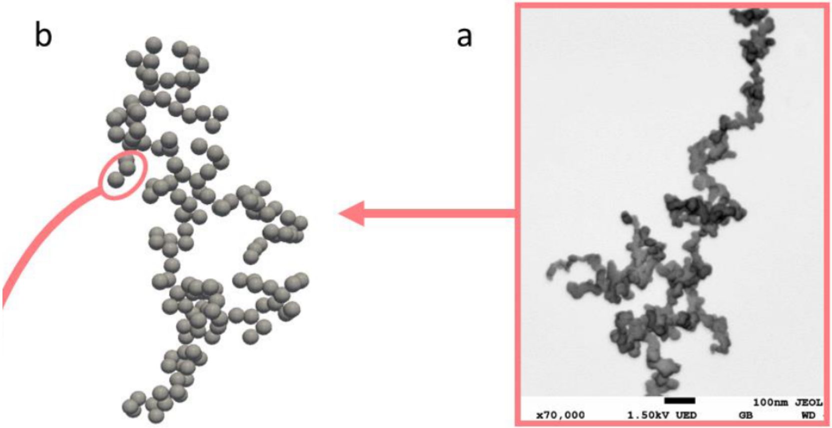


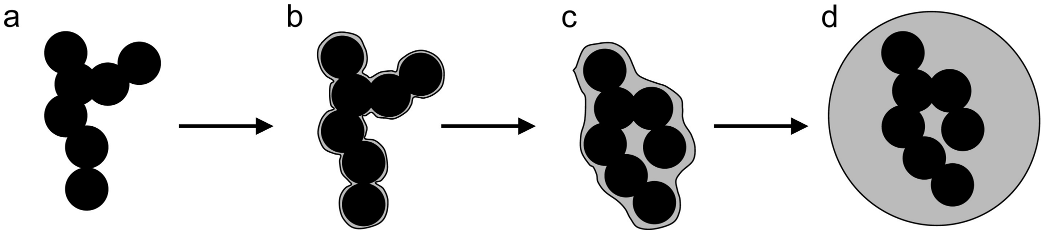
Soot is a fractal-like agglomerate of carbon particles

Soot and its morphology



We can represent it as an agglomerate of rigid spherical particles

Soot and its morphology



Condensation drives restructuring of agglomerates (the agglomerate rearranges due to forces exerted by the liquid)

Supplemental: animations

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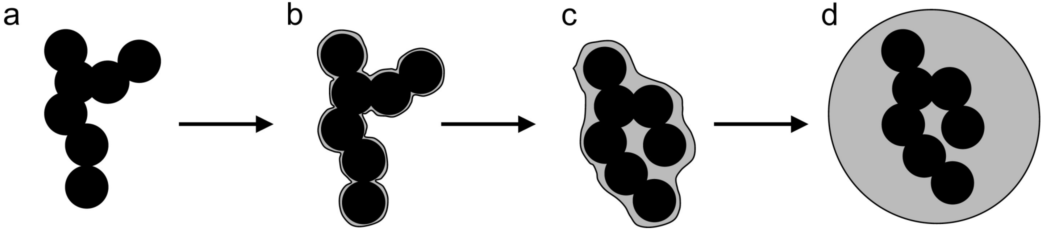
Particle dynamics



- We model restructuring by
  - Calculating the forces acting on every particle
  - Integrating 2^{nd} Law

Particle dynamics

$$m\frac{d^2\mathbf{x}}{dt^2} = \sum_i \mathbf{f}_i$$

$$I\frac{d^2\theta}{dt^2} = \sum_i \boldsymbol{\tau}_i$$

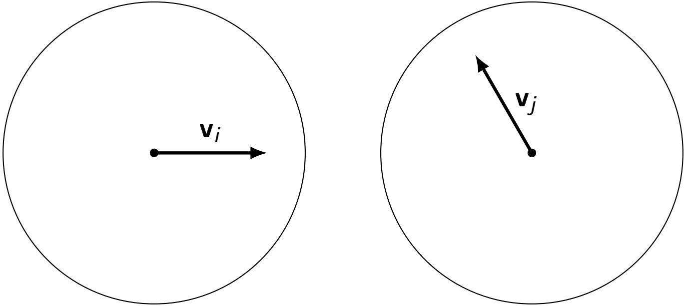
Particle dynamics

$$m\frac{d^2\mathbf{x}}{dt^2} = \sum_i \mathbf{f}_i$$

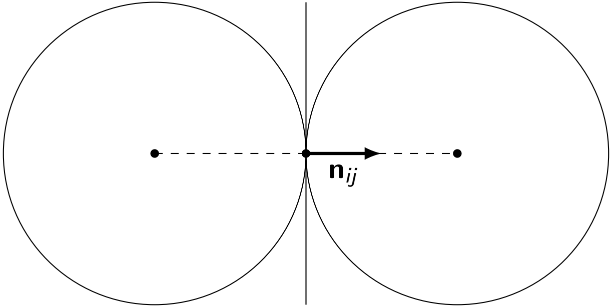
$$\boxed{I\frac{d^2\theta}{dt^2} = \sum_i \boldsymbol{\tau}_i}$$

- Unlike in molecular dynamics
  - Particles (atoms) are not point-masses
  - Particles have nonzero moment of inertia and undergo rotational motion
  - Frictional forces between contacting particles need to be considered

Contact forces

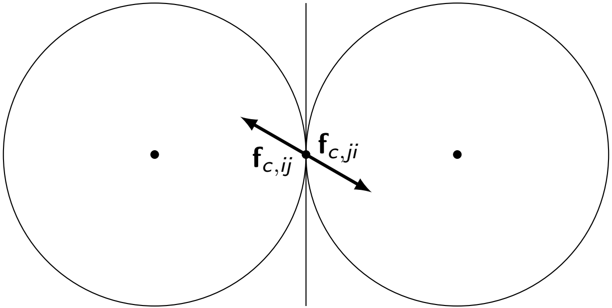


Contact forces



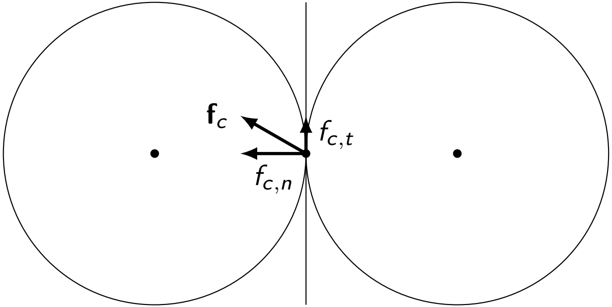
Contact plane between particles i and j is defined by normal vector $\mathbf{n}_{ij}$ connecting centers of respective particles

Contact forces



Contact will result in particle i experiencing force $\mathbf{f}_{c,ij}$ and particle j experiencing an equal in magnitude and opposite force $\mathbf{f}_{c,ji} = -\mathbf{f}_{c,ij}$ applied at the contact point

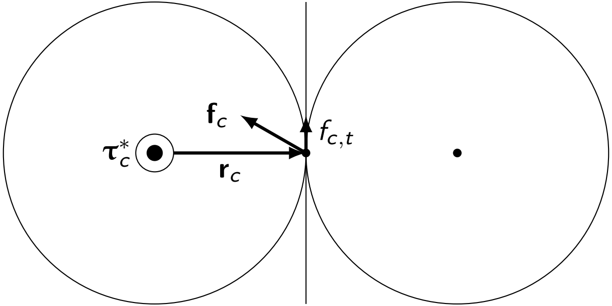
Contact forces



Contact force $\mathbf{f}_c$ can be decomposed into normal and tangential components $f_{c,n}$ and $f_{c,t}$, where $f_{c,n}$ is related to elasticity and $f_{c,t}$ is related to friction:

$$\mathbf{f}_c = f_{c,n}\mathbf{n} + f_{c,t}\mathbf{t}$$

Contact forces



* $\boldsymbol{\tau}_c$ is directed out-of-plane

Since the contact force is applied to the contact point, it will result in a torque:

$$\boldsymbol{\tau}_c = \mathbf{r}_c \times \mathbf{f}_c = f_{c,t} \left(\mathbf{r}_c \times \mathbf{t} \right)$$

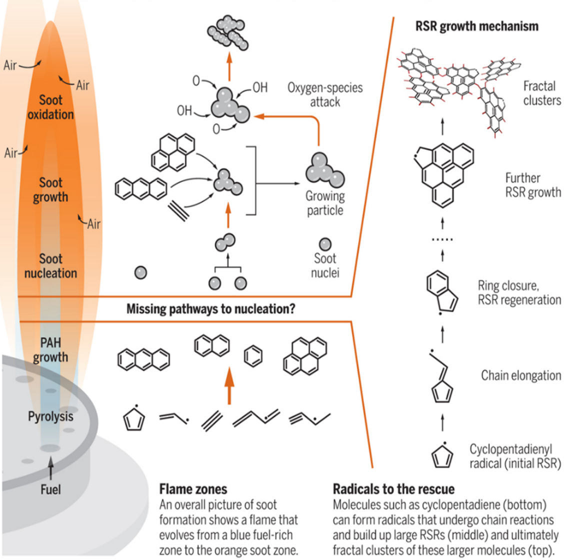
Contact forces

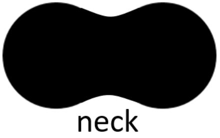
Recap:

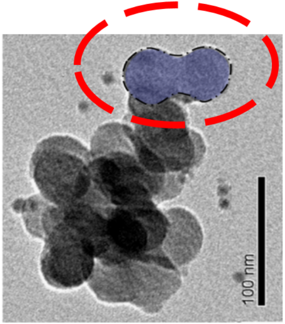
- Contact forces are expressed in terms of elasticity and friction coefficients
- They only act on free particles that come into contact
- Various models exist, including ones that simulate energy dissipation

Supplemental: animations Supplemental: Luding 2008

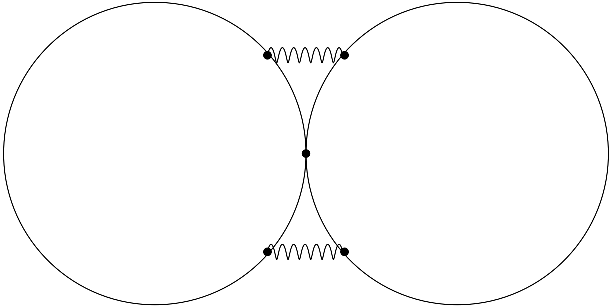
Sinter bridges





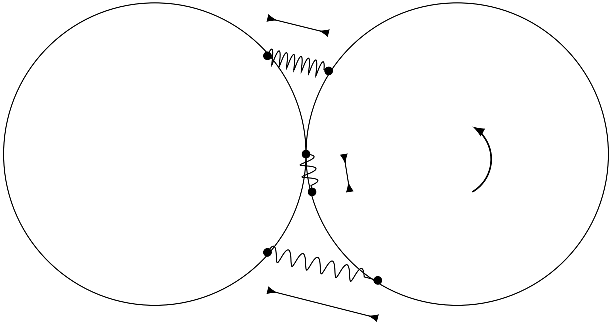


Sinter bridges



Three (2D) / five (3D) springs are inserted between sintered particles

Sinter bridges



Translation / rotation of one particle gives rise to forces that restore the reference configuration of the pair

Sinter bridges

Numerical implementation:

Motion of a spring connector **s** attached to particle i with center at **x**:

$$\frac{d\mathbf{s}}{dt} = \mathbf{v}_i + \boldsymbol{\omega}_i \times (\mathbf{s} - \mathbf{x}_i)$$

Spring displacement, force, and torque:

$$\Delta l = \|\mathbf{s}_i - \mathbf{s}_j\| - l_0$$

$$\mathbf{f}_n = -k_n \Delta l \frac{\mathbf{s}_i - \mathbf{s}_j}{\|\mathbf{s}_i - \mathbf{s}_j\|}$$

$$\boldsymbol{\tau}_n = \mathbf{r}_n \times \mathbf{f}_n$$

Sinter bridges

Breaking criterion:

Potential energy stored in a neck - sum of PEs stored in constituent springs:

$$E_{\mathrm{neck}} = \sum E_{\mathrm{spring}}$$

$$E_{\mathrm{spring}} = \frac{1}{2} k_n \left(l - l_0\right)^2$$

Let us break the neck when

$$E_{\mathrm{neck}} \geq E_{\mathrm{crit}}$$

where E_{crit} is an attribute of the neck and is assigned at its creation

Supplemental: animations

Non-contact / body forces

Hamaker (Van der Waals) attraction:

$$\mathbf{f}_{VdW} = \frac{2AR}{(\|\mathbf{x}_i - \mathbf{x}_j\| - 2R)^2}\mathbf{n} \qquad \text{if } \|\mathbf{x}_i - \mathbf{x}_j\| - 2R > h_0$$

$$\mathbf{f}_{VdW} = \frac{2AR}{h_0^2}\mathbf{n} \qquad \text{if } \|\mathbf{x}_i - \mathbf{x}_j\| - 2R \leq h_0$$

Coating forces: to be implemented

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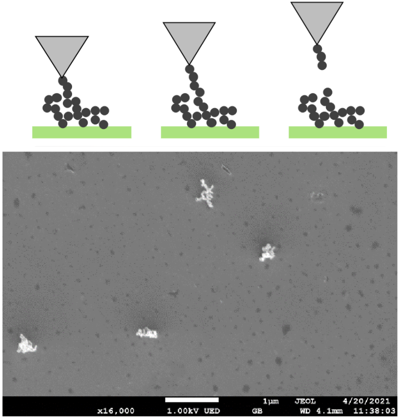
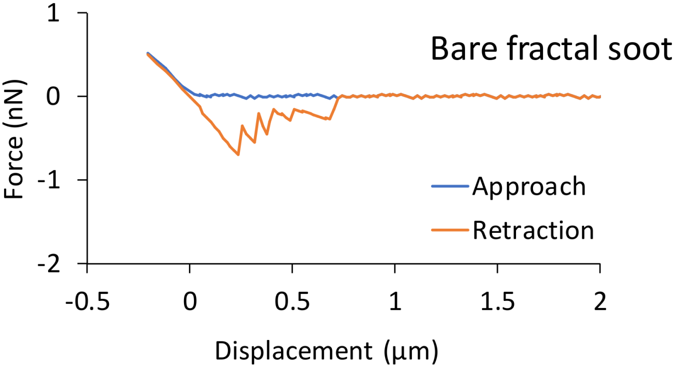
Mechanics only simulations

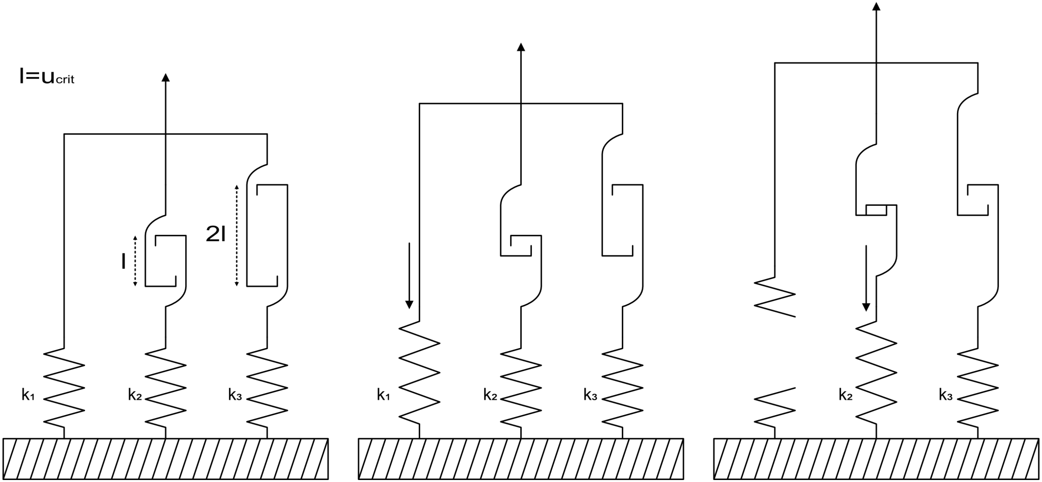
Before coating is implemented, AFM experiments[1] and TEM tomography can be used to parametrize the model:



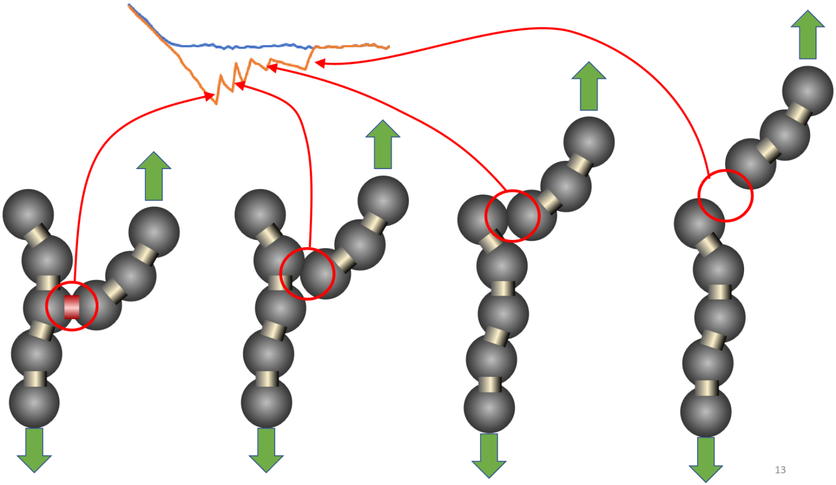


[1]Khalizov and Hasani, AAAR 2023

Mechanics only simulations



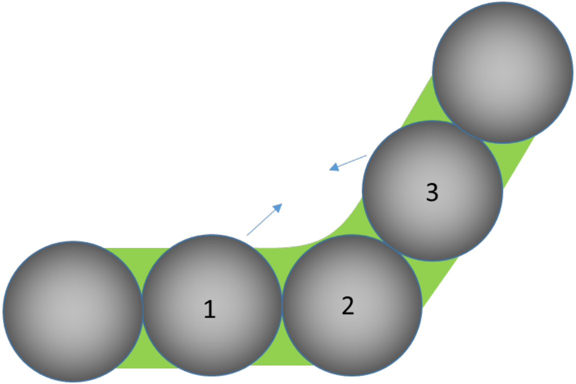
Mechanics only simulations



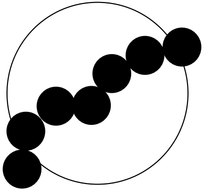
Supplemental: animations

Adding capillary forces to the DEM model

Proposed model - "ternary" force:



Proposed model - interface force:



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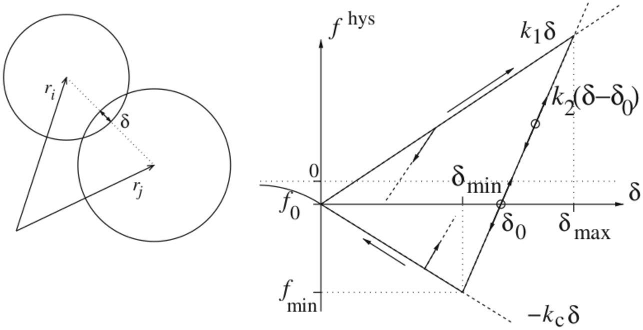
Animations

- Contact forces (Luding 2008)
  - No resistance
  - Rolling resistance
  - Torsion resistance
- Necks
  - Trimer
  - Y-shape
  - Aggregate (central force)

Return: soot and its morphology | Return: contact forces | Return: sinter bridges | Return: mechanics only simulations

Luding 2008[1] contact model

Normal force, friction, rolling and torsion resistance



Return: contact forces

[1] Stefan Luding. "Cohesive, frictional powders: contact models for tension". In: *Granular matter* 10.4 (2008), pp. 235–246

AFM transfer function

Cantilever dynamics:

$$m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + kx = g(t)$$

where x is cantilever displacement and $g(t)$ is the forcing function on the cantilever.

Apparent force $f(t)$:

$$f(t) = kx(t)$$

$$\frac{m}{k}\frac{d^2f}{dt^2} + \frac{\gamma}{k}\frac{df}{dt} + f(t) = g(t)$$

AFM transfer function

For a critically damped cantilever:

$$\gamma = 2\sqrt{mk}$$

Transfer function becomes:

$$\frac{F(s)}{G(s)} = \frac{\omega_0^2}{(s+\omega_0)^2}$$

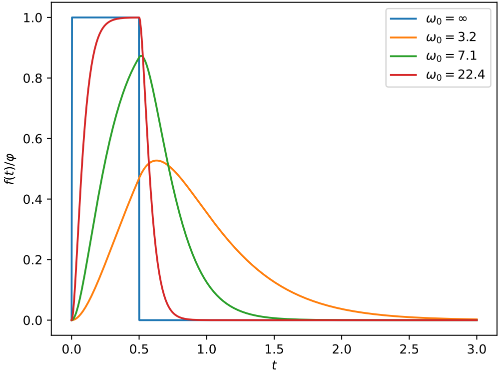
Where ω_0 is the natural angular frequency of the undamped system:

$$\omega_0 = \sqrt{\frac{k}{m}}$$

AFM transfer function

Response to step input (Heaviside step function):

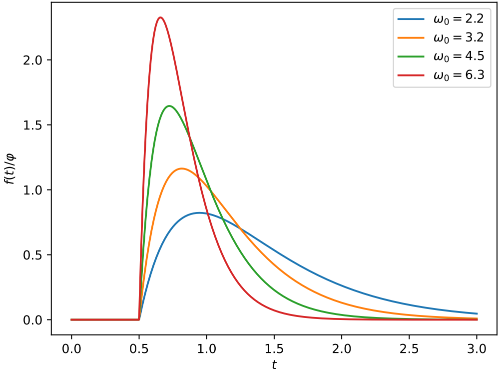
$$f(t) = \varphi\left(1 - e^{-\omega_0 t}\left(\omega_0 t + 1\right)\right)$$



AFM transfer function

Response to unit impulse (Dirac delta function):

$$f(t) = \varphi \omega_0^2 e^{-\omega_0 (t)}$$



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Bibliography I

- Luding, Stefan. "Cohesive, frictional powders: contact models for tension". In: *Granular matter* 10.4 (2008), pp. 235–246.
- Zhang, Renyi et al. "Variability in morphology, hygroscopicity, and optical properties of soot aerosols during atmospheric processing". In: *Proceedings of the National Academy of Sciences* 105.30 (2008), pp. 10291–10296.