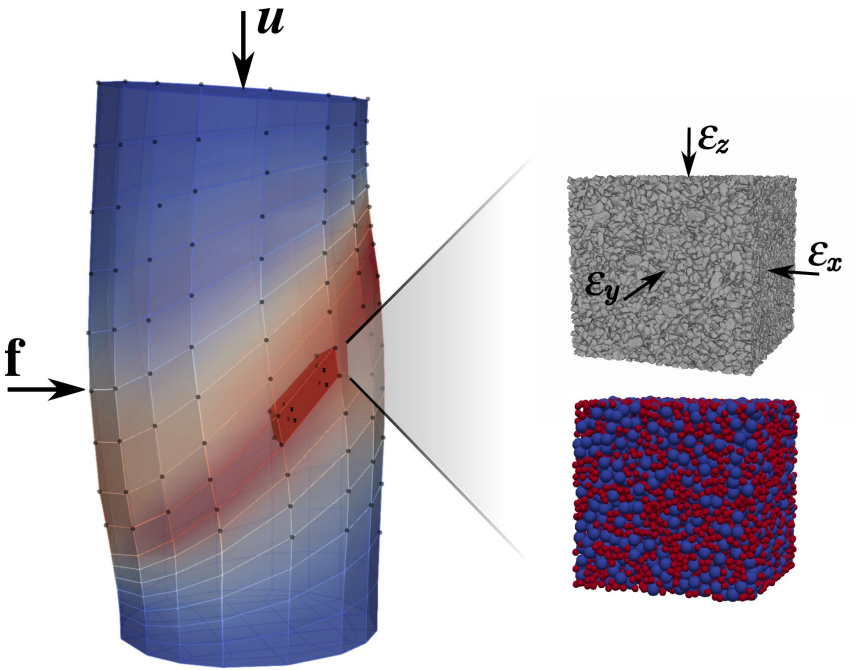


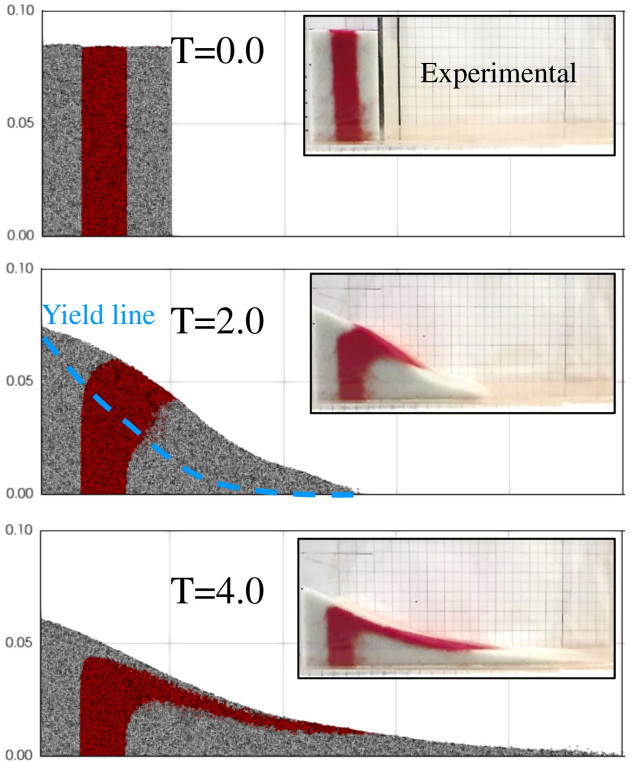
CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

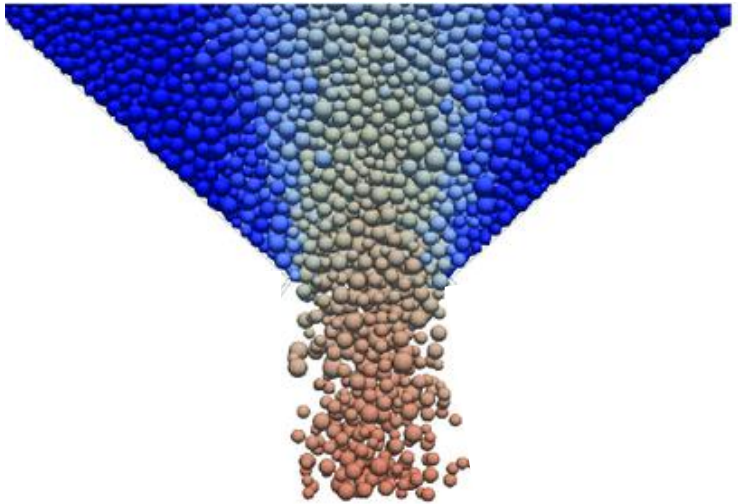
Week 6

Modeling granular materials

Geophysics/geotechnical engineering



Industrial flows

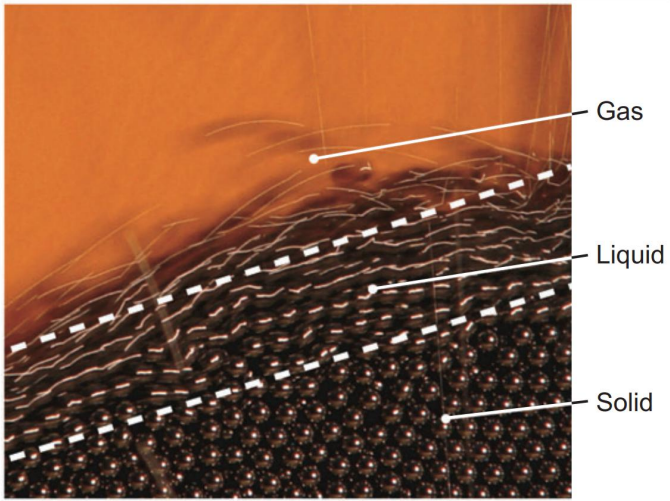


Collection of interacting **athermal** particles

Solids, liquids and gases

Granular materials may exist in **three phases** (**solid**, **liquid** and **gas**) and experience transitions between those three phases.

No general constitutive model exists for all phases.



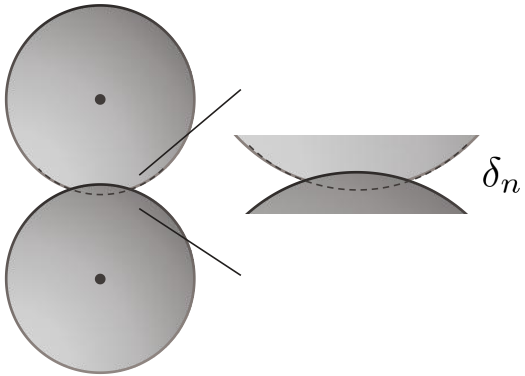
Multiscale modeling presents a viable alternative.

But first let's dive into direct modeling at the grain scale.

Modeling granular materials

Soft-particle approach (Discrete Element Method)

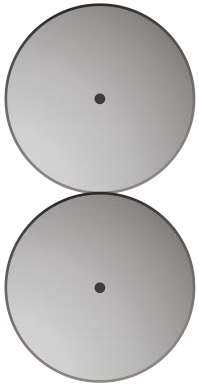
Models “soft” particles by allowing a local interpenetration (contact regularization).



Explicit (fast, easily parallelizable)
Approximate

Hard-particle approach (Contact Dynamics)

Models rigid particles without allowing any interpenetration.



Implicit (requires solving nonlinear system)
Accurate

The Discrete Element Method (DEM)

General principles

Update particle positions

Forces and moments on particles:

$$\boldsymbol{f}_i^c = f_i^n \boldsymbol{n}^c + f_i^t \boldsymbol{t}^c$$

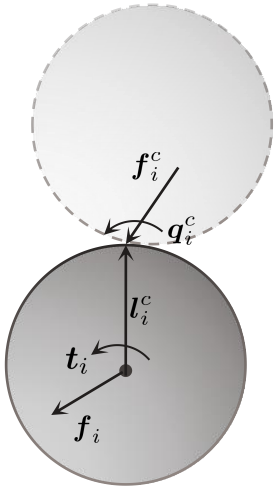
$$\boldsymbol{f}_i = \sum_c \boldsymbol{f}_i^c \qquad \text{: Total force acting on particle i}$$

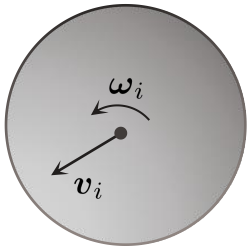
$$\boldsymbol{t}_i = \sum_c (\boldsymbol{l}_i^c \times \boldsymbol{f}_i^c + \boldsymbol{q}_i^c) \qquad \text{: Total torque acting on particle i}$$

Equations of motion:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{f}_i \qquad \text{: Linear momentum balance}$$

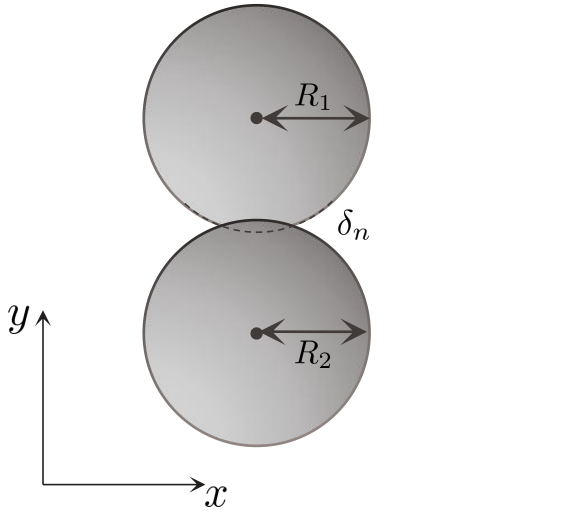
$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \boldsymbol{t}_i \qquad \text{: Angular momentum balance}$$





Accounting for particle shape

Disk/spheres



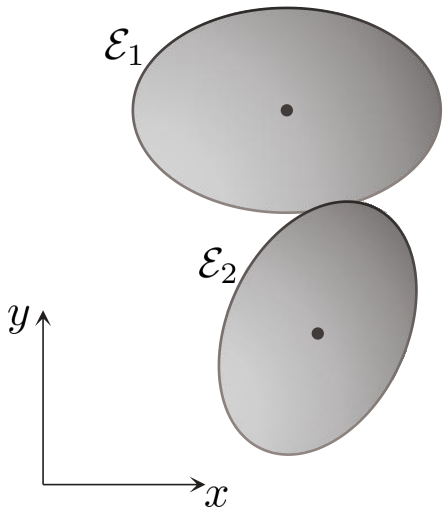
Overlap:

$$\delta_n = R_1 + R_2 - \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Contact normal:

$$\boldsymbol{n} = \frac{\boldsymbol{x}_1 - \boldsymbol{x}_2}{||\boldsymbol{x}_1 - \boldsymbol{x}_2||}$$

Ellipses/Ellipsoids

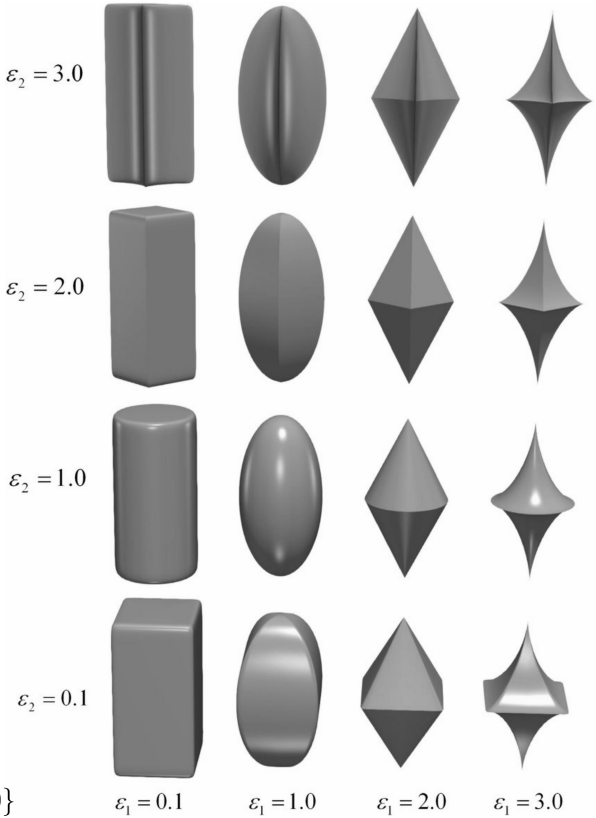


Overlap requires solution of a min problem:

$$\delta_n = \arg\min ||\hat{x}_1 - \hat{x}_2||$$
$$\text{s.t. } x_1 \in \mathcal{E}_1,\ x_2 \in \mathcal{E}_2$$

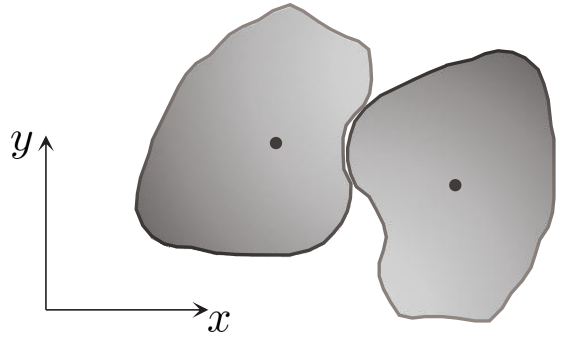
$$\mathcal{E}_1 = \{\hat{\boldsymbol{x}}_1 \in \mathbb{R}^2 : (\hat{\boldsymbol{x}}_1 - \boldsymbol{c})^T \boldsymbol{Q} (\hat{\boldsymbol{x}}_1 - \boldsymbol{c}) - 1 = 0\}$$

Superquadrics

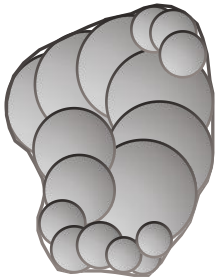


Accounting for particle shape

Arbitrary shapes



Sphere clumps

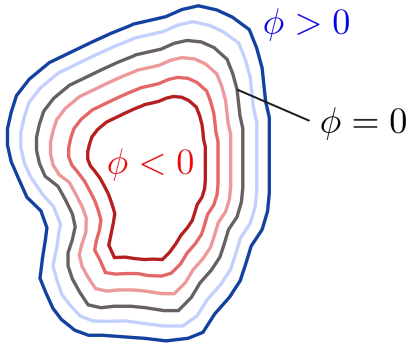


Each sphere of particle 1 checked against each sphere of particle 2

Polygons/polyhedra

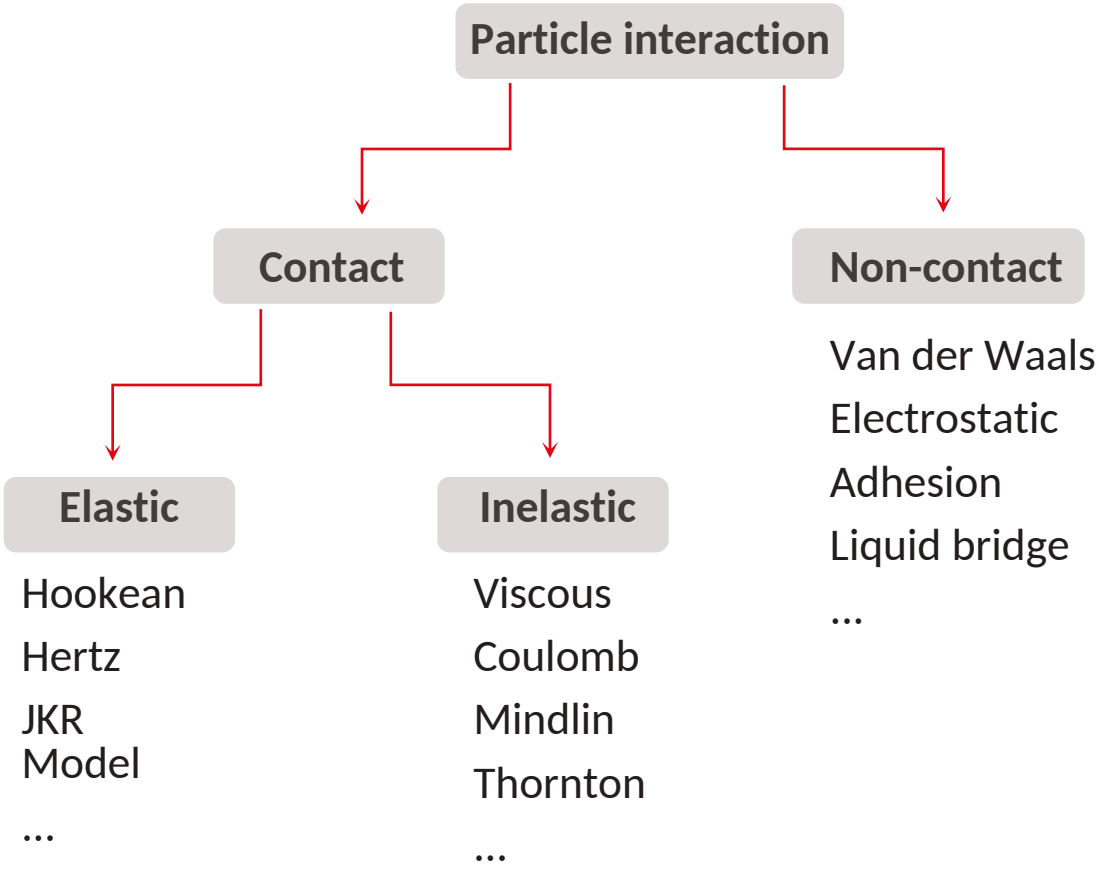
Each node of particle 1 checked against each face of particle 2

Level sets



Each node of particle 1 checked against the level set of particle 2

Particle interactions



Contact laws - Normal contact

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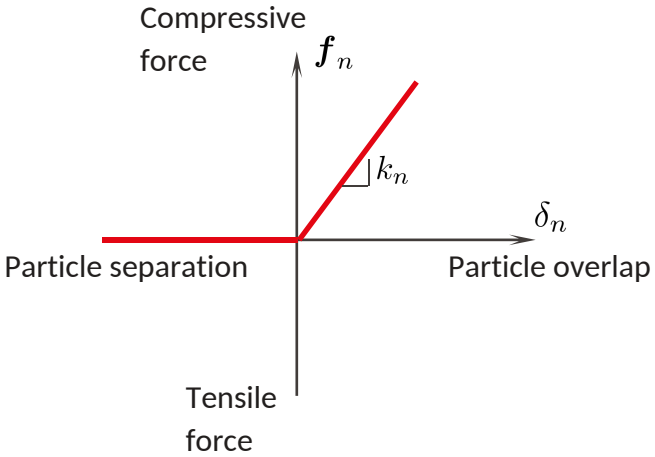
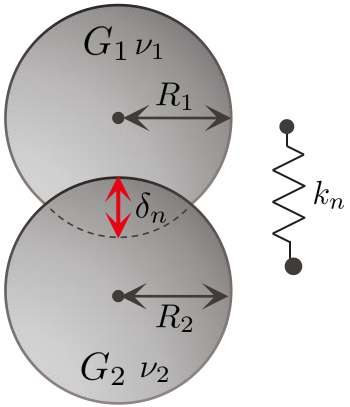
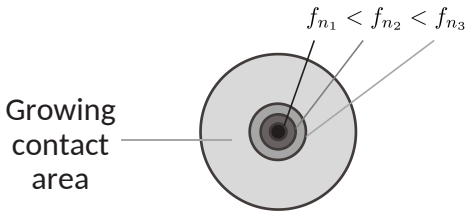
Linear (**Hookean**) contact



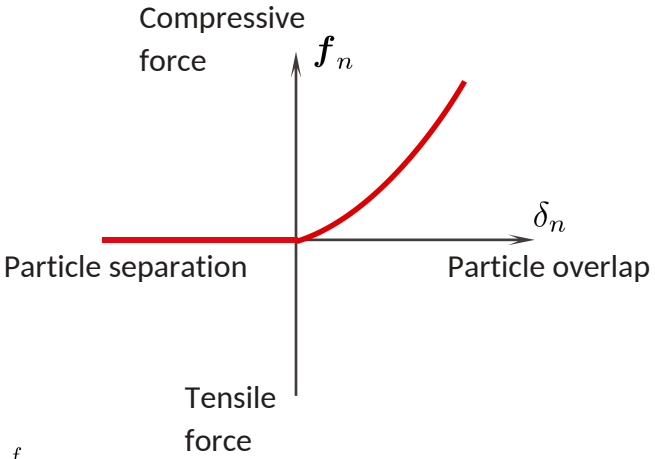
$$f_n = k_n \delta_n$$
$$k_n = \text{const}$$





Hertz theory captures increase in contact area with increasing force

Nonlinear (**Hertzian**) contact



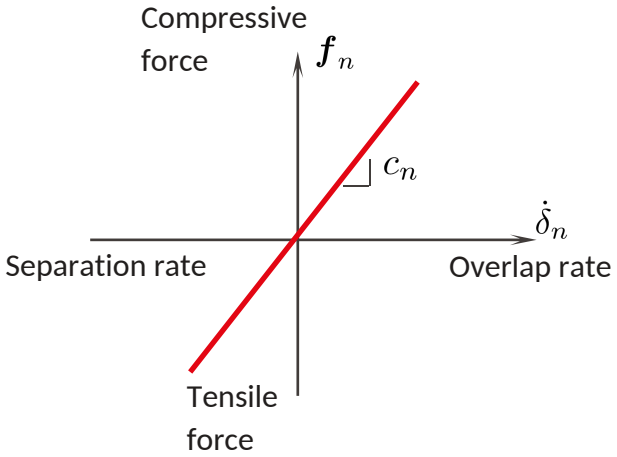
$$f_n = k_n \delta_n$$

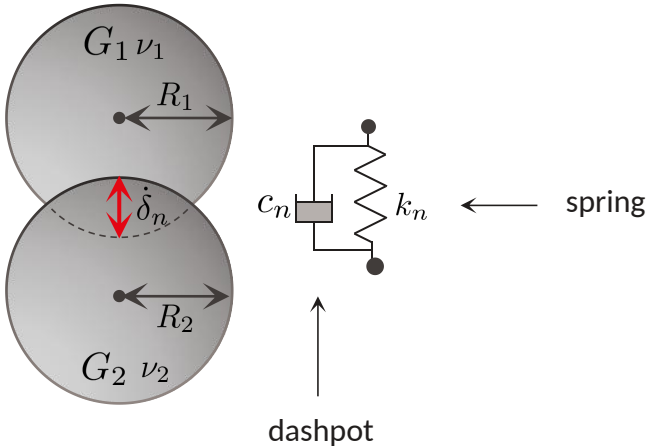
$$k_n = \frac{2G^* \sqrt{2R^*}}{3(1-2\nu^*)} \sqrt{\delta_n}$$

$$R^* = \frac{2R_1 R_2}{R_1 + R_2} \quad G^* = \frac{G_1 + G_2}{2} \quad \nu^* = \frac{\nu_1 + \nu_2}{2}$$

Contact laws - Normal contact

Accounting for **viscous** energy dissipation due to **restitution**





$$f_n = k_n \delta_n + c_n \dot{\delta}_n$$

$$c_n = -2\frac{\ln e}{\sqrt{\pi^2 + \ln e^2}}\sqrt{m^* k_n}$$

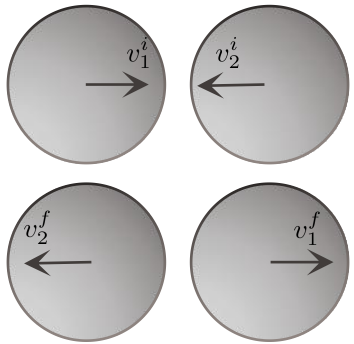
$$m^* = \frac{m_1 m_2}{m_1 + m_2}$$

Coefficient of restitution:

$$e = \frac{|v_2^f - v_1^f|}{|v_1^i - v_2^i|}$$

Initial: before collision

Final: after collision



Contact laws - Tangential contact

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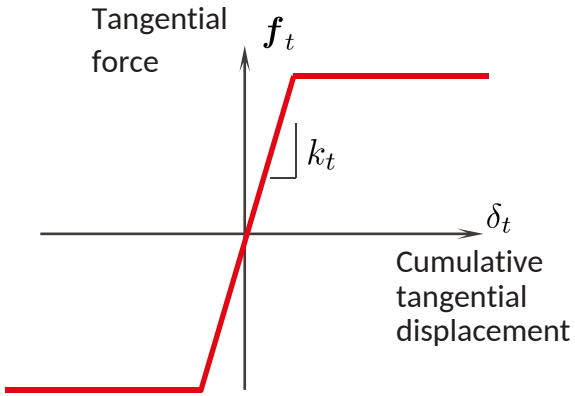
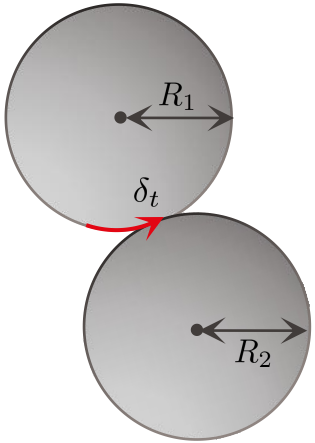
Regularized **Coulomb** friction



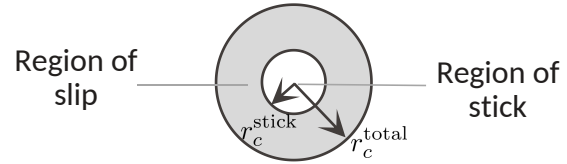


$$f_t < \mu f_n \quad \text{: Stick}$$
$$f_t = \mu f_n \quad \text{: Slip}$$
$$\longrightarrow \quad f_t = -\min(|\mu f_n|, f_t(\delta_t, \dot{\delta}_t))\frac{\dot{\delta}_t}{|\dot{\delta}_t|}$$

where $\quad f_t(\delta_t, \dot{\delta}_t) = k_t \int_{t_c^0}^{t} \dot{\delta}_t \, dt$

Mindlin theory

Mindlin theory resolves the tangential traction at a distance r from the center of the contact area



$$f_t(r) = \frac{3\mu f_n}{2\pi r_c^{\text{total}}} \sqrt{r_c^{\text{total}^2} - r^2}, \quad r \in [r_c^{\text{stick}}, r_c^{\text{total}}]$$

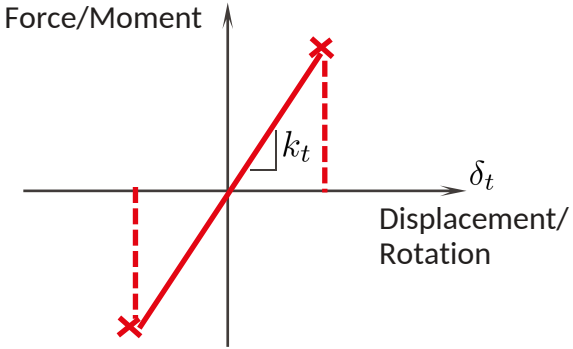
$$f_t(r) = \frac{3\mu f_n}{2\pi r_c^{\text{total}}} \left(\sqrt{r_c^{\text{total}^2} - r^2} - \sqrt{r_c^{\text{stick}^2} - r^2}\right), \quad r \in [r_c^{\text{stick}}, r_c^{\text{total}}]$$

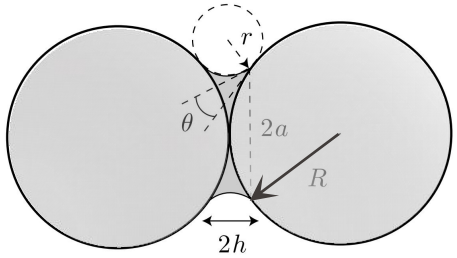
Tangential force acting in the direction opposite to the apparent tangential sliding velocity

Other particle interactions

Cohesion

Due to the formation of a solid bond between the particles



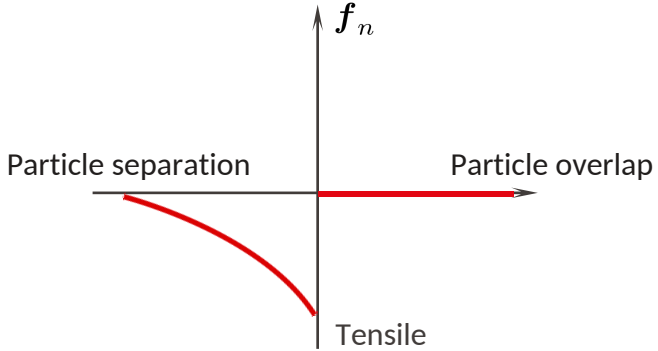


$$f_n = k_n^b A \delta_n$$
$$f_t = k_t^b A \delta_t \quad \text{if } |f_n|/A + |M_t|R/I < \sigma_c$$
$$M_n = k_t^b J \Delta\theta_n \quad \text{and } |f_t|/A + |M_n|R/J < \tau_c$$
$$M_t = k_n^b I \Delta\theta_t$$

Describes an elastic-brittle Euler-Beroulli beam

Capillary forces

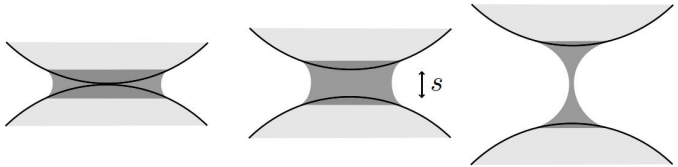
Due to the formation of liquid bridges between grains



$$f_n = 2\pi\gamma_{LV} R \cos\theta$$

liquid-air surface tension

contact angle of the liquid on the solid



Equations of motion & Time integration

Equations of motion:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{f}_i \qquad I_i \frac{d\boldsymbol{\omega}_i}{dt} = \boldsymbol{t}_i$$

Implicit: Backward Euler (hard-sphere DEM)

It's unconditionally stable, but requires solution on nonlinear system of equations

Explicit: Velocity Verlet/Central difference scheme (soft-sphere DEM)

Does not require solution of system of equations, is only conditionally stable

$$\boldsymbol{v}_i^{t+\Delta t/2} = \boldsymbol{v}_i^{t-\Delta t/2} + \Delta t\, \boldsymbol{m}_i^{-1} \boldsymbol{f}_i^t \qquad \boldsymbol{x}_i^{t+\Delta t} = \boldsymbol{x}_i^t + \Delta t\, \boldsymbol{v}_i^{t+\Delta t/2} \qquad \boldsymbol{\omega}_i^{t+\Delta t/2} = \boldsymbol{\omega}_i^{t-\Delta t/2} + \Delta t\, \boldsymbol{I}_i^{-1} \boldsymbol{t}_i^t$$

Stability of time integration

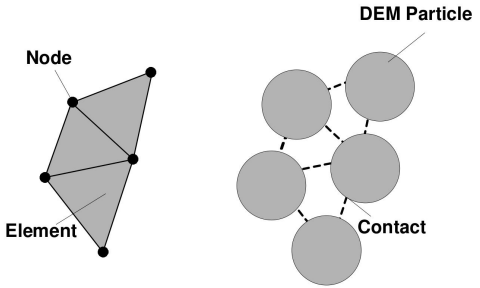
In general for dynamical systemns, the critical time increment for stable analysis is obtained using stability analysis by considering the amplification matrix ***A***:

$$\boldsymbol{x}_{t+\Delta t} = \boldsymbol{A}\boldsymbol{x}_t$$

If any eigenvalue of ***A*** has magnitude exceeding 1, then any initially small errors (unavoidable in any numerical scheme) will increase without bound!

A simple estimate can be found by considering the analogy between a particle packing and a structural system via the eigenvalues of the stiffness:

$$\Delta t_{\text{crit}} = \frac{2}{\omega_{\max}}$$



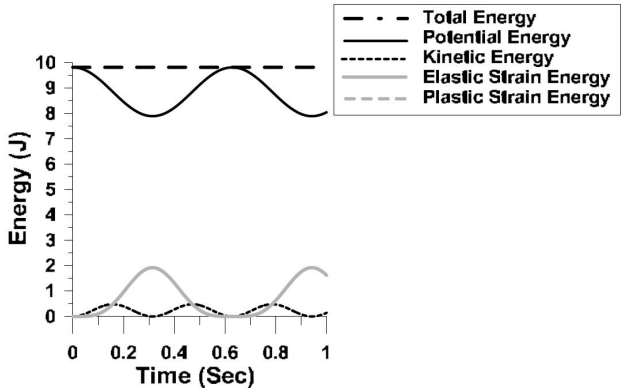
Critical time step:

An even simpler estimate is obtained by equivalence to a linear strut model connecting two particles in the assembly:

$$\Delta t_{\text{crit}} = \alpha\sqrt{m/k_n}$$

Enhancing stability

We can monitor development of instabilities by considering the energy balance in the system.



Since the critical time step is proportional to the (square root of the) particle mass, a common strategy is to artificially increase particle density to be able to take larger time steps. This is called **density scaling**. May only be applied to quasistatic problems or when the steady state solution is of interest.

The other possible strategy is to switch to an **implicit scheme**, but this might be **complex** to implement and often requires **computationally expensive** iterations within each time increment.

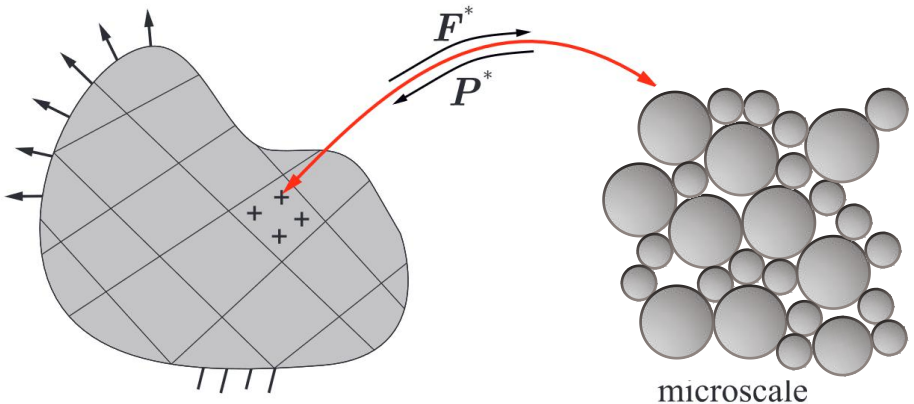
Global damping

Typically for quasistatic problems, to dampen out particle vibrations, we also introduce numerical global damping. Care should be taken to keep numerical damping low, and monitor its effect (e.g. through energy balance analysis).

This can also to account for mechanisms not described by the particle interactions e.g. simulate the effect of **movement through a viscous fluid**.

Outlook

- Computional homogenization and coarse-graining
- Analysis of fabric and structural signatures
- Periodic boundary conditions
- Various numerical/algorithmic aspects



Discussion

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Particulate Discrete Element Modeling,
C. O'Sullivan

Chapters 5,7,9,10