

Discrete Models for Granular Materials

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Multiscale Mathematics and Engineering
Seminar Series

Outline

- 1 Introduction & Scope
- 2 Examples of Granular Behavior
 - Softening examples
 - Instability examples
 - Localization example
- 3 Origins and Scaling of Behavior
 - Softening
 - Instability
 - Localization
- 4 Summary

Introduction & Scope

Limitations of the talk !!

- Possible ranges of behavior
 - Rapid flows (single- and multi-phase)
 - Quasi-static behavior — small strains
 - **Quasi-static behavior — large strains**
- Quasi-static (time-invariant) behavior of dense packings
- Emphasis on behavior at large strains
- Emphasis on micro- and meso- scales

Introduction

Discrete simulation models:

- Discrete Element Method (DEM, Cundall) —
Molecular Dynamics (MD)
- Discontinuous Deformation Analysis (DDA, Shi) —
Granular Element Method (GEM, Kishino)
- Contact Dynamics (CD, Moreau)

Five Examples of Granular Behavior

Dominant behaviors at **large strains**:

- Softening (2 examples)
- Instability (2 examples)
- Localization (1 example)

Outline

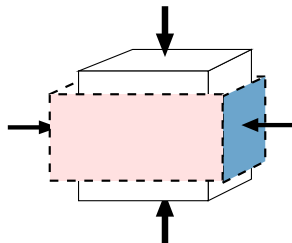
- 1 Introduction & Scope
- 2 **Examples of Granular Behavior**
 - **Softening examples**
 - Instability examples
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Example #1: Granular Softening

Softening of 4096 spheres — DEM simulation

Densely packed

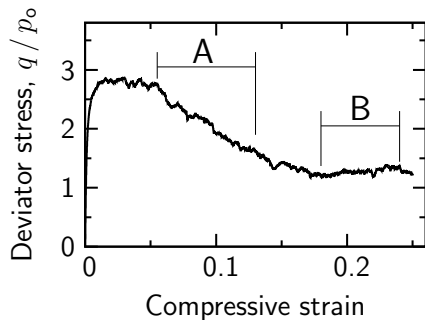
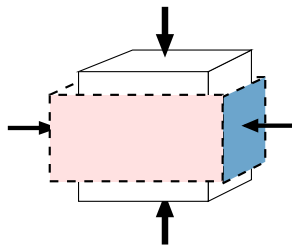
Plane-strain, biaxial compression



Example #1: Granular Softening

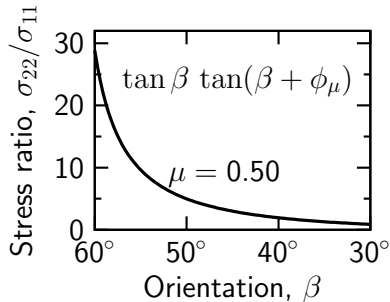
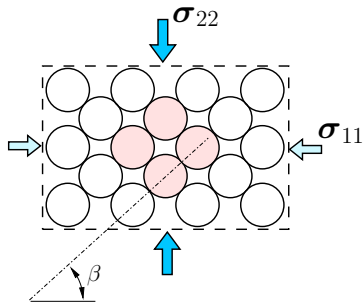
Softening of 4096 spheres — DEM simulation

Plane-strain, biaxial compression



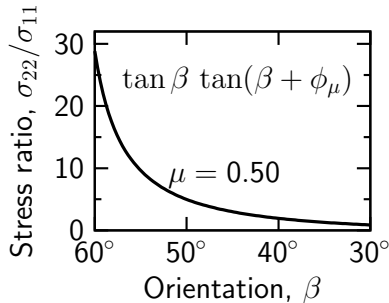
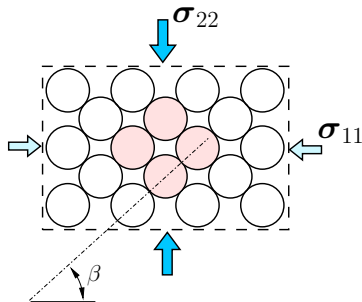
Example #2: Granular Softening

Softening of a regular 2D array



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Softening of a regular 2D array



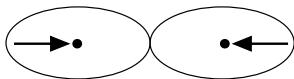
$$\int_{\partial V} (d\mathbf{u} \cdot d\mathbf{f}) < 0 \quad \text{or} \quad [d\mathbf{u}]^T [d\mathbf{f}] < 0$$

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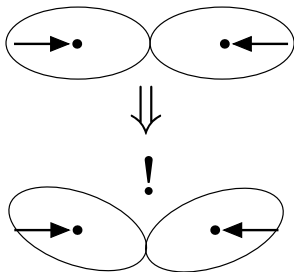
Example #3: Instability

Instability of 2-particle systems



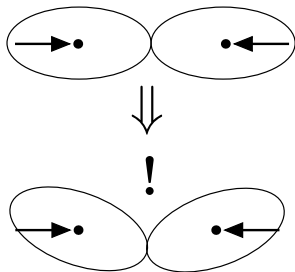
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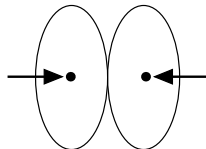


Example #3: Instability

Instability of 2-particle systems



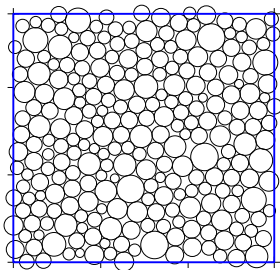
Stable system:



Example #4: Instability

Instability in 256 disks — DEM simulation

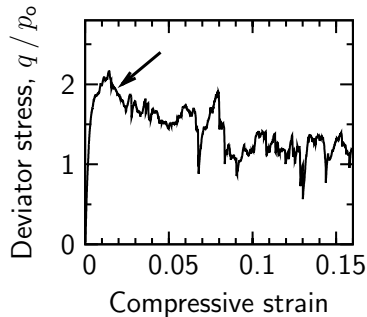
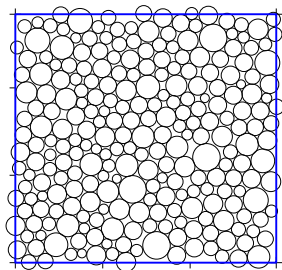
Biaxial compression



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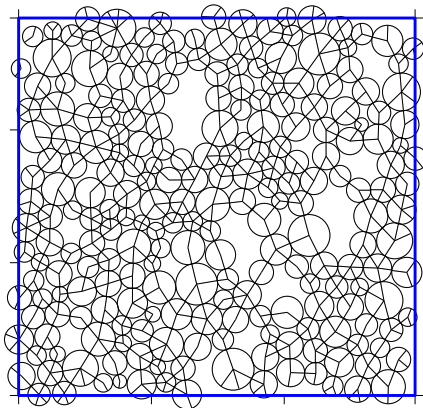
Instability in 256 disks — DEM simulation

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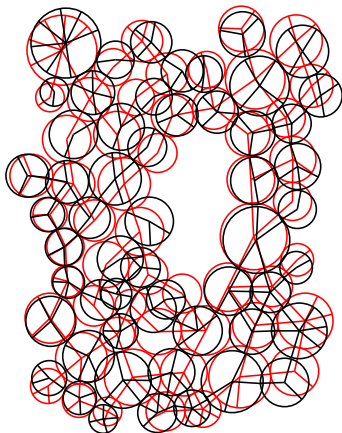
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256 disks — DEM simulation



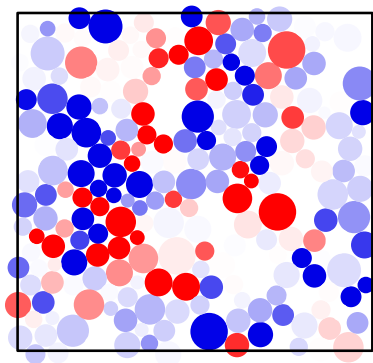
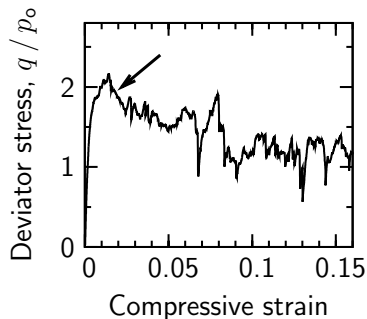
Example #4: Instability

256 disks — Detail around a granular “hole”



Example #4: Instability

256 disks — Plot of internal instability

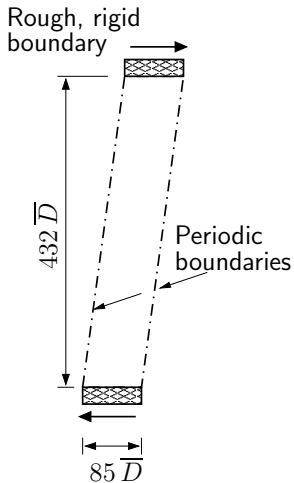


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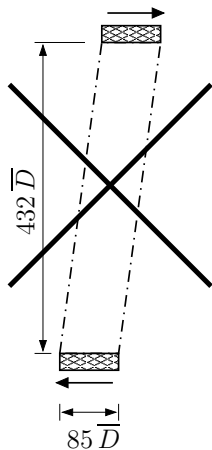
Example #5: Localization

Localization in 40,500 disks — DEM simulation



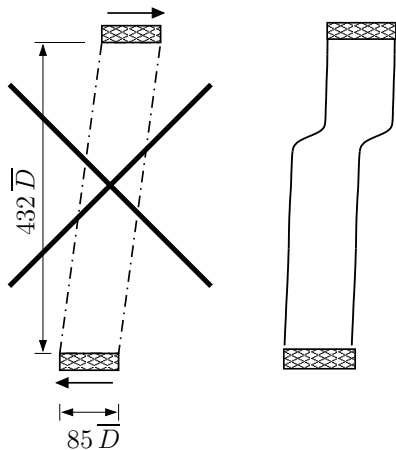
Example #5: Localization

40,500 disks — Localized shearing



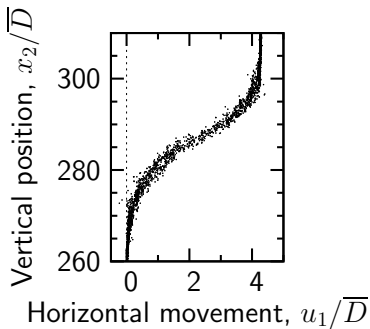
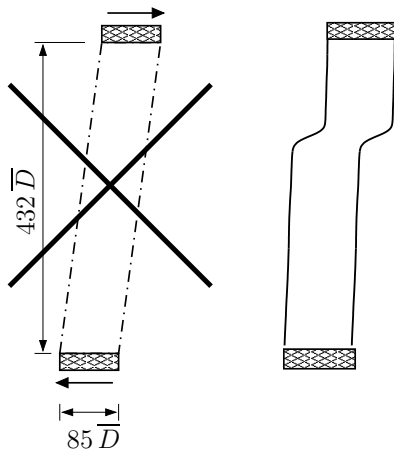
Example #5: Localization

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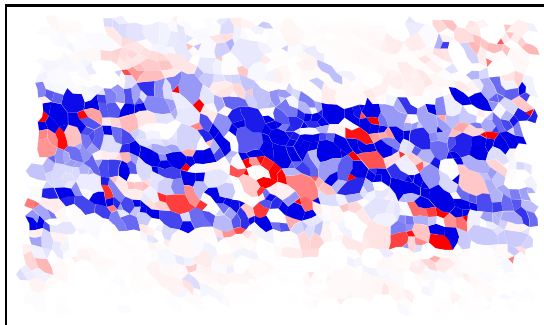
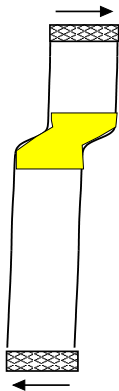
Example #5: Localization

40,500 disks — Localized shearing



Localization

Localization inside of a shear band



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Granular Softening

Origins of granular softening:

1) Mechanical

Produced by contact deformations

Depends upon particle material properties

Granular Softening

Origins of granular softening:

1) Mechanical

Produced by contact deformations

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2) Geometric

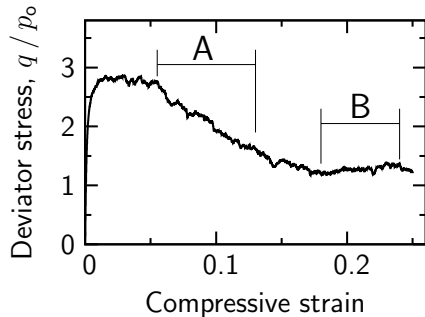
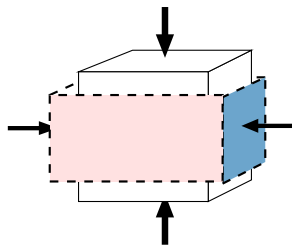
Produced by contact re-orientations

Depends upon particle shapes

Example: Granular Softening

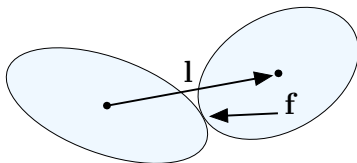
Softening of 4096 spheres — DEM results

Plane-strain, biaxial compression



Granular Softening

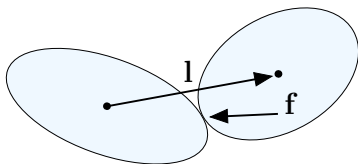
Calculation of average stress



$$\sigma = \frac{1}{V} \sum \mathbf{l} \otimes \mathbf{f}$$

Granular Softening

Calculation of **stress increment**

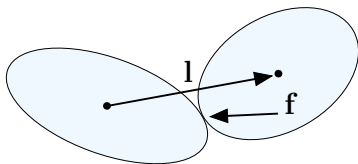


$$\sigma = \frac{1}{V} \sum \mathbf{l} \otimes \mathbf{f}$$

$$d\sigma = -\frac{dV}{V}\sigma + \underbrace{\frac{1}{V} \sum \mathbf{l} \otimes d\mathbf{f}}_{\text{Mechanical}} + \underbrace{\frac{1}{V} \sum d\mathbf{l} \otimes \mathbf{f}}_{\text{Geometric}}$$

Granular Softening

Calculation of **stress increment**

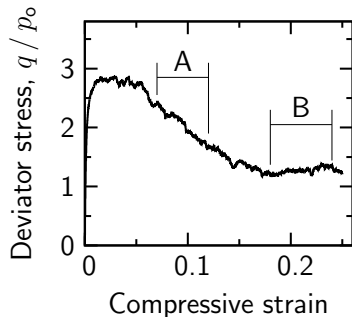


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Granular Softening — Example

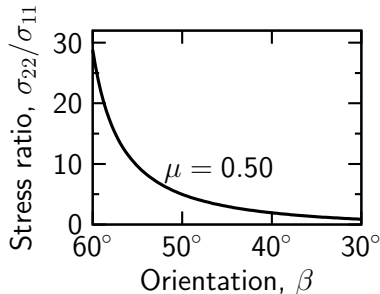
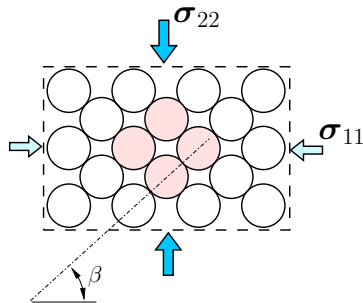
Stress rates during loading, $d\sigma/k d\epsilon \times 1000$



	A	B
Mechanical	-2.9	+1.4
Geometric	-1.7	-1.4
$\Sigma =$	-4.6	0

Granular Softening — Another Example

Softening of a regular array of disks



Here, softening is entirely *geometric* !

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Granular Instability

Origins of granular stiffness:

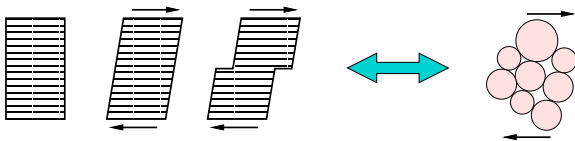
- 1) Mechanical
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Granular Instability

Origins of granular stiffness:

- 1) Mechanical
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Example:

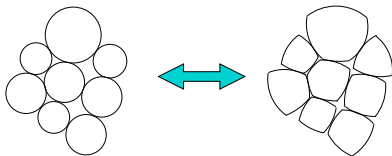


Granular Instability

Origins of granular stiffness:

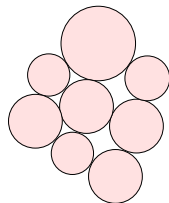
- 1) Mechanical
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Another example:



Granular Stiffness and Instability

Incremental stiffness of a particle assembly:



Particle
movements

$$\left[\frac{d\mathbf{u}}{d\theta} \right]$$



External
forces & moments

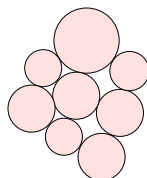
$$\left[\frac{d\mathbf{f}}{d\mathbf{m}} \right]$$

Contact model: soft contacts, time invariant

GEM, Y. Kishino, 1989

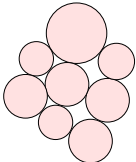
Granular Stiffness and Instability

Incremental stiffness matrix:


$$\left[\mathbf{K} \right] \left[\frac{d\mathbf{u}}{d\theta} \right] = \left[\frac{df}{dm} \right]$$

Granular Stiffness and Instability

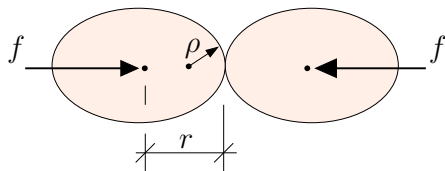
Incremental stiffness matrix:



$$\left(\left[\mathbf{K}^{\text{Mechanical}} \right] + \left[\mathbf{K}^{\text{Geometric}} \right] \right) \left[\frac{d\mathbf{u}}{d\theta} \right] = \left[\frac{d\mathbf{f}}{d\mathbf{m}} \right]$$

Kuhn & Chang 2005, PG2005

Granular Stiffness — Example

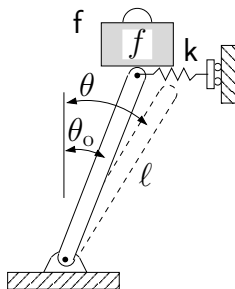


2-particle example,
 6×6 stiffness matrix

$$\underbrace{k \begin{bmatrix} 1 & 0 & 0 & | & -1 & 0 & 0 \\ 0 & 1 & r & | & 0 & -1 & r \\ 0 & r & r^2 & | & 0 & -r & r^2 \\ \hline -1 & 0 & 0 & | & 1 & 0 & 0 \\ 0 & -1 & -r & | & 0 & 1 & -r \\ 0 & r & r^2 & | & 0 & -r & r^2 \end{bmatrix}}_{\text{Mechanical}} + \frac{f}{2\rho} \underbrace{\begin{bmatrix} 0 & 0 & 0 & | & 0 & 0 & 0 \\ 0 & -1 & \rho - r & | & 0 & 1 & \rho - r \\ 0 & \rho - r & \rho^2 - r^2 & | & 0 & r - \rho & (\rho - r)^2 \\ \hline 0 & 0 & 0 & | & 0 & 0 & 0 \\ 0 & 1 & r - \rho & | & 0 & -1 & r - \rho \\ 0 & \rho - r & (\rho - r)^2 & | & 0 & r - \rho & \rho^2 - r^2 \end{bmatrix}}_{\text{Geometric}}$$

Structural Stiffness — Analogy

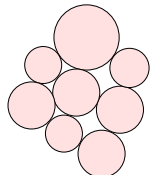
Mechanical and geometric stiffnesses of a simple structure:



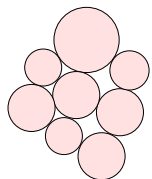
$$[\mathbf{K}][d\theta] = [df]$$

$$\underbrace{\left[k \left(\sin \theta_0 + \frac{\cos 2\theta}{\sin \theta} \right) \right]}_{\text{Mechanical}} - \underbrace{\left[\frac{f}{l} \cot \theta \right]}_{\text{Geometric}} l d\theta = df$$

Instability and Softening — Criteria


$$\left(\left[\mathbf{K}^{\text{Mechanical}} \right] + \left[\mathbf{K}^{\text{Geometric}} \right] \right) \left[\frac{d\mathbf{u}}{d\theta} \right] = \left[\frac{d\mathbf{f}}{d\mathbf{m}} \right]$$

Instability and Softening — Criteria

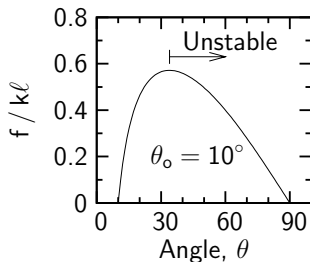
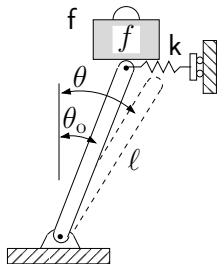


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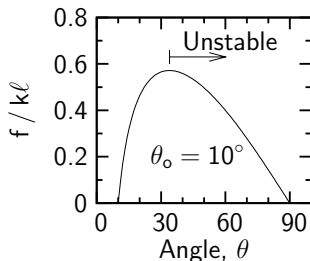
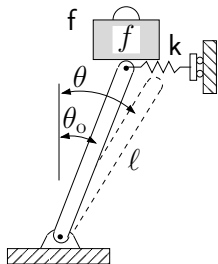
Second-order work criteria for discrete systems:

$$\delta^2 W = \left[\frac{d\mathbf{u}}{d\theta} \right]^T \left[\frac{d\mathbf{f}}{d\mathbf{m}} \right] < 0 \quad \left\{ \begin{array}{l} 1) \text{ Necessary for instability} \\ 2) \text{ Sufficient for softening} \\ \quad \text{in the direction } [d\mathbf{u}/d\theta] \end{array} \right.$$

Structural Instability and Softening — Analogy



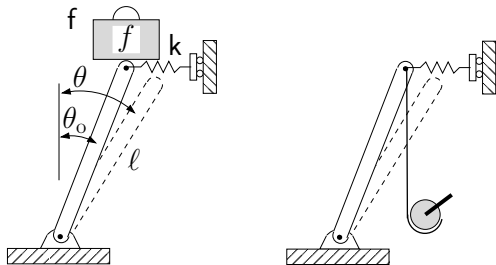
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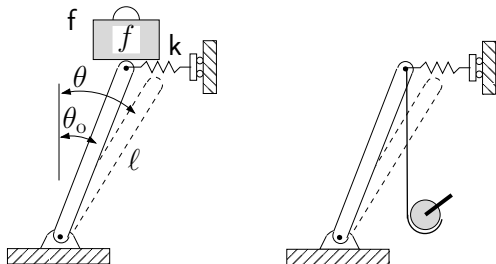
Second-order work criteria:

$$\delta^2 W = l d\theta \cdot df < 0 \quad \Rightarrow \quad \begin{array}{c} \text{Unstable} \\ \text{and} \\ \text{Softening} \end{array}$$

Structural Instability and Softening — Analogy



Structural Instability and Softening — Analogy



Second-order work criteria:

$$\delta^2 W = l d\theta \cdot d\mathbf{f} < 0 \quad \Rightarrow \quad \begin{array}{c} \text{Stable} \\ \text{but} \\ \text{Softening} \end{array}$$

Granular Instability and Softening

Investigating granular instability, $\delta^2 W < 0$:

Discrete systems \longrightarrow Search eigenvalues of $[\mathbf{K}]^{\text{Symmetric}}$

Difficulties:

- 1) Non-symmetric, $[\mathbf{K}] = [\mathbf{K}^{\text{Mechanical}}] + [\mathbf{K}^{\text{Geometric}}]$
- 2) Incrementally non-linear \Rightarrow Multiple stiffness branches,

$$[\mathbf{K}] = \{ [\mathbf{K}^1], [\mathbf{K}^2], \dots \}$$

Must check multiple branches to investigate directional stability.

Granular Instability and Softening

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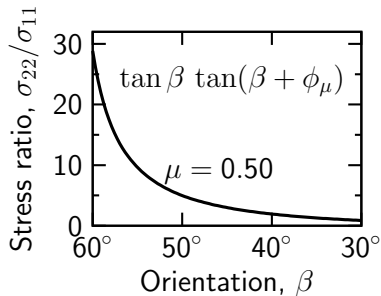
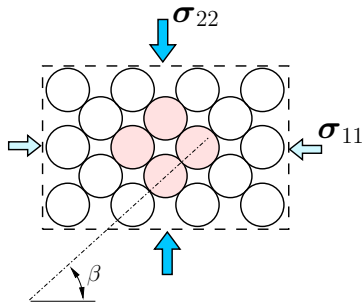
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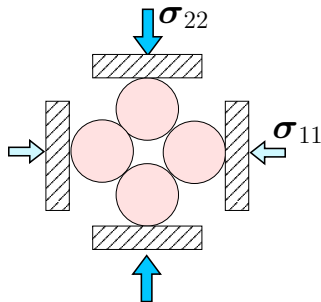
Granular Instability and Softening — Example

Internal instability during softening



Granular Instability and Softening — Example

Instability of 4 particles

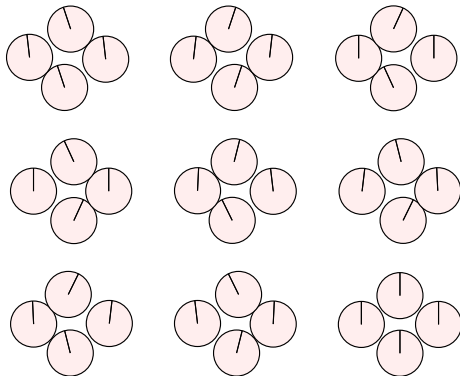


Search for unstable eigenmodes:

$$\lambda < 0 \Rightarrow \delta^2 W < 0$$

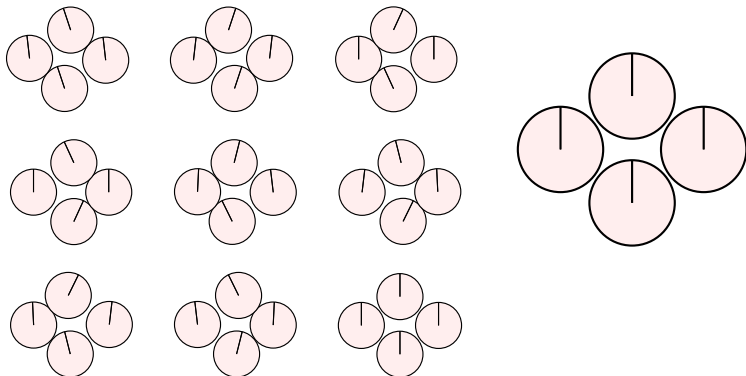
Granular Instability and Softening — Example

9 Unstable eigenmodes, with $\lambda < 0$:



Granular Instability and Softening — Example

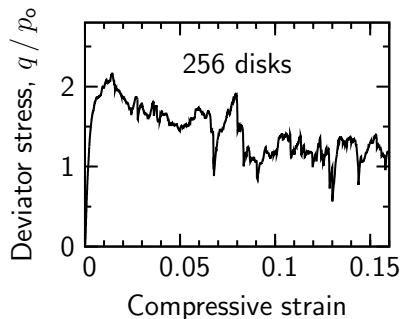
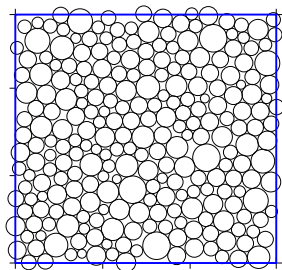
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Granular Instability and Softening — Another Example

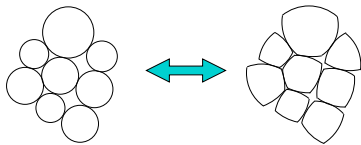
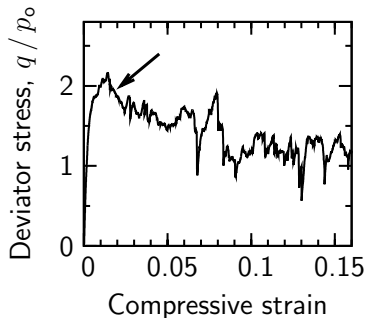
Softening and instability of 256 disks — DEM simulation

Biaxial compression



Granular Instability and Softening — Another Example

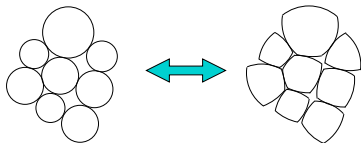
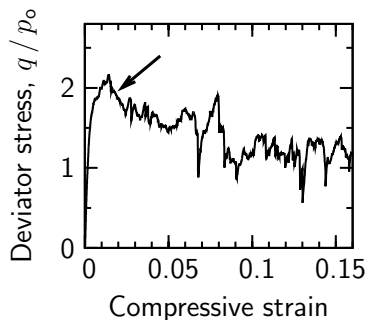
Softening — **effect of contact curvatures**



Incremental softening is **halted** when curvatures " ρ " are increased by 12%.

Granular Instability and Softening — Another Example

Softening — **effect of contact curvatures**

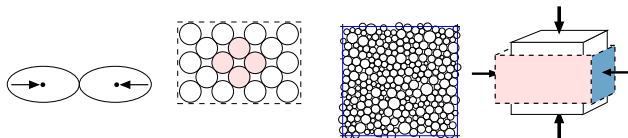


Incremental softening is **halted** when curvatures “ ρ ” are increased by 12%.

Granular Instability and Softening

Sources of instability and softening (negative 2nd-order work)

1) Geometric stiffness



2) Mechanical stiffness

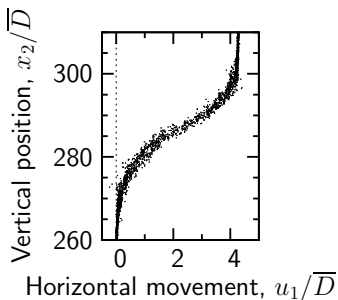
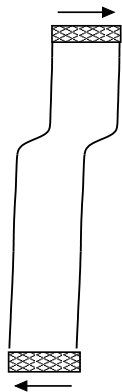
- a) Contact friction
- b) Particle fracture

Outline

- 1 Introduction & Scope
- 2 Examples of Granular Behavior
 - Softening examples
 - Instability examples
 - Localization example
- 3 Origins and Scaling of Behavior
 - Softening
 - Instability
 - **Localization**
- 4 Summary

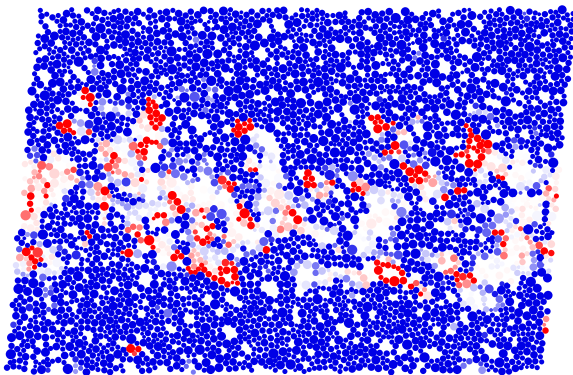
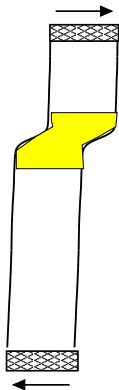
Localization — Softening — Instability

Localization in the shearing of 40,500 disks



Localization — Softening — Instability

Hardening and softening inside a shear band — $\delta^2 W$



Summary

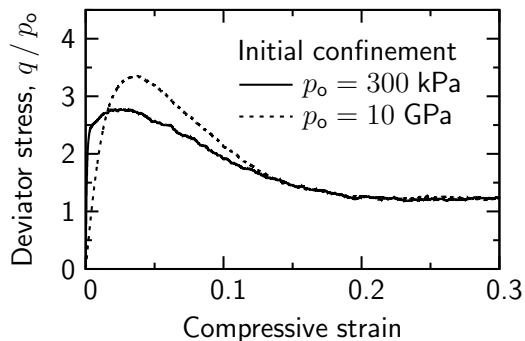
At large strains . . .

- Discrete simulation models, such as the DEM, permit the study of micro-, meso-, and macro-scale behaviors.
- At the micro-scale, the DEM reveals exceedingly complex micro-scale behavior.
- This complexity gives rise to macro-scale phenomena: softening, instability, and localization.
- Stiffness (matrix) models offer a means of studying these phenomena.

Questions

Scaling of Granular Behavior

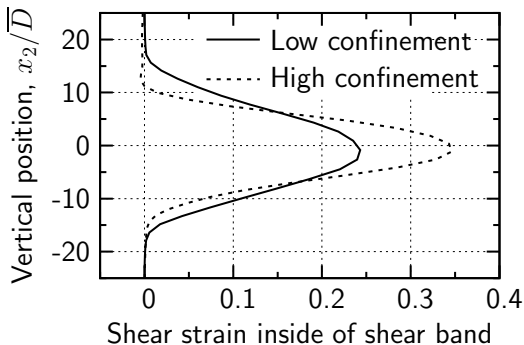
Effect of confinement pressure on strength
4096 “durable” spheres — DEM simulations



Scaling of Granular Behavior

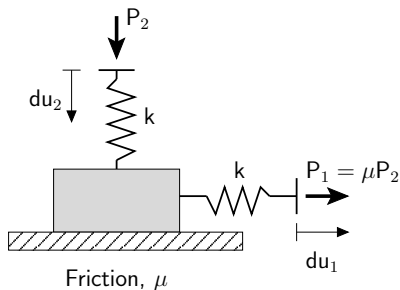
Effect of confinement pressure on **shear band thickness**

4096 “durable” spheres — DEM simulations



Granular Instability and Softening

Contact friction can produce instability and softening:



Negative 2nd-order work,

$$\delta^2 W = du_1 dP_1 + du_2 dP_2 < 0$$

when $du_2 < 0$ and $du_1 > \frac{1}{\mu} |du_2|$

(Mandel, Bažant)