

# Multi-scale Phenomena in Granular Materials

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Workshop on Multi-scale Modeling of Materials  
*University of Puget Sound, Tacoma, WA*



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# Outline

- 1 Introduction & scope
- 2 Scale-dependent phenomena
- 3 Obstacles to multi-scale modeling
- 4 Possible multi-scale models

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- 1 Introduction & scope
  - Introduction
  - Behavior domains
  - Macro-scale behavior
- 2 Scale-dependent phenomena
- 3 Obstacles to multi-scale modeling
- 4 Possible multi-scale models

# Introduction

## Granular materials:

- Assemblies of particles
- Bulk behavior is a consequences of particle interactions
- The “micro-scale” is well defined: individual particles
- The good news: amenable to direct, computational simulation
- The bad news: bulk behavior is complex, with multiple domains of behavior.

# Introduction

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- **The bad news: bulk behavior is complex, with multiple domains of behavior.**

# Behavior domains

Domains of granular behavior:

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Slow deformation	or	Rapid flow
Small-strain behavior	or	Large-strain behavior
Unbonded particles	or	Bonded particles
Contact interaction	or	Long-range interaction
Soft particles	or	Hard particles
Single phase	or	Multiple phases
2D	or	3D

---

# Behavior domains

Domains of granular behavior:

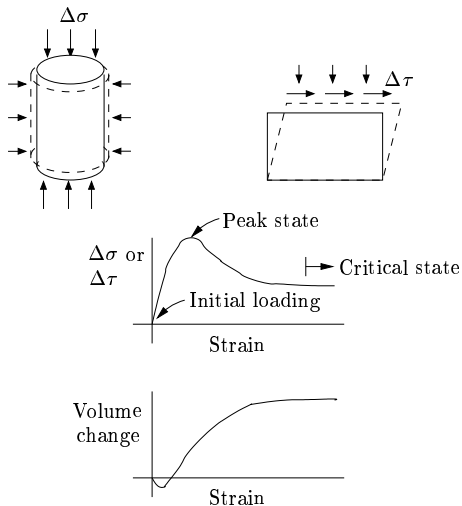
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# Typical macro-scale behavior (slow loading)



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- 1 Introduction & scope
- 2 Scale-dependent phenomena**
  - Force chains — Circulation cells — Rotation chains
  - Micro-bands — Dilation clusters
  - Crushing — Shear bands
- 3 Obstacles to multi-scale modeling
- 4 Possible multi-scale models

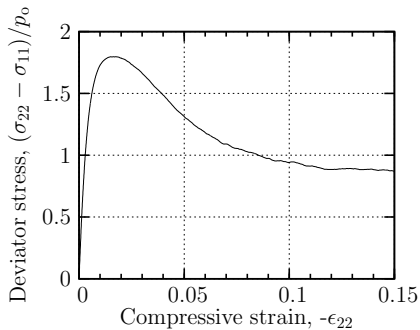
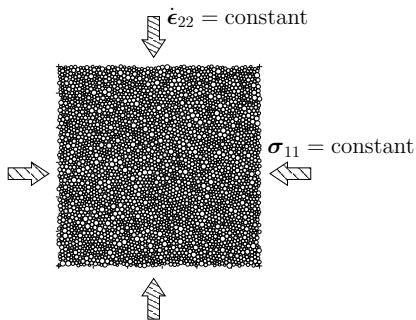
## Internal behavior — localization

### Scale-dependent, localization phenomena

- Force chains
- Circulation cells
- Rotation chains
- Micro-bands
- Dilation clusters
- Size-dependent crushing
- Shear bands and faulting

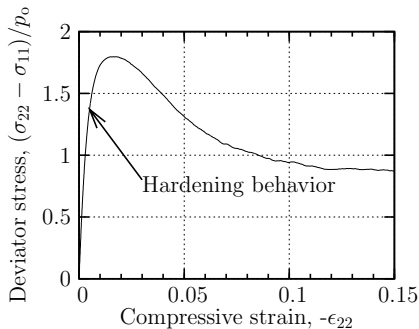
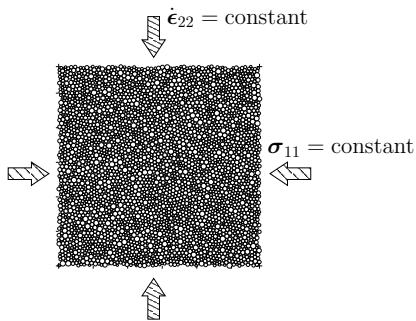
## 2D simulations

Biaxial compression of 4096 disks:

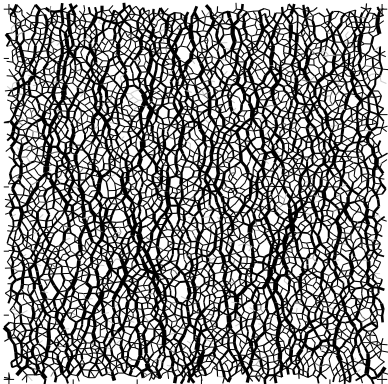


## 2D simulations

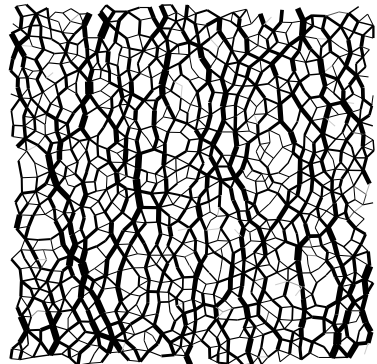
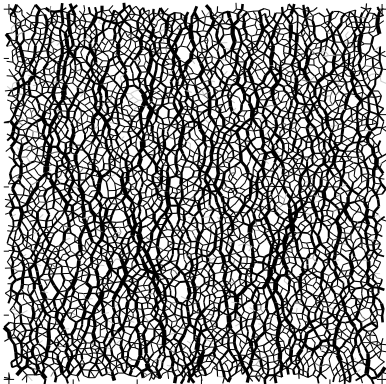
Biaxial compression of 4096 disks:



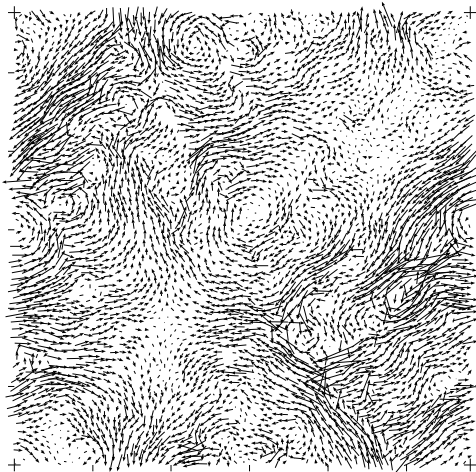
# Force chains



# Force chains

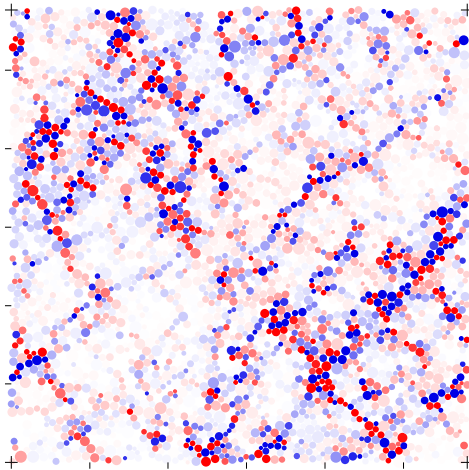


# Circulation cells





# Rotation chains

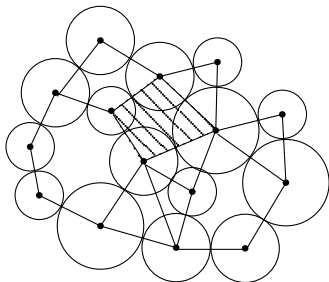


## Internal behavior — localization, cont.

### Localization phenomena

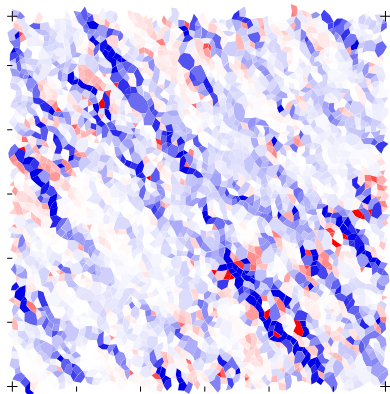
- Force chains
- Circulation cells
- Rotation chains
- **Micro-bands**
- **Dilation clusters**
- Size-dependent crushing
- Shear bands and faulting

## Particle graph — 2D

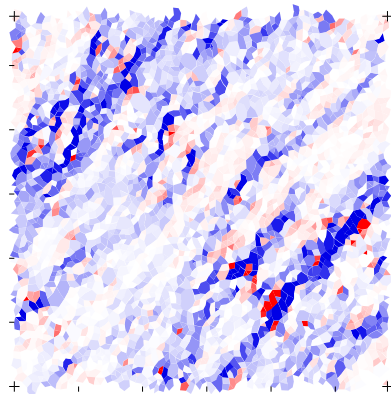
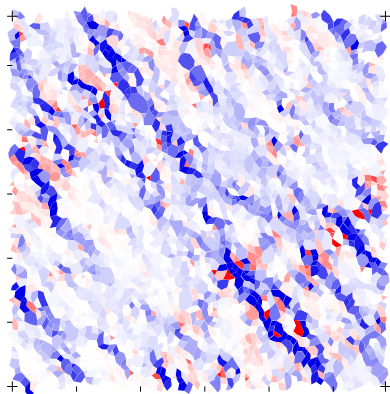


vertices → particles  
edges → contacts  
faces → void cells

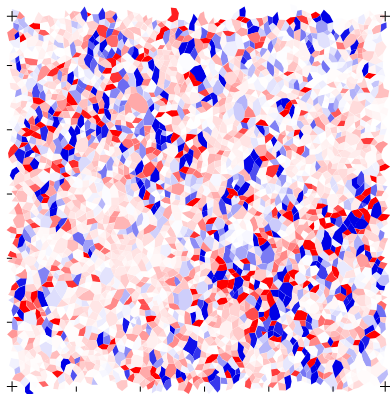
# Micro-bands



# Micro-bands



# Dilation clusters



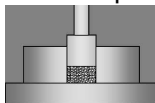
## Internal behavior — localization

### Scale-dependent, localization phenomena

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# Size-dependent crushing

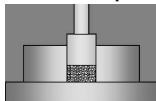
Uniaxial compression of an embedded agglomerate  
1MPa normal pressure





# Size-dependent crushing

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1MPa normal pressure



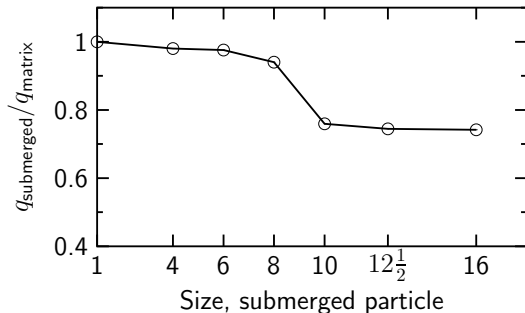
Size ratio  $\approx 3.5$



Size ratio  $\approx 10$

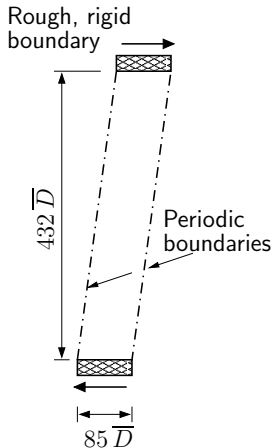
# Size-dependent crushing

Crushing tendency vs. Size of embedded particle



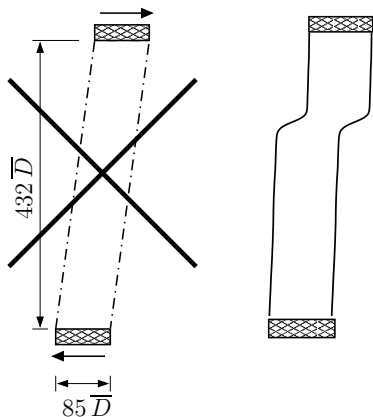
# Shear band localization

## Localization in 40,500 disks — DEM simulation



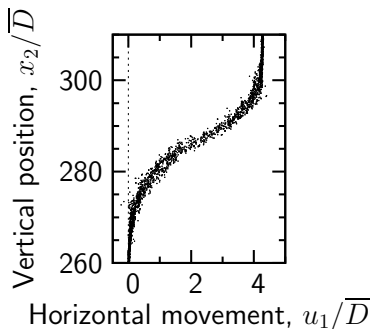
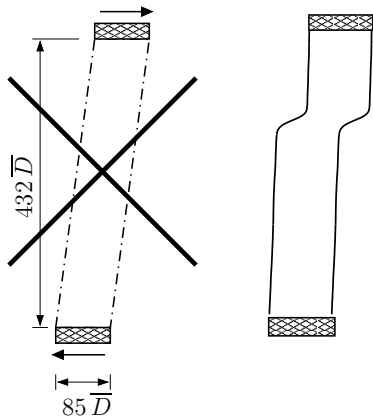
# Shear band localization

40,500 disks — Localized shearing



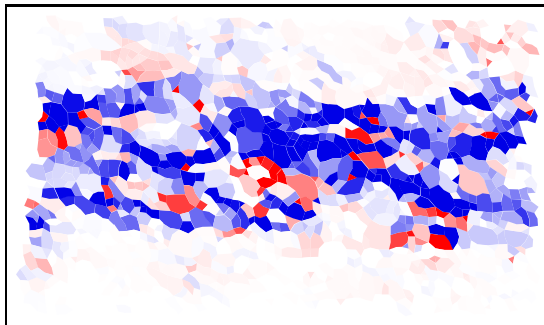
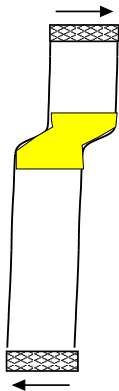
# Shear band localization

40,500 disks — Localized shearing



# Shear band localization

Localization inside of a shear band



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- 1 Introduction & scope
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- 3 Obstacles to multi-scale modeling**
  - Complex topology — Particle rotations
  - Heterogeneity
  - Misconceptions of friction
- 4 Possible multi-scale models

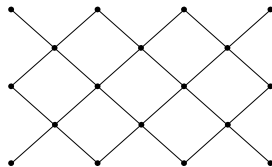
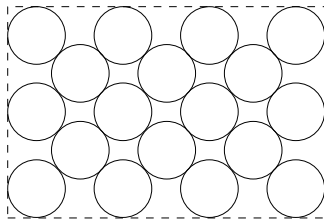
# Multi-scale modeling

Obstacles to the transition from micro to larger scales:

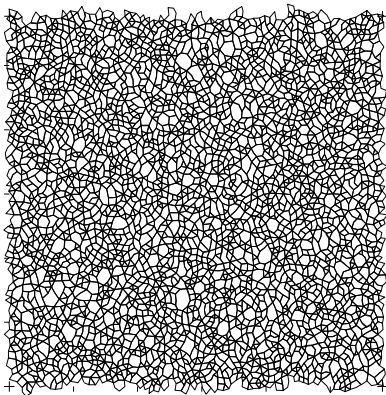
- **Complex micro-topology**
- Particle rotations
- Heterogeneous micro-scale deformation and stress
- Strength heterogeneity
- Misconceptions of friction



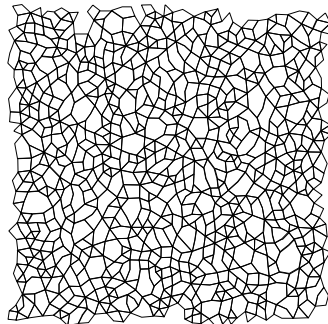
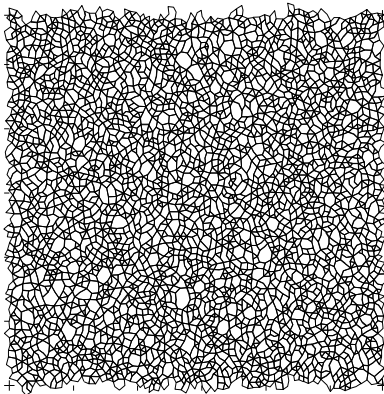
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# Obstacles to multi-scale modeling

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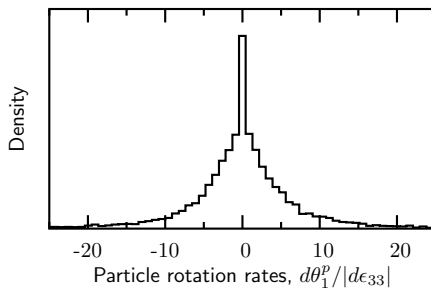
# Particle rotation complications

Particle rotations complicate the transition from micro to macro:

- 1) Particle rotations are large
- 2) Particle rotations soften/weaken the material response
- 3) Particle rotations are patterned *and* spatially organized

# Particle rotations are large

Histogram of particle rotations



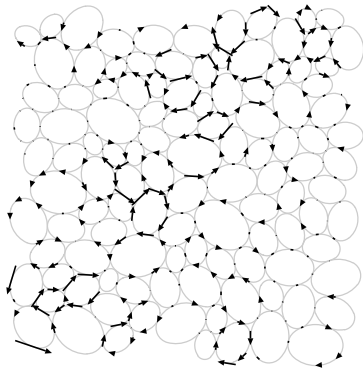
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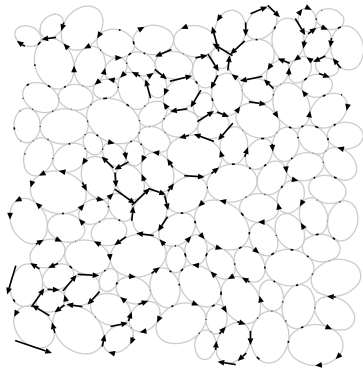
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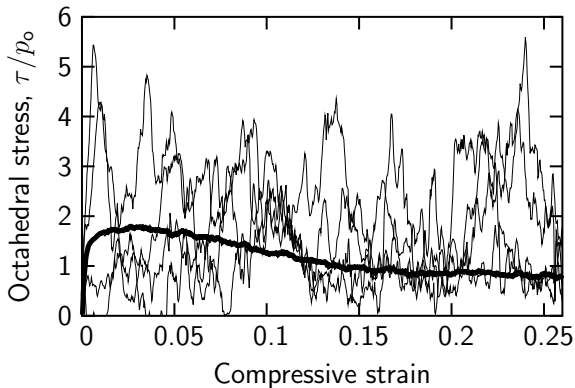
# Obstacles to multi-scale modeling

Obstacles to the transition from micro to larger scales:

- Complex micro-topology
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- Heterogeneous micro-scale deformation and stress
- Strength heterogeneity
- Misconceptions of friction

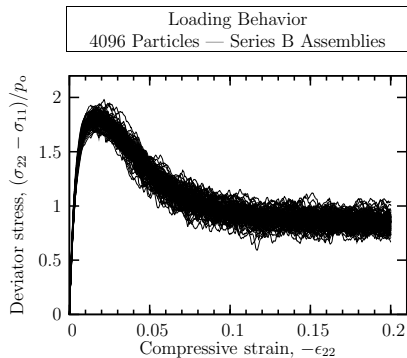
# Heterogeneous micro-scale stress

Stresses in **four** individual particles  
&  
Average stress among 4096 particles



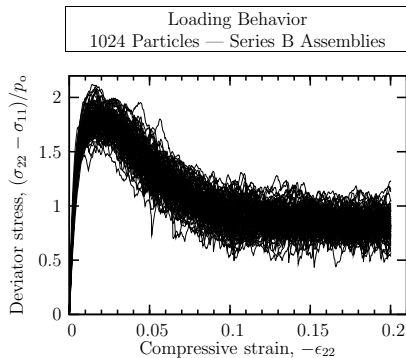
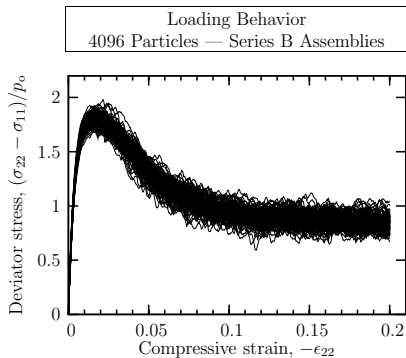
# Strength heterogeneity

Tests on 100 different assemblies:



# Strength heterogeneity

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# Obstacles to multi-scale modeling

Obstacles to the transition from micro to larger scales:

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- Heterogeneous micro-scale deformation and stress
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- **Misconceptions of friction**

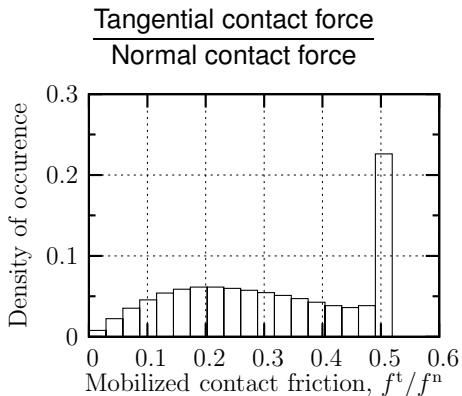
# Friction

## Misconceptions of friction

- Only a small minority of particle contacts are “slipping”
- Slipping contacts are spatially dispersed
- Micro- and macro-scale friction are poorly correlated

# Friction

Histogram of contact forces:





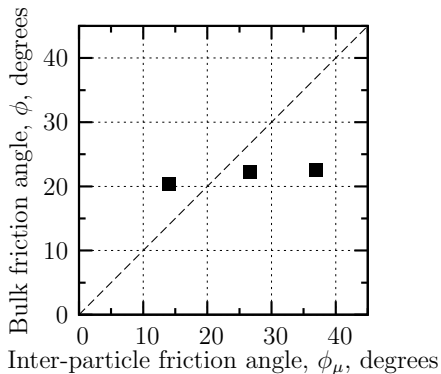
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## Misconceptions of friction

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# Friction

## Macro-scale vs. contact friction



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- 1 Introduction & scope
- 2 Scale-dependent phenomena
- 3 Obstacles to multi-scale modeling
- 4 Possible multi-scale models
  - Strain gradient dependent models
  - Non-local, integral-type models
  - Discrete stiffness models

# Strain gradient dependent models

Simple materials:

$$\sigma = f(\epsilon, \text{material parameters})$$

Gradient-dependent materials:

$$\sigma = f(\epsilon, \partial\epsilon/\partial\mathbf{x}, \partial^2\epsilon/\partial\mathbf{x}^2, \dots, \text{material parameters})$$

Are granular materials gradient-dependent?

# Strain gradient dependent models

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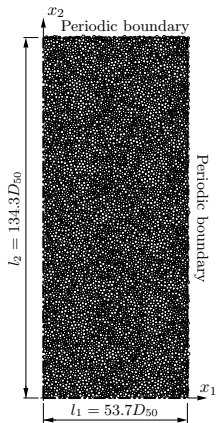
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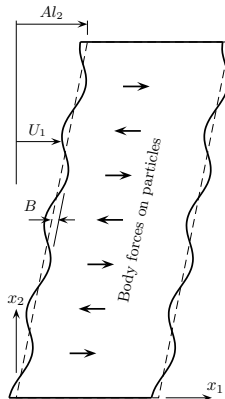
Are granular materials gradient-dependent?

# Strain gradient dependent models

## Experiments to determine strain gradient-dependence



Undeformed assembly

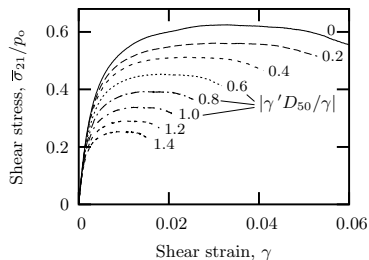


Boundary displacements

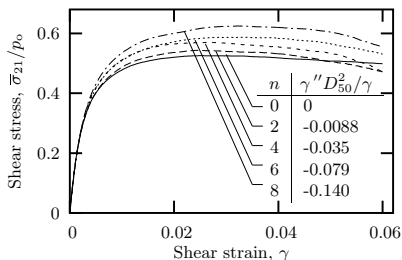
# Strain gradient dependent models

Experimental results:

Effect of the 1st gradient,  
 $d\epsilon_{12}/dx_2$



Effect of the 2nd gradient,  
 $d^2\epsilon_{12}/dx_2^2$





## Non-local models

In non-local models, stress at a point depends on an averaged strain  $\bar{\epsilon}$  within a region  $\mathcal{B}$  around the point:

$$\sigma = f(\bar{\epsilon}, \text{material parameters})$$

where

$$\bar{\epsilon} = \int_{\mathcal{B}} \Phi(\mathbf{x} - \mathbf{x}') \epsilon(\mathbf{x}') dV$$

The weighting kernel  $\Phi$  is usually a norm  $\rightarrow |\mathbf{x} - \mathbf{x}'|$ .

## Non-local models

An example non-local model:

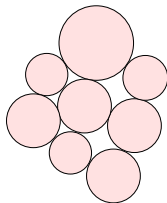
$$\bar{\epsilon} = \int_B \left( \frac{1}{\ell \sqrt{\pi}} e^{-\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\ell}\right)^2} \right) \epsilon(\mathbf{x}') dV$$

Unfortunate deficiencies:

- 1) When applied to experimental results, the length scale  $\ell$  is abnormally small: less than 2 particle diameters.
- 2) Experimental results suggest that the kernel  $\Phi$  must be asymmetric.

# Discrete stiffness models

Incremental stiffness of a particle assembly:



Particle  
movements

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

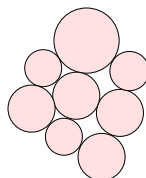


External  
forces & moments

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

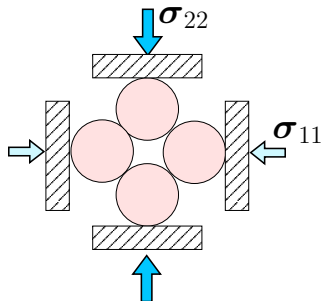
# Discrete stiffness models

Incremental stiffness matrix:


$$\left[ \mathbf{K} \right] \left[ \frac{d\mathbf{u}}{d\theta} \right] = \left[ \frac{d\mathbf{f}}{d\mathbf{m}} \right]$$

## Discrete stiffness models — example

Instability of 4 particles?

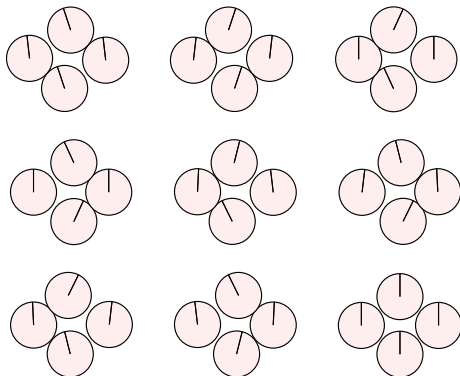


Search for unstable eigenmodes:

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

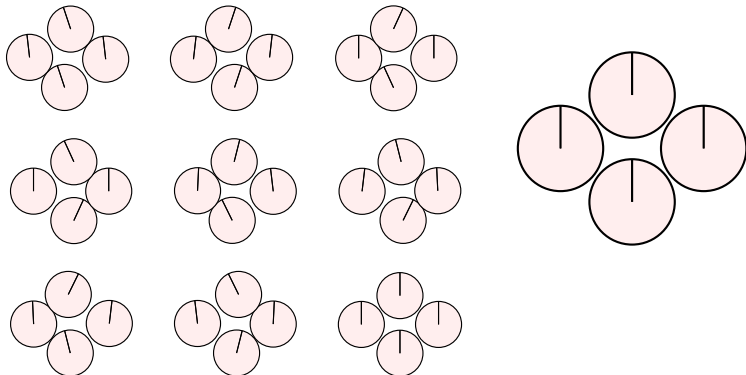
## Discrete stiffness models — example

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



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# Questions?