Entropy model for granular materials at the critical state

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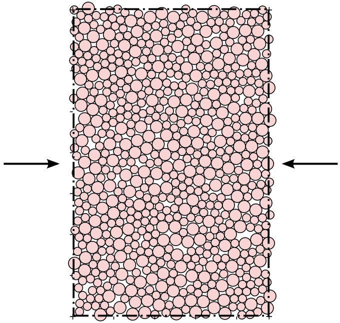
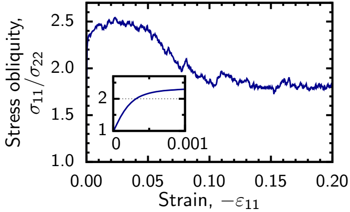
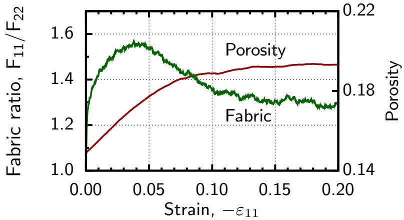
The Critical State in Geomechanics

Bi-axial compression of a 2D disk assembly:







Critical State at the Micro-scale

Questions:

- At a micro-scale, is anything unusual at the critical state?

- Can we predict micro-scale statistics of fabric?

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- Focus: Contact forces, movements, and orientations at the critical state.
- 2D materials only. Biaxial loading conditions.
- Six contact quantities
- Objective: Probability density distributions of these quantities

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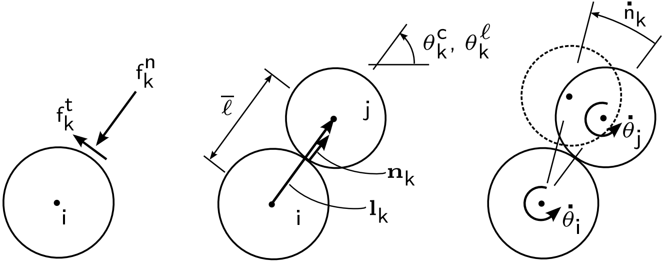

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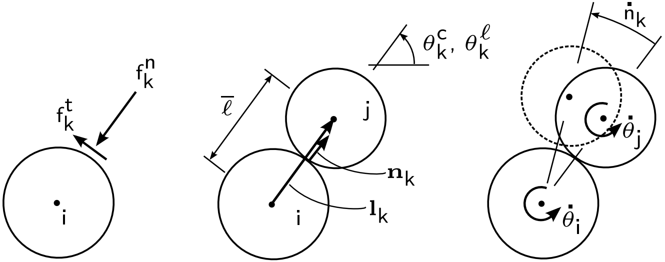

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Contact model

Contact model:

- We focus on the contacts, ignoring the particles
- No contact elasticity — a purely rigid-frictional model
- No application of affine fields — no static or kinematic hypotheses
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- A flow model — contacts are either sliding or non-sliding

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Contact model

Rigid-frictional contact restrictions:

$$g_k^{\mathrm{n}} \in \mathbb{R}^+$$

Contact sliding

$$g_k^{\mathrm{t}} \in \begin{cases} -\mu g_k^{\mathrm{n}} & \Leftarrow \quad \dot{n}_k - \dot{\phi}_k < 0 \\ (-\mu g_k^{\mathrm{n}}, \mu g_k^{\mathrm{n}}) & \Rightarrow \quad \dot{n}_k - \dot{\phi}_k = 0 \\ \mu g_k^{\mathrm{n}} & \Leftarrow \quad \dot{n}_k - \dot{\phi}_k > 0 \end{cases}$$

Probability density

Probability density function of the six contact quantities:

$$p(\cdots) = p(f^{\mathrm{n}}, f^{\mathrm{t}}, \theta^{\mathrm{c}}, \theta^{\ell}, \dot{n}, \dot{\phi})$$

This probability density must conform to certain constraints

$$\int_{\{f^{\mathrm{n}}, f^{\mathrm{t}}, \theta^{\mathrm{c}}, \theta^{\ell}, \dot{n}, \dot{\phi}\}} \cdots \int \Gamma_i(\cdots)\, p(\cdots) = \overline{\Gamma}_i$$

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Constraint #1

Constraint #1: mean stress = p_o

$$\int_{\{f^n, f^t, \theta^c, \theta^\ell, \dot{n}, \dot{\phi}\}} \cdots \int f^n p(\cdots) = 2p_o\bar{\ell}\left(\frac{M}{A}\right)^{-1}$$

Constraint #2

Constraint #2: frictional dissipation at the contacts must be consistent with the stress-work

$$\frac{1}{A}\sum f_k^{\mathrm{t}}\,\overline{\ell}\,(\dot{n}_k - \dot{\phi}_k) = \boldsymbol{\sigma} : \mathbf{D} \qquad \text{with} \quad \mathbf{D} = \begin{bmatrix} -\dot{\varepsilon} & 0 \\ 0 & \dot{\varepsilon} \end{bmatrix}$$

or

$$\int \cdots \int_{\{f^{\mathrm{n}}, f^{\mathrm{t}}, \theta^{\mathrm{c}}, \theta^{\ell}, \dot{n}, \dot{\phi}\}} \Big[f^{\mathrm{t}}(\dot{n}_k - \dot{\phi}_k) + \dot{\varepsilon} f^{\mathrm{n}}(-\cos^2\theta^{\mathrm{c}} + \sin^2\theta^{\mathrm{c}}) - \dot{\varepsilon} f^{\mathrm{t}}(-2\cos\theta^{\mathrm{c}}\sin\theta^{\mathrm{c}}) \Big] \; p(\cdots) = 0$$

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Constraint #3

Constraint #3: isochoric flow

$$\mathrm{tr}(\mathbf{D}) = 0$$

or

$$\underbrace{\int \cdots \int}_{\{f^{\mathrm{n}}, f^{\mathrm{t}}, \theta^{\mathrm{c}}, \theta^{\ell}, \dot{n}, \dot{\phi}\}} K(\theta^{\mathrm{c}}, \theta^{\ell})\, \dot{n}\, (\sin\theta^{\mathrm{c}} \sin\theta^{\ell} + \cos\theta^{\mathrm{c}} \cos\theta^{\ell})\, p(\cdots) = 0$$

$$K(\theta^{\mathrm{c}}, \theta^{\ell}) = \begin{cases} \frac{1}{2} - \frac{1}{2\pi}\mathrm{mod}(\theta^{\ell} - \theta^{\mathrm{c}}, 2\pi) & \theta^{\ell} \neq \theta^{\mathrm{c}} \\ 0 & \theta^{\ell} = \theta^{\mathrm{c}} \end{cases}$$

Constraint #4

Constraint #4: 11.2% of contacts are sliding (from DEM data).

These constraints do not (by themselves) determine the full probability density $p(\cdots)$. Example...

Constraint #1: mean stress = p_{o}

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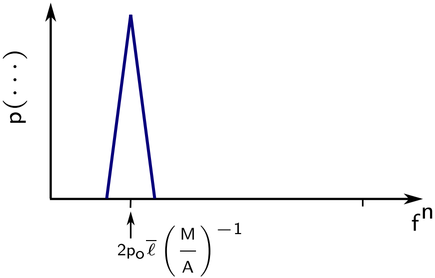

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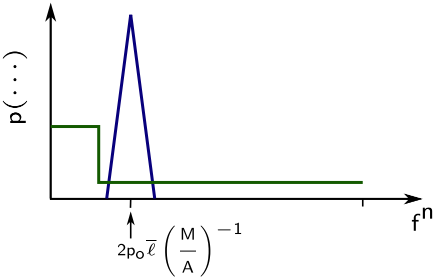

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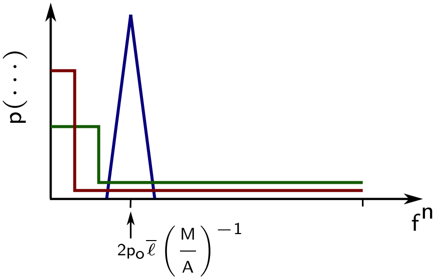

Disorder

The Shannon entropy associated with the probability density:

$$H\{p(\cdots)\} = -\underset{\{f^{\mathrm{n}}, f^{\mathrm{t}}, \theta^{\mathrm{c}}, \theta^{\ell}, \dot{n}, \dot{\phi}\}}{\int \cdots \int} p(\cdots) \ln(p(\cdots))$$

The density $p(\cdots)$ with the largest entropy corresponds to the most likely "macro-state" and encompasses the broadest combination of the 6 contact quantities.

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Disorder, continued

Entropy H is maximized with the following probability density:

$$p(\cdots) = \frac{1}{Z(\cdots)} \exp\left(- \sum_{i=1}^{4} \lambda_i \Gamma_i(\cdots) \right)$$

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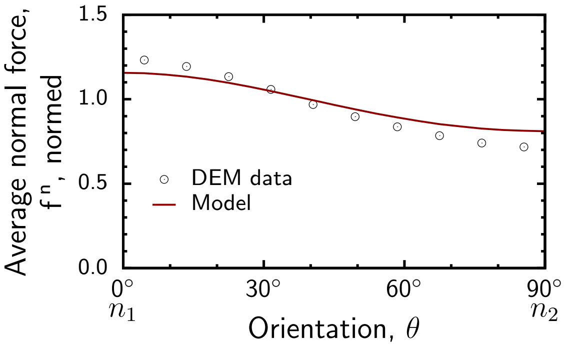
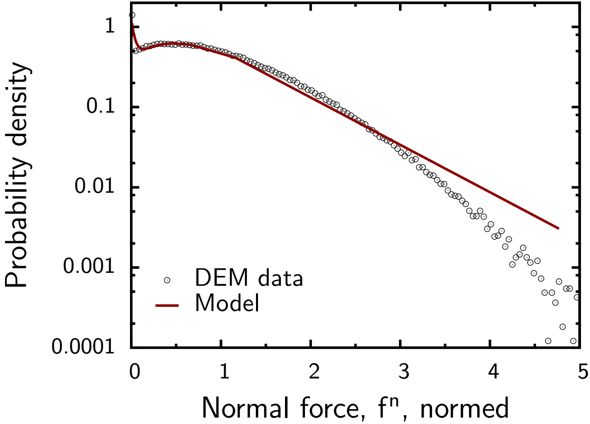
Anisotropy

Anisotropy of contact forces:



Normal forces

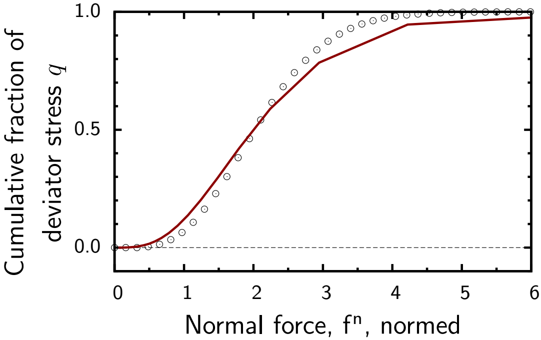
Probability density of the normal contact forces:



Weak-strong contacts

Contribution of contacts to the bulk deviatoric stress.

Other investigators have found that the most heavily loaded contacts account for nearly the entire deviatoric stress.



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References

- M. R. Kuhn, "Boundary integral for gradient averaging in two dimensions: application to polygonal regions in granular materials," *Int. J. Num. Methods Engrg.*, (2004) Vol. 59, No. 4, 559–576.
- M. R. Kuhn, "Dense granular flow at the critical state: maximum entropy and topological disorder," *Granular Matter*, (2014) Vol. 16, No. 4, 499–508.