Multiscale characterization & modeling of granular matter

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Outline

• Motivation
• Elastoplasticity framework
• Multiscale framework
  • Semi-concurrent & Hierarchical schemes
• Representative examples
• Closure
Family of geomaterials across scales
Elastoplastic framework

Hooke’s law \[ \dot{\sigma} = c^{ep} : \dot{\varepsilon} \]

Additive decomposition of strain \[ \dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p \]

Convex elastic region \[ F(\sigma, \alpha) = 0 \]

Non-associative flow \[ \dot{\varepsilon}^p = \lambda g, \quad g := \partial G/\partial \sigma \]

K-T optimality \[ \lambda F = 0 \quad \chi H = -\partial F/\partial \alpha \cdot \dot{\alpha} \]

Elastoplastic constitutive tangent

\[ c^{ep} = c^e - \frac{1}{\chi} c^e : g \otimes f : c^e, \quad \chi = H - g : c^e : f \]
Simple plasticity model

**Yield function**

\[ F(I_1, I_2, \alpha) = \sqrt{\frac{3}{2}} I_2 + m(I_1, \alpha) - c(\alpha) \]

**Plastic potential**

\[ G(I_1, I_2, \alpha) = \sqrt{\frac{3}{2}} I_2 + \tilde{m}(I_1, \alpha) - \tilde{c}(\alpha) \]

**Friction**

\[ \mu = 3 \frac{\partial m}{\partial I_1} \]

**Dilatancy**

\[ \beta = 3 \frac{\partial \tilde{m}}{\partial I_1} \]

\[ 2\mu = -3\sqrt{6} \frac{\partial I_2}{\partial I_1} \]

\[ \beta = \frac{\partial \varepsilon^p_v}{\partial \varepsilon^p_s} \]
Simple plasticity model

\[ f = \frac{1}{3} \mu 1 + \sqrt{\frac{3}{2}} \hat{n} \]

\[ g = \frac{1}{3} \beta 1 + \sqrt{\frac{3}{2}} \hat{n} \]

friction & dilation affect constitutive response

hardening law

\[ \frac{\partial F}{\partial \mu} \dot{\mu} = -\lambda H \]

stress-dilatancy relation

\[ \begin{align*}
\mu &= \beta + \bar{\mu} \\
\text{friction strength} & \quad \text{dilatancy strength} & \quad \text{residual strength}
\end{align*} \]
Multiscale framework

$E, \nu$  
external elastic constants

$\beta \approx \frac{\partial \bar{\epsilon}_v}{\partial \bar{\epsilon}_s}$  
external extract dilation from micromechanics

$2\mu = -3\sqrt{6} \frac{\bar{I}_2}{\bar{I}_1}$  
external extract friction from micromechanics

total number of parameters: 2

$E, \nu$  
calibrated once for given material

warning: bypassing phenomenological hardening
experiments

extract strains $\Rightarrow$ dilatancy

Unit cell concept: experiments Vs. calculations

calculations

extract strains $\Rightarrow$ dilatancy
AND
extract stress $\Rightarrow$ friction

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Multiscale schemes: Semi-concurrent & Hierarchical
Semi-concurrent multiscale scheme
Hierarchical multiscale scheme

EXTRACT MICRO-MECHANICAL STATE

\[ \bar{\sigma} \quad \bar{\epsilon} \]

CONTINUUM MODEL

DISCRETE MODEL

PIV

DEFORMATION

UPDATE CONTINUUM PLASTICITY

\[ F(., \mu) Q(., \beta) \]

Hierarchical multiscale scheme

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Homogeneous predictions

DEM-based calcs with multi-cell computations
Semi-concurrent DEM-based multiscale
\[
\bar{\sigma} = \text{sym} \left[ \frac{1}{V} \sum_{n=1}^{N_c} l^n \otimes d^n \right]
\]

\[
\bar{\epsilon} = \text{sym} \left[ \frac{1}{V} \sum_{n=1}^{N_t} u^n \otimes \nu^n A^n \right]
\]

Hierarchical multi-cell calculations
Hierarchical triaxial compression simulations
Hierarchical triaxial compression simulations
Inhomogeneous predictions

experiment-based calcs with shear band using DIC
In-situ X-ray CT data from Grenoble
Strain fields and dilatancy
Strain prediction Vs. experiment

- $\epsilon_s \leq 0.15$
- $0.15 < \epsilon_s \leq 0.30$
- $\epsilon_s > 0.30$

EXPERIMENT  MULTISCALE
Kinematics Vs. Elastostatics

- Kinematics can be measured @ grain scale
- Stresses cannot be measured @ grain scale
Kinematics Vs. Elastostatics

- Kinematics can be measured @ grain scale
- Stresses cannot be measured @ grain scale

need to fill this gap
Can contact forces be measured?

- 3DXRCT & 3DXRD: grain topology, kinematics & average grain strains

- Fundamental question: how to use information (constitutive modeling)?

- Missing link: grain contact forces Vs. stress
Isaac Newton: 1643-1727

\[ f = ma \]

force relates to momentum

Robert Hooke: 1635-1703

\[ f = k\delta \]

\textit{ut tensio sic vis}

The \textbf{concept} of force
fundamental relationships @ particle level

\[
\bar{\sigma}^p = \frac{1}{\Omega_p^p} \sum_{\alpha=1}^{N_c^p} f^\alpha \otimes x^\alpha
\]

static equilibrium

\[
\sum_{\alpha=1}^{N_c^p} f^\alpha = 0
\]

\[
\sum_{\alpha=1}^{N_c^p} f^\alpha \times x^\alpha = 0
\]

balance of linear momentum
Result 1

\[ \langle \sigma \rangle = \frac{1}{\Omega} \sum_{p=1}^{N_p} \sum_{\alpha=1}^{N_c^p} f^{\alpha} \otimes \mathbf{x}^{\alpha} \]

directly recovers Christoffersen et al., 1981

Linkage between grain-scale and macro-scale

Result 2

If particle elastic:

\[ \bar{\sigma}^p = c : \bar{\varepsilon}^p \]

average grain strains furnish average stresses

\[ \bar{\sigma}^p = \frac{1}{\Omega_p} \sum_{\alpha=1}^{N_c^p} f^{\alpha} \otimes \mathbf{x}^{\alpha} \]

‘known’ from 3DXRD

‘want’ for macro stress

KEY: ut tensio sic vis
macroscopic loading → strain measurement

experiment + GEM concept

use GEM to calculate contact forces
Array grain geometry and position is given (e.g., from 3DXRCT)

\[ N_p = 15 \quad \text{# of particles} \]
\[ N_c = 33 \quad \text{# of contacts} \]

Get \( 15 \times 3 = 45 \) eqn from statics

Have \( 33 \times 2 = 66 \) unknowns

Statically Indeterminate Problem!
Ko compression

\[ \sigma = 0.5 \text{ kPa} \]

smooth walls
infinite friction

numerical experiment

\begin{align*}
\text{‘measured’ ave strains} & \\
6.823 & 6.117 \\
1.3122 & 1.0126 \\
0.7007 & 1.6241 \\
7.2948 & 5.7052
\end{align*}
GEM Ko compression

\[ \sigma = 0.5 \text{ kPa} \]

distribution of contact forces in sample

compare with FEM

\begin{align*}
\text{FEM} & : 6.823 & 6.117 \\
\text{GEM} & : 1.3122 & 1.0126 & 0.7007 & 1.6241 & 1.0126 & 7.2948 & 5.7052
\end{align*}
GEM Ko compression

\[ \sigma = 0.5 \text{ kPa} \]

distribution of contact forces in sample

\[ \langle \sigma \rangle = \begin{bmatrix} -0.085 & 0.001 \\ 0.001 & -0.496 \end{bmatrix} \]

principal grain stress directions

quasi-Ko

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• Multiscale can bypass phenomenology
• Hierarchical works well with experiments
• Combine imaging & computing: predict
• First predictive multiscale framework
• See the unseen, measure the unmeasured
The future...

EXACT particle shape for DEM
Collaborators:
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S. Hall & G. Viggiani, Grenoble
T. Belytschko, Northwestern


Tu et al. Return mapping for nonsmooth and multiscale elastoplasticity. CMAME. 198:2286-2296, 2009