Multiscale characterization & modeling of granular matter

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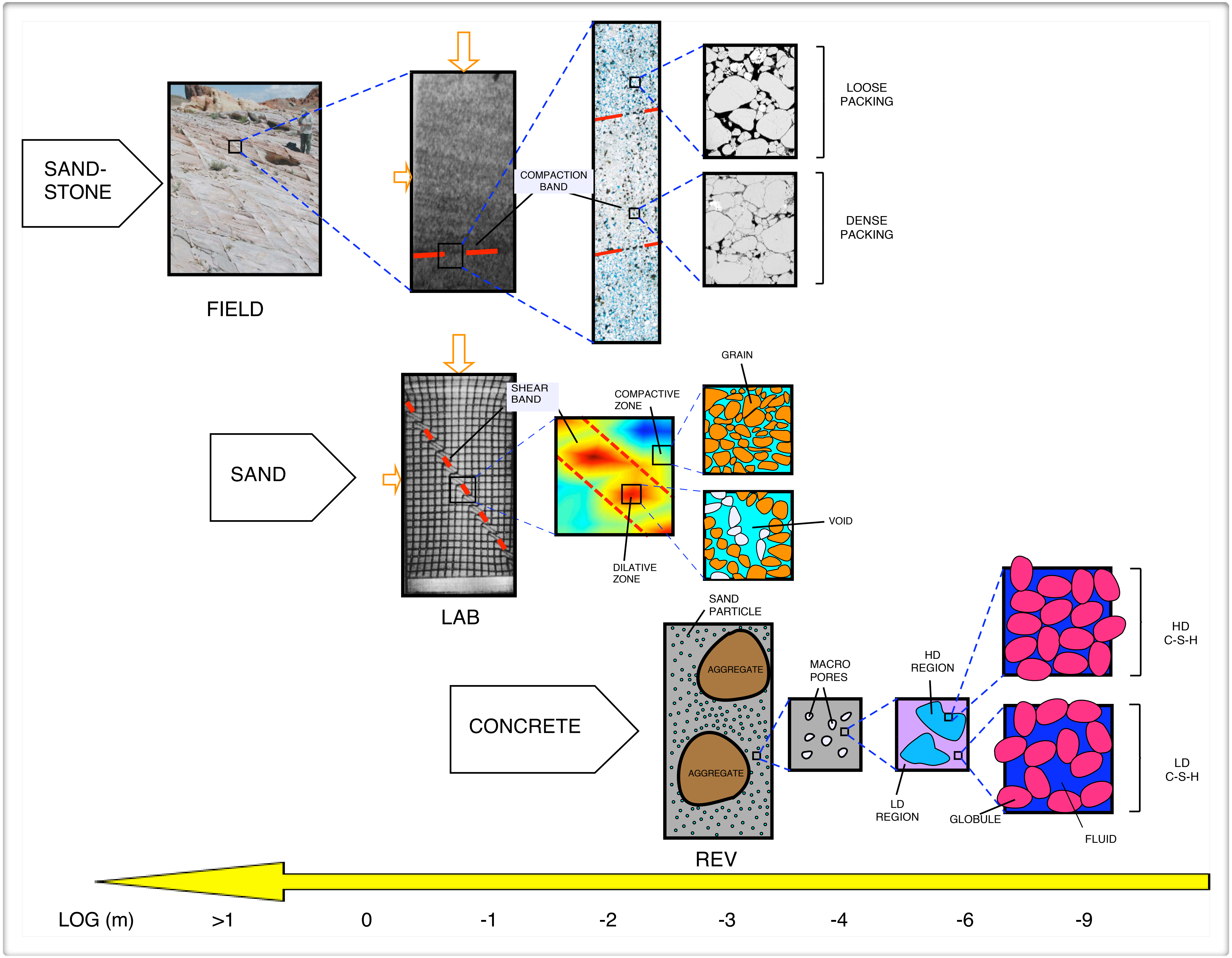
KISS xTerramechanics, June 2011

Outline

- Motivation
- Elastoplasticity framework
- Multiscale framework
- Semi-concurrent & Hierarchical schemes
- Representative examples
- Closure



Family of geomaterials across scales

Elastoplastic framework

Hooke's law $\dot{\boldsymbol{\sigma}} = \boldsymbol{c}^{\mathrm{ep}} : \dot{\boldsymbol{\epsilon}}$

Additive decomposition of strain $\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^{\mathrm{e}} + \dot{\boldsymbol{\epsilon}}^{\mathrm{p}}$

Convex elastic region $F(\boldsymbol{\sigma}, \boldsymbol{\alpha}) = 0$

Non-associative flow $\dot{\boldsymbol{\epsilon}}^{\mathrm{p}} = \dot{\lambda}\boldsymbol{g}, \quad \boldsymbol{g} := \partial G / \partial \boldsymbol{\sigma}$

K-T optimality $\dot{\lambda} F = 0 \quad \dot{\lambda} H = -\partial F / \partial \boldsymbol{\alpha} \cdot \dot{\boldsymbol{\alpha}}$

Elastoplastic constitutive tangent

$$\boldsymbol{c}^{\mathrm{ep}} = \boldsymbol{c}^{\mathrm{e}} - \frac{1}{\chi} \boldsymbol{c}^{\mathrm{e}} : \boldsymbol{g} \otimes \boldsymbol{f} : \boldsymbol{c}^{\mathrm{e}}, \qquad \chi = H - \boldsymbol{g} : \boldsymbol{c}^{\mathrm{e}} : \boldsymbol{f}$$

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

$$G(I_1, I_2, \alpha) = \sqrt{\frac{3}{2}} I_2 + \bar{m}(I_1, \alpha) - \bar{c}(\alpha)$$

friction

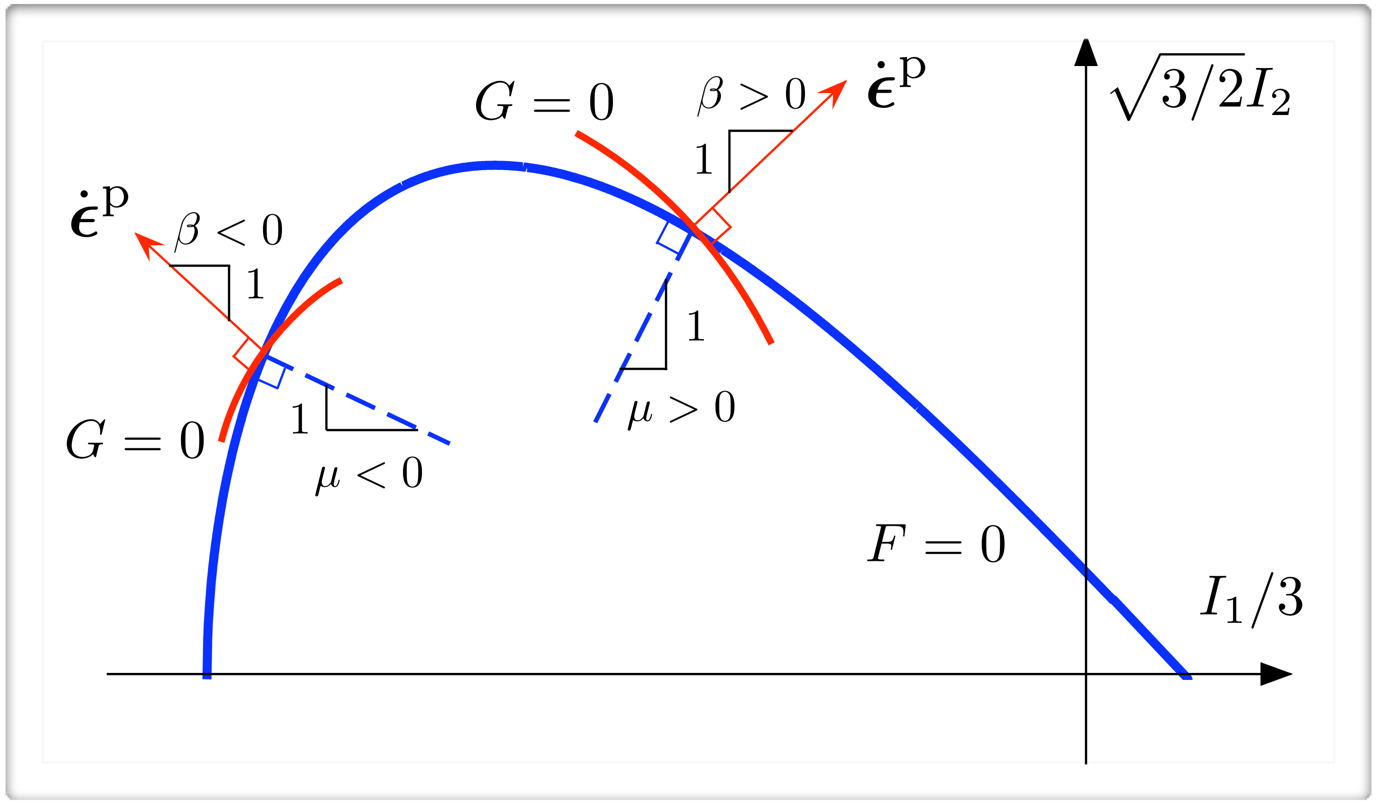
$$\mu = 3\frac{\partial m}{\partial I_1}$$

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

dilatancy

$$\beta = 3\frac{\partial \bar{m}}{\partial I_1}$$

$$\beta = \frac{\partial \epsilon_v^p}{\partial \epsilon_s^p}$$



Simple plasticity model

$$\boldsymbol{f} = \frac{1}{3}\mu\mathbf{1} + \sqrt{\frac{3}{2}}\hat{\boldsymbol{n}}$$

$$\boldsymbol{g} = \frac{1}{3}\beta\mathbf{1} + \sqrt{\frac{3}{2}}\hat{\boldsymbol{n}}$$

friction & dilation
affect constitutive response

hardening law $$\frac{\partial F}{\partial \mu}\dot{\mu} = -\dot{\lambda}H$$

stress-dilatancy relation

$$\underbrace{\mu}_{\text{friction strength}} = \underbrace{\beta}_{\text{dilatancy strength}} + \underbrace{\bar{\mu}}_{\text{residual strength}}$$

Multiscale framework

$E,\ \nu$ elastic constants

$$\beta \approx \frac{\partial \bar{\epsilon}_{\mathrm{v}}}{\partial \bar{\epsilon}_{\mathrm{s}}}$$

extract dilation from micromechanics

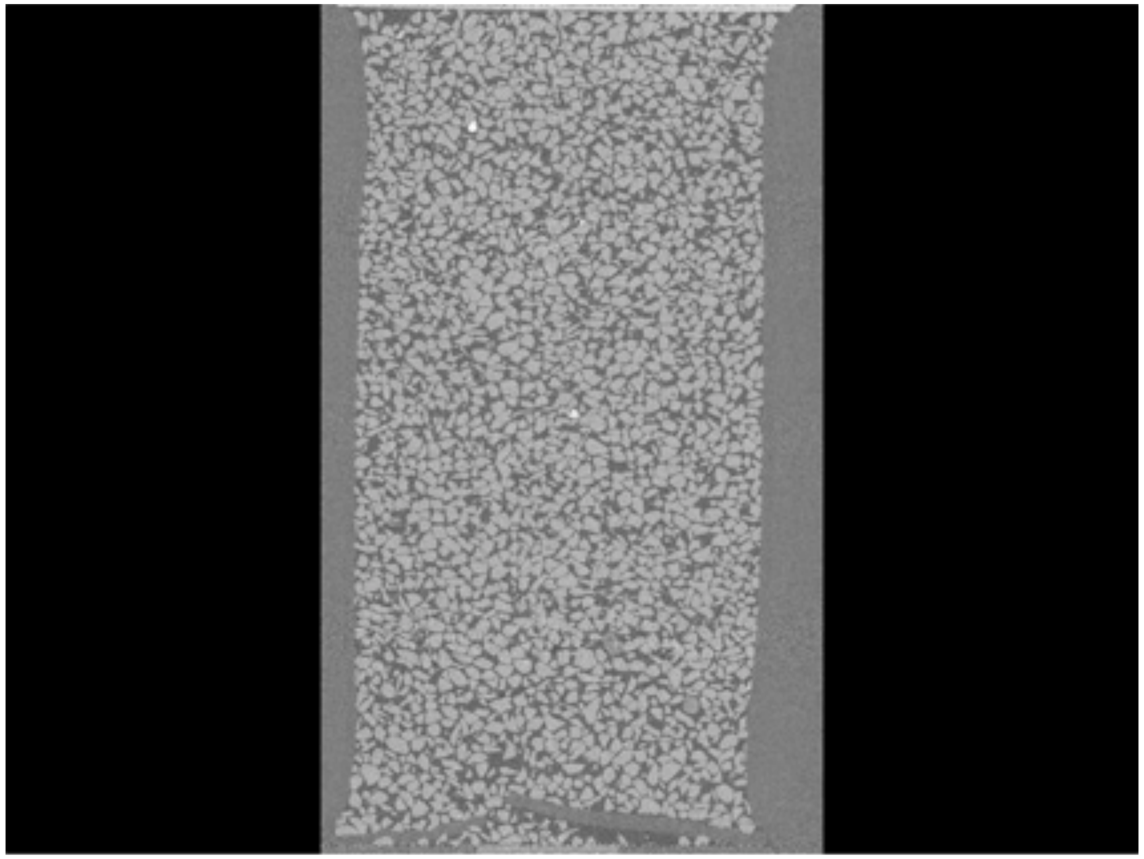
$$2\mu = -3\sqrt{6}\frac{\bar{I}_2}{\bar{I}_1}$$

extract friction from micromechanics

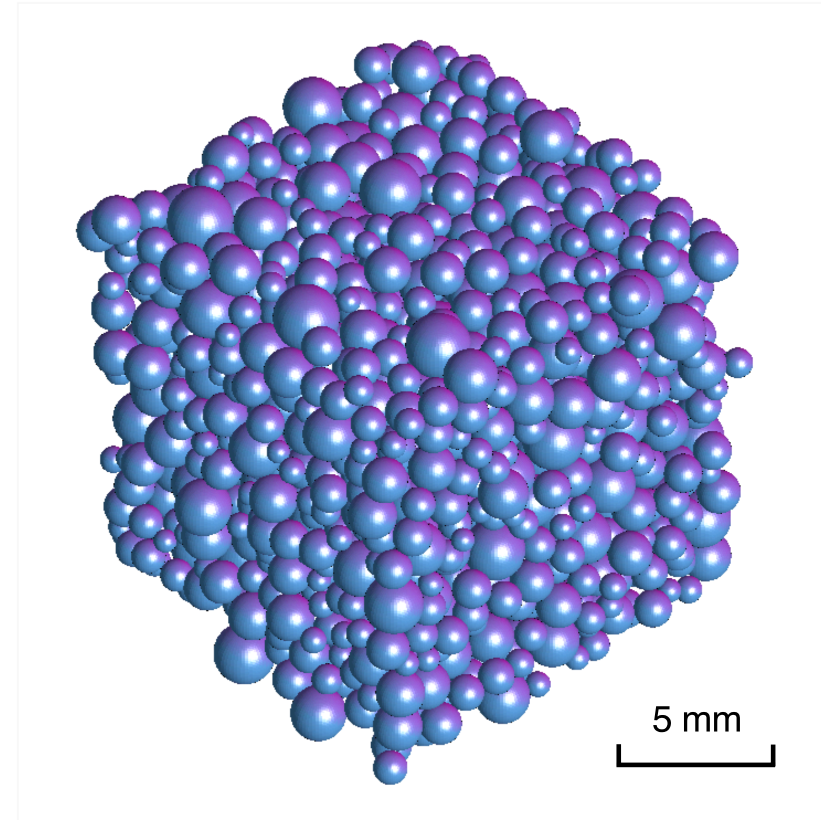
total number of parameters: 2

$E,\ \nu$ calibrated once for given material

warning: bypassing phenomenological hardening experiments



calculations

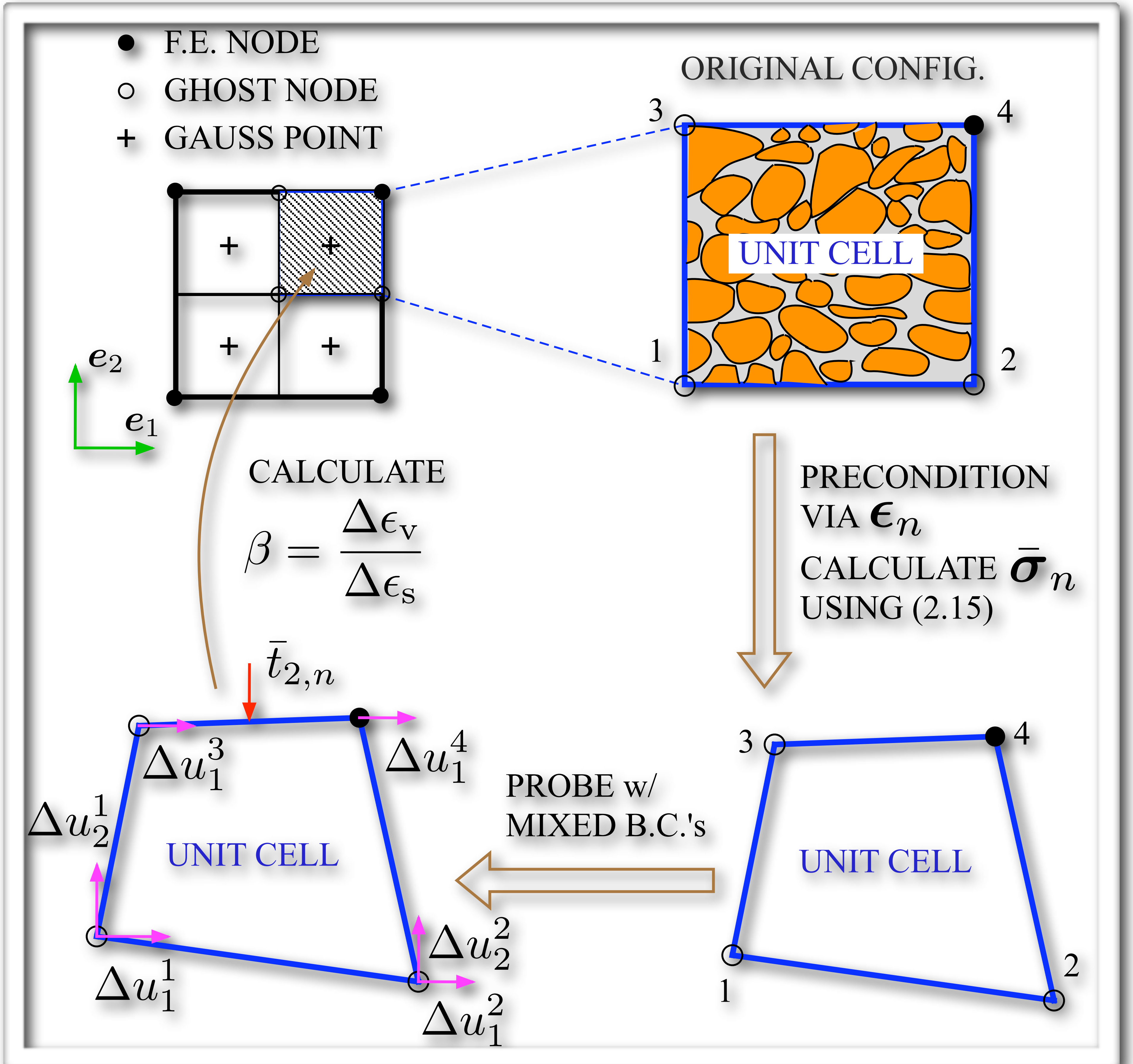


extract strains=>
dilatancy

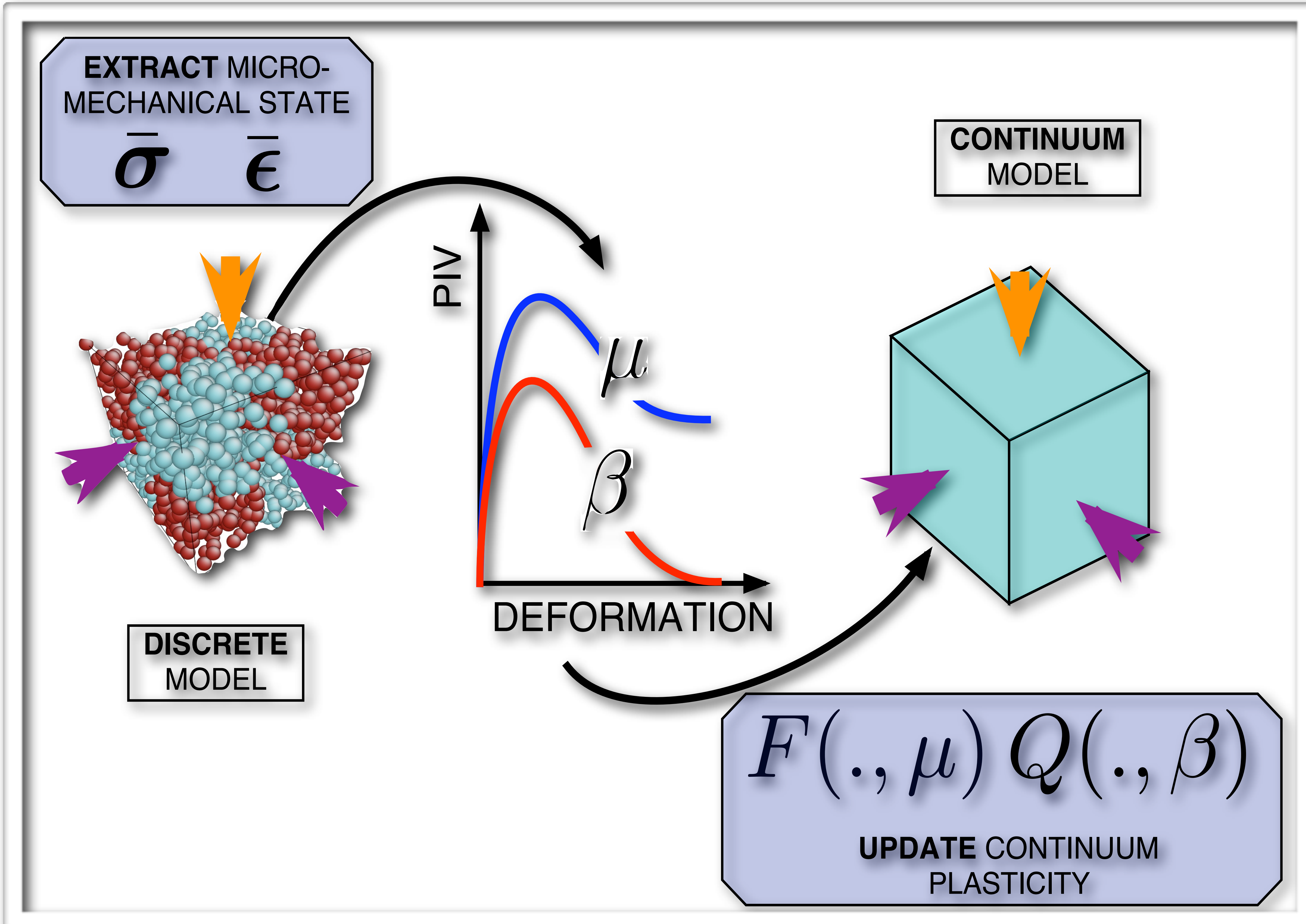
extract strains=>
dilatancy
AND
extract stress=>
friction

Unit cell concept: experiments
Vs. calculations

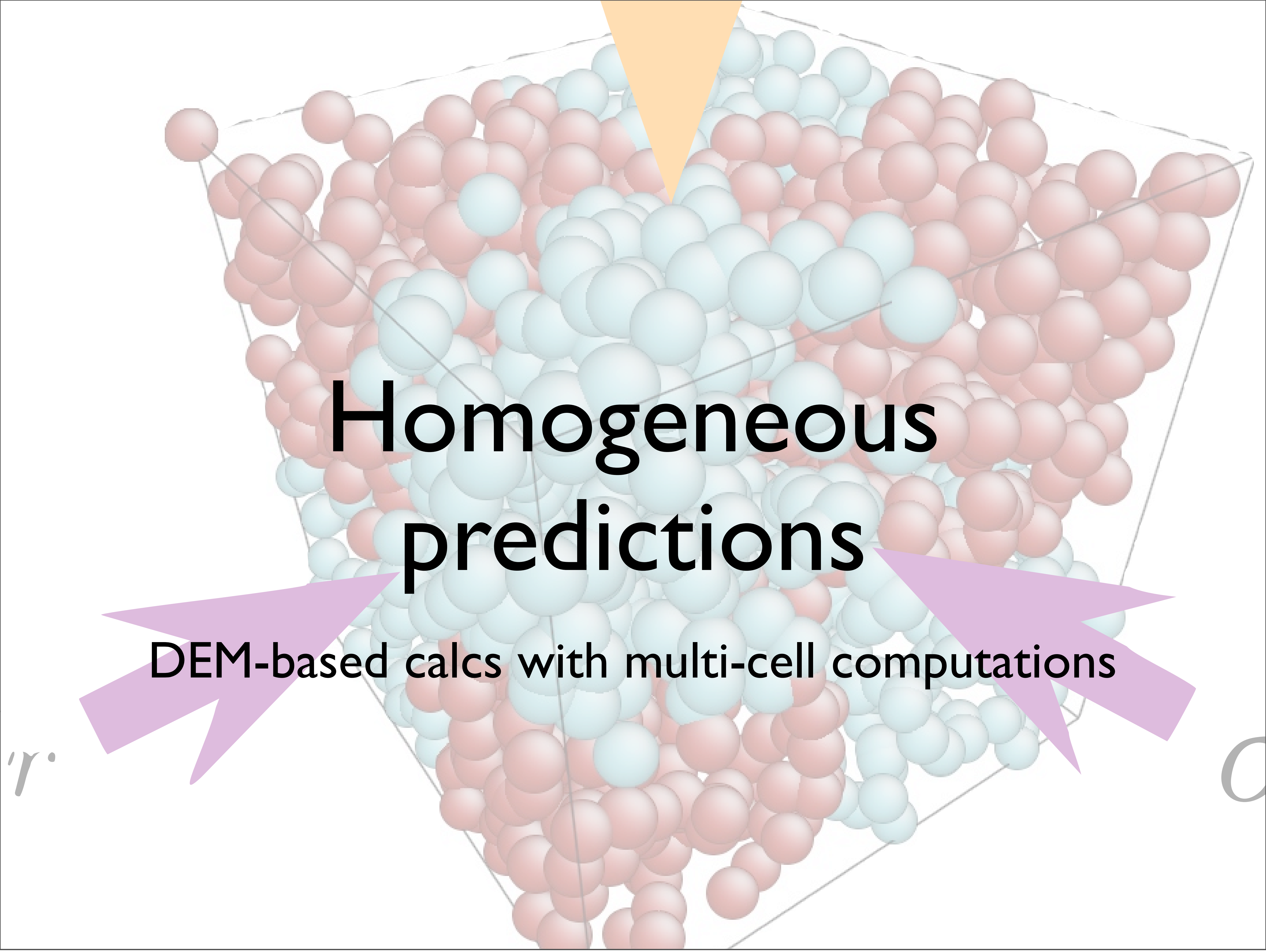
Multiscale schemes: Semi-concurrent & Hierarchical



Semi-concurrent multiscale scheme

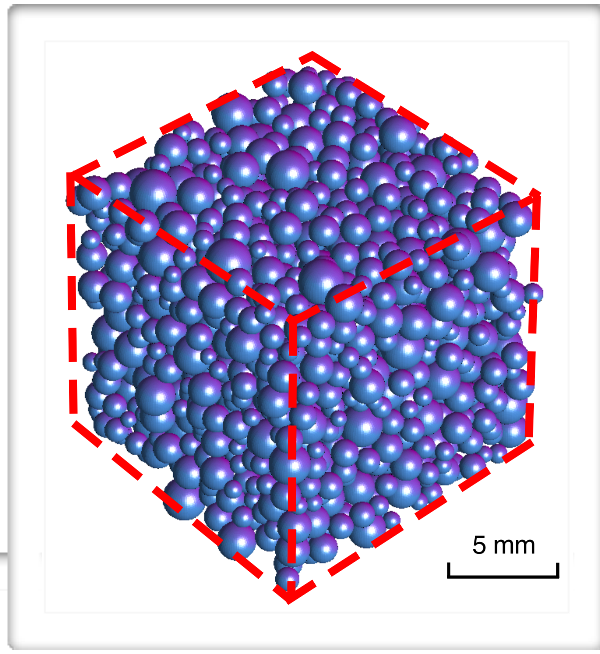


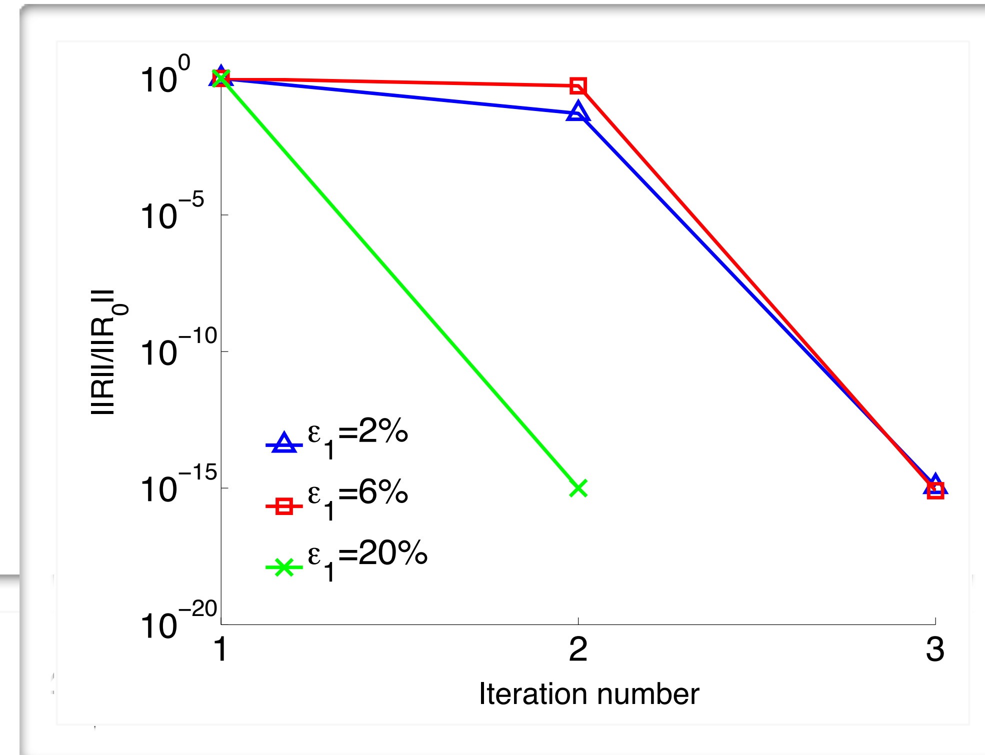
Hierarchical multiscale scheme

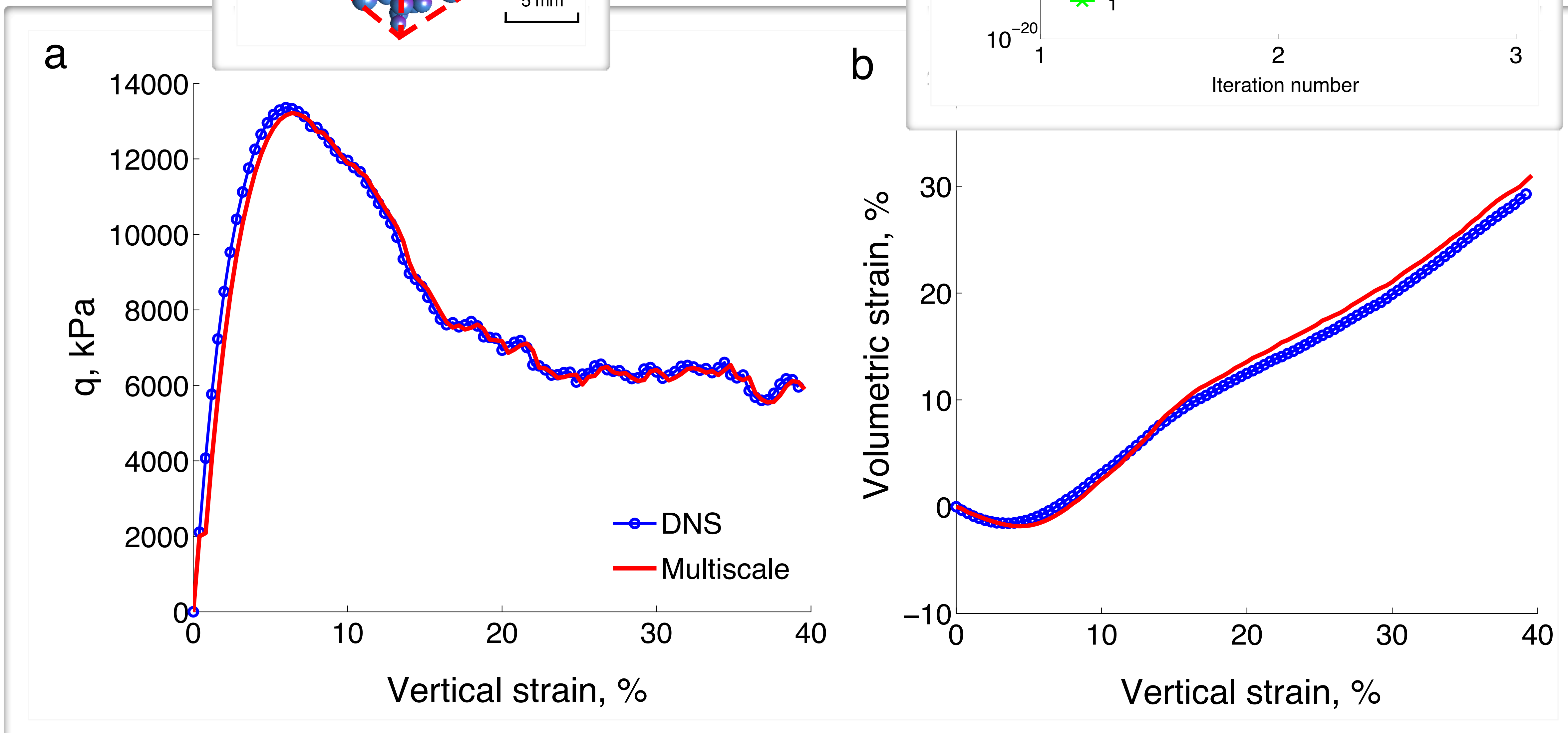


Homogeneous predictions

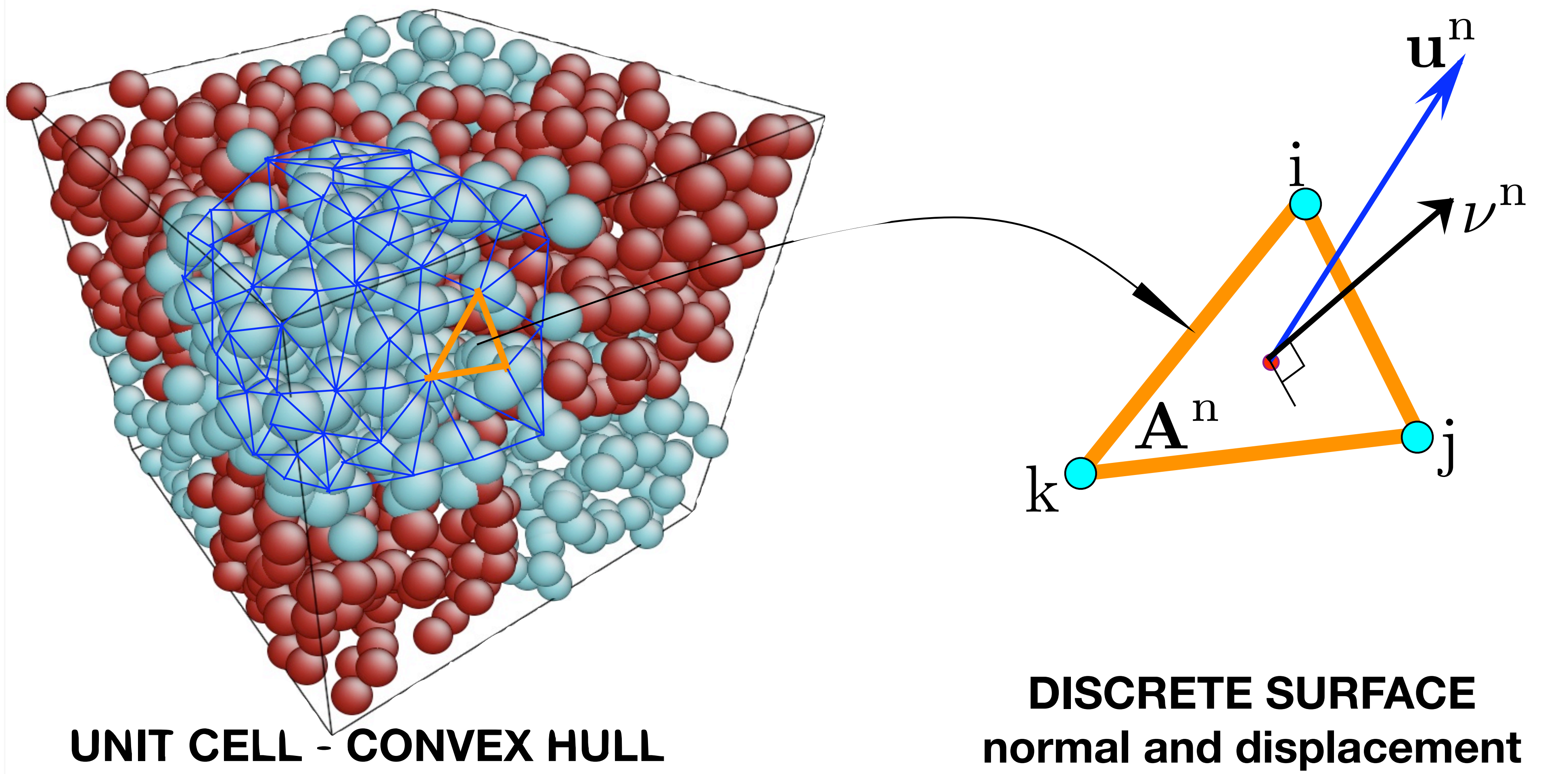
DEM-based calcs with multi-cell computations unit cell







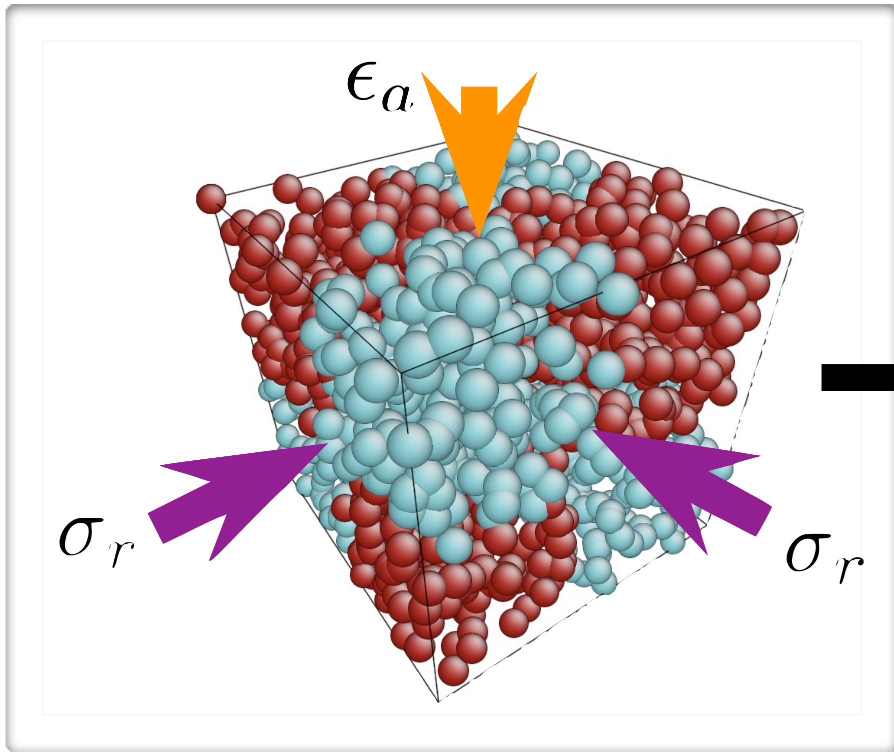
Semi-concurrent DEM-based multiscale

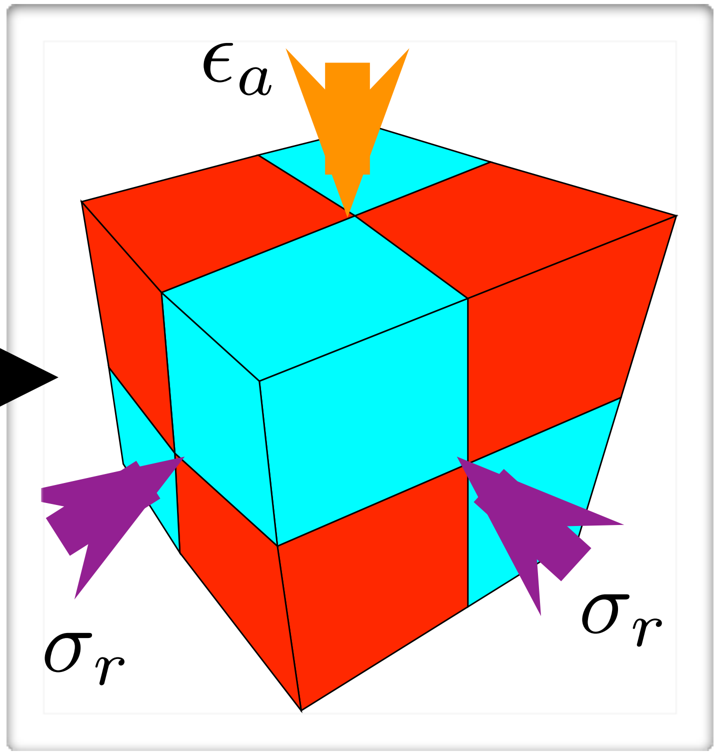


$$\bar{\boldsymbol{\sigma}} = \mathrm{sym}\left[\frac{1}{V}\sum_{\mathrm{n}=1}^{N_c} \boldsymbol{l}^{\mathrm{n}} \otimes \boldsymbol{d}^{\mathrm{n}}\right]$$

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

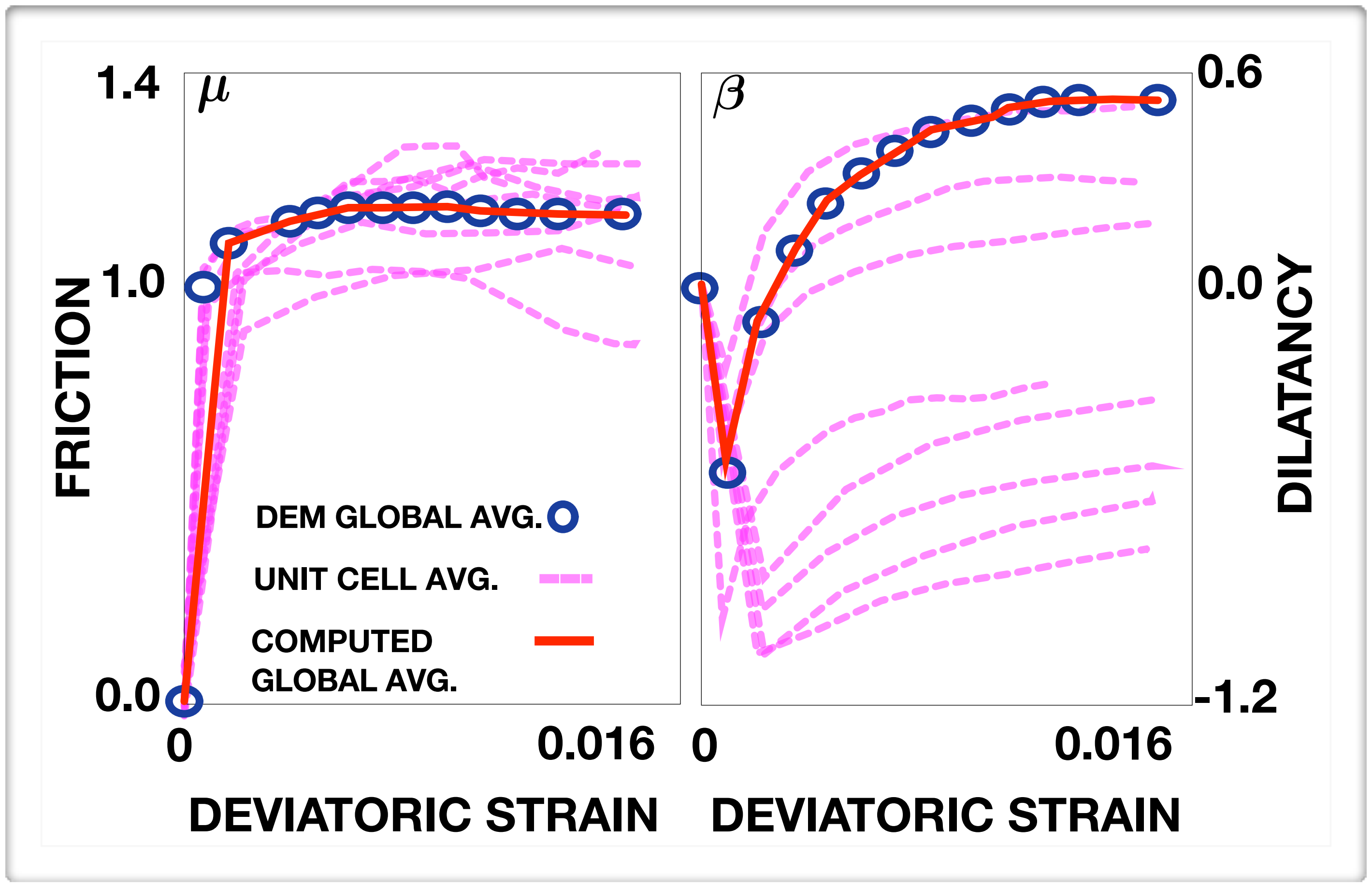
Hierarchical multi-cell calculations



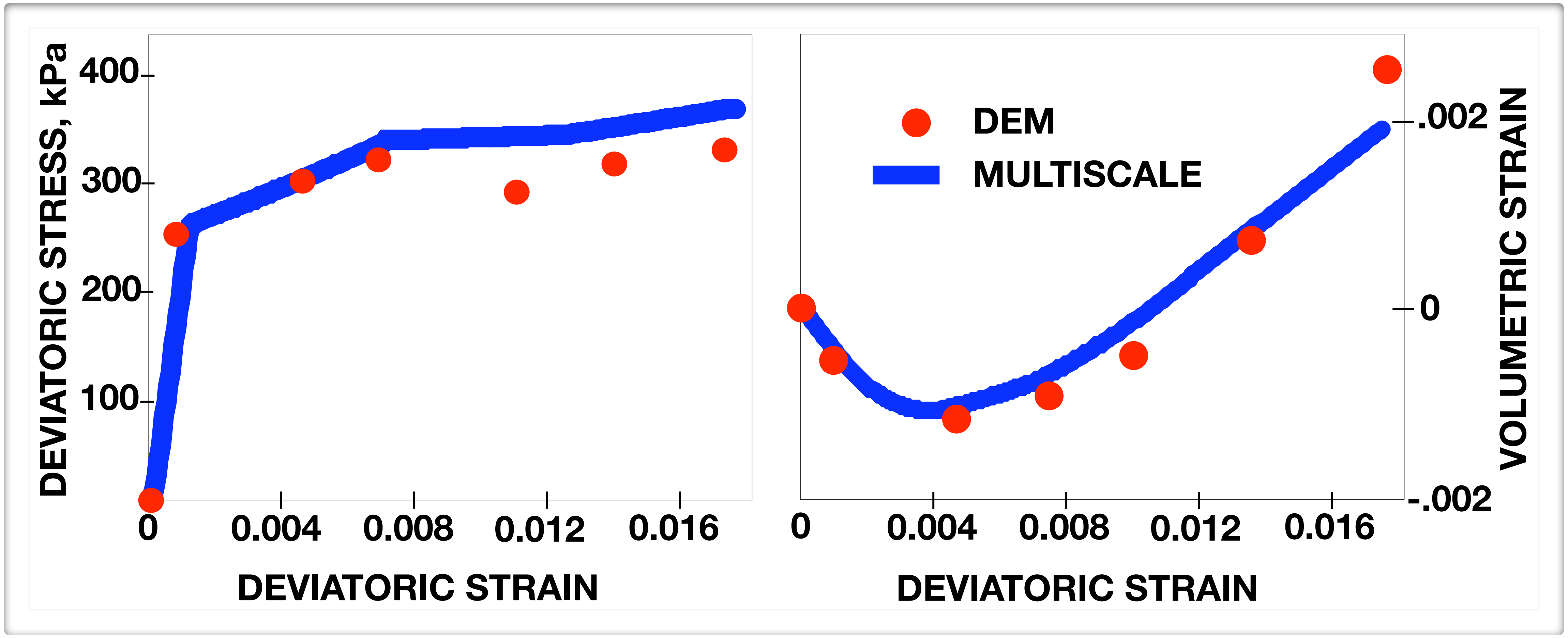


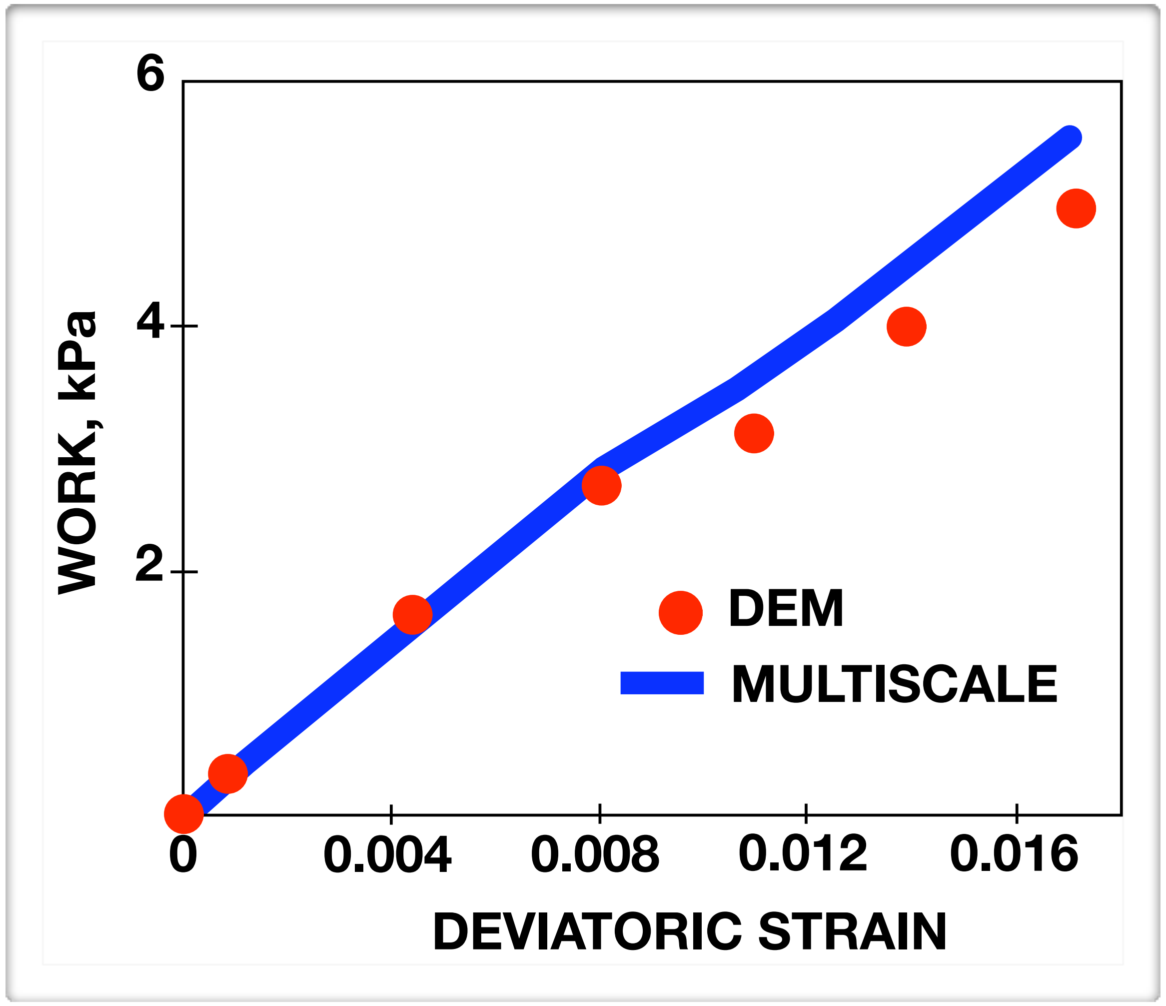
DEM

FEM



Hierarchical triaxial compression simulations

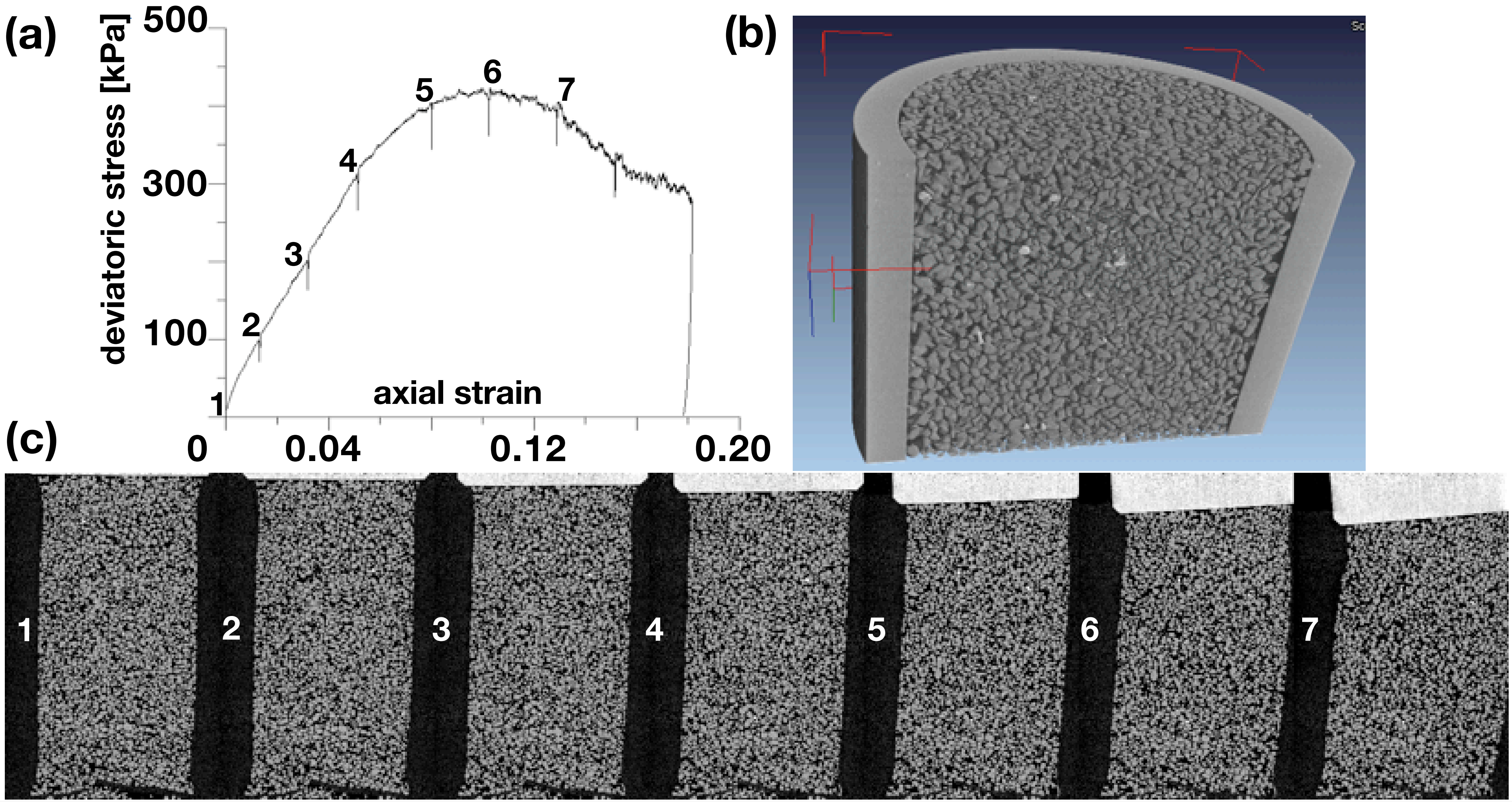




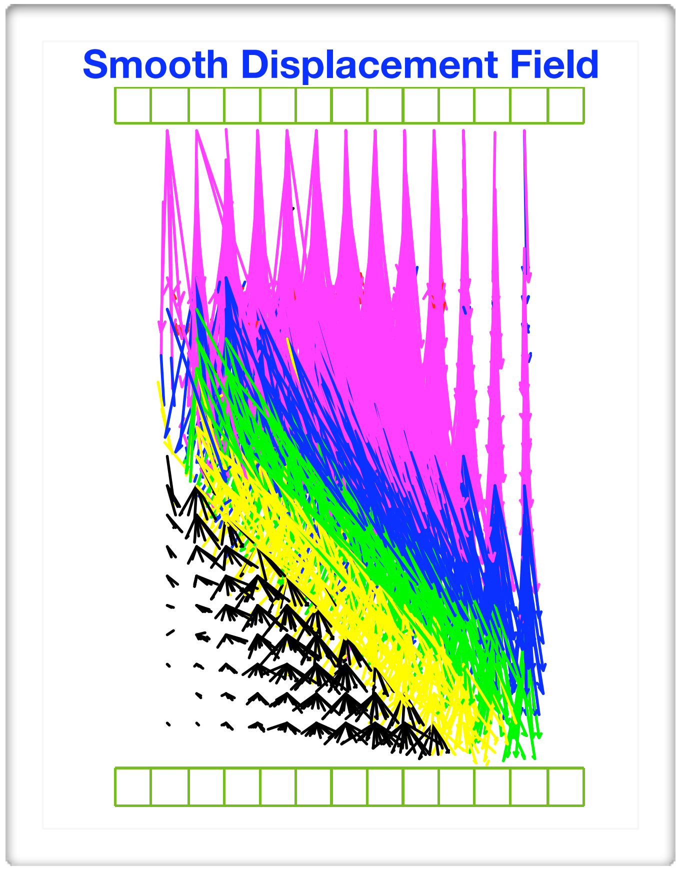
Hierarchical triaxial compression simulations

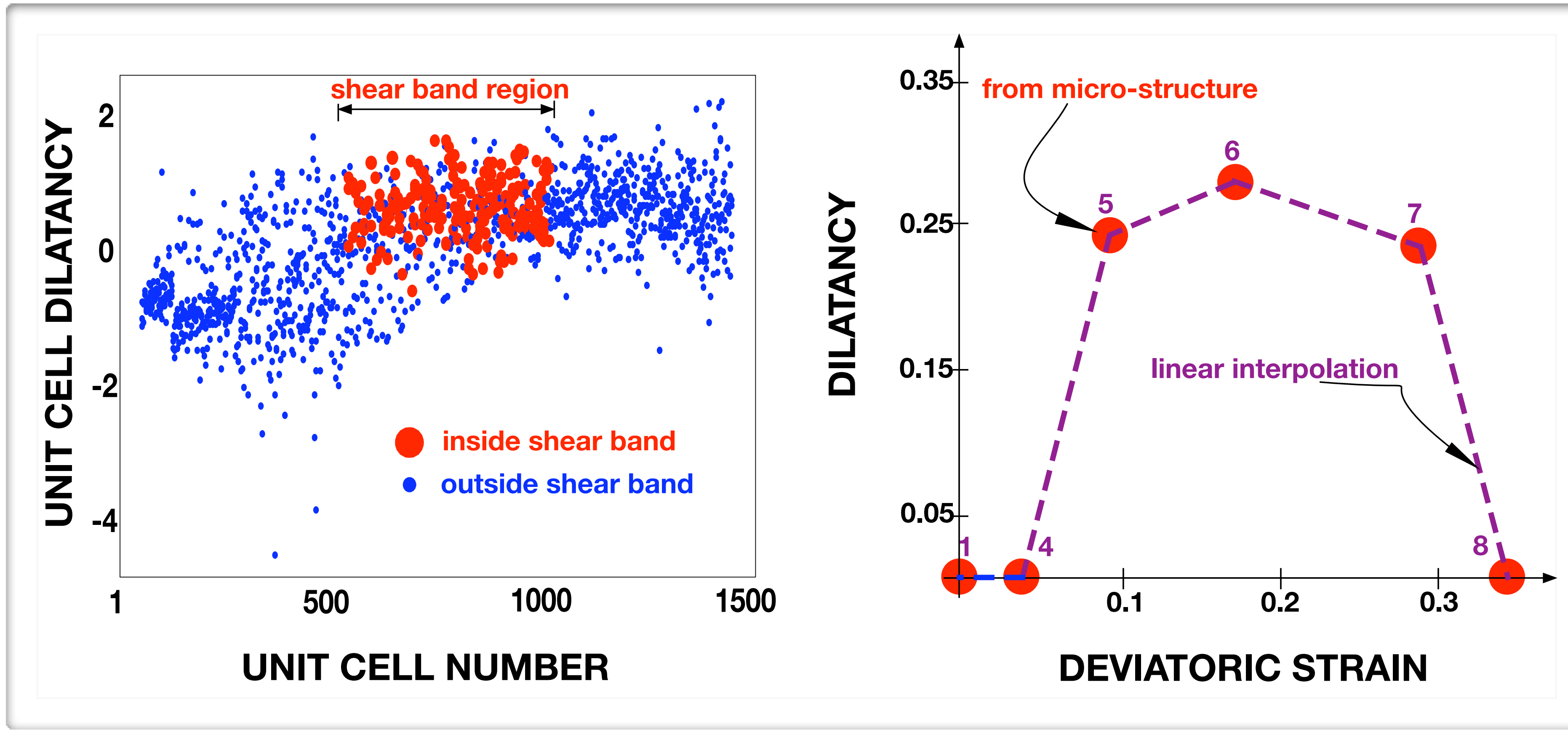
Inhomogeneous predictions

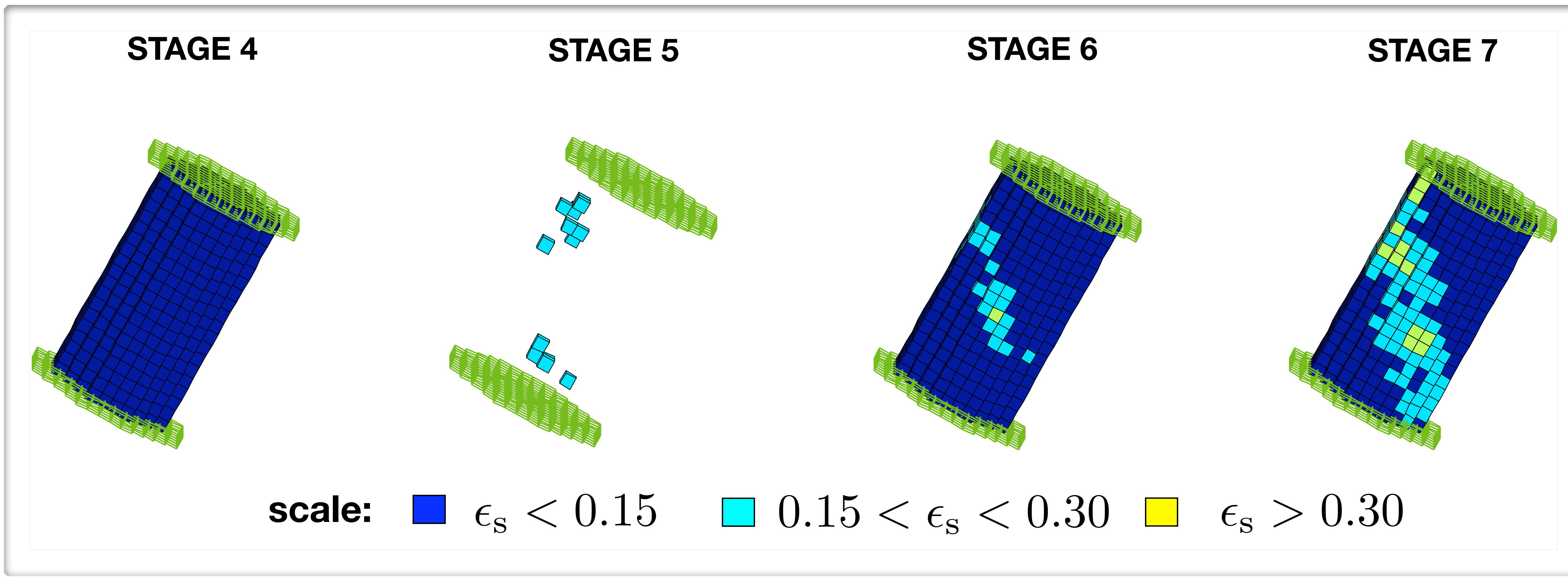
experiment-based calcs with shear band using DIC



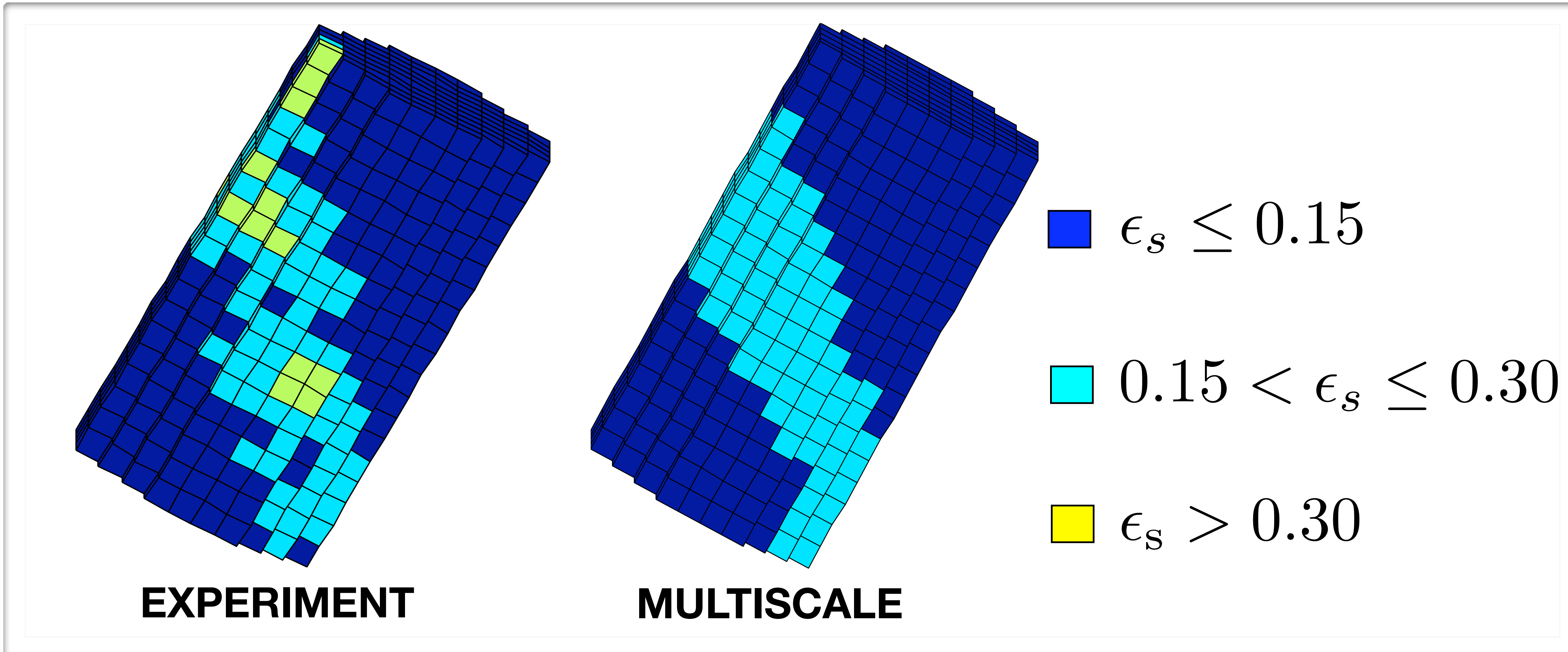
In-situ X-ray CT data from Grenoble

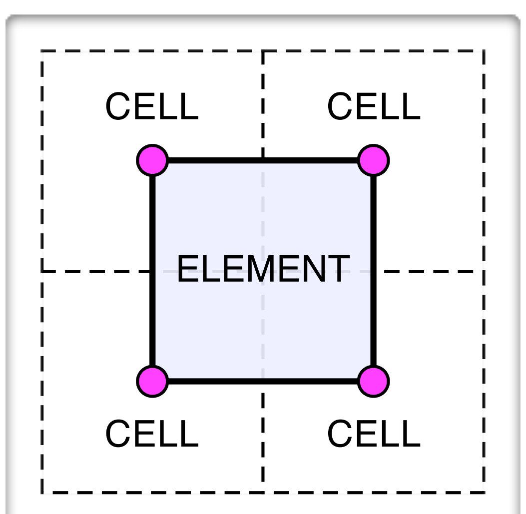




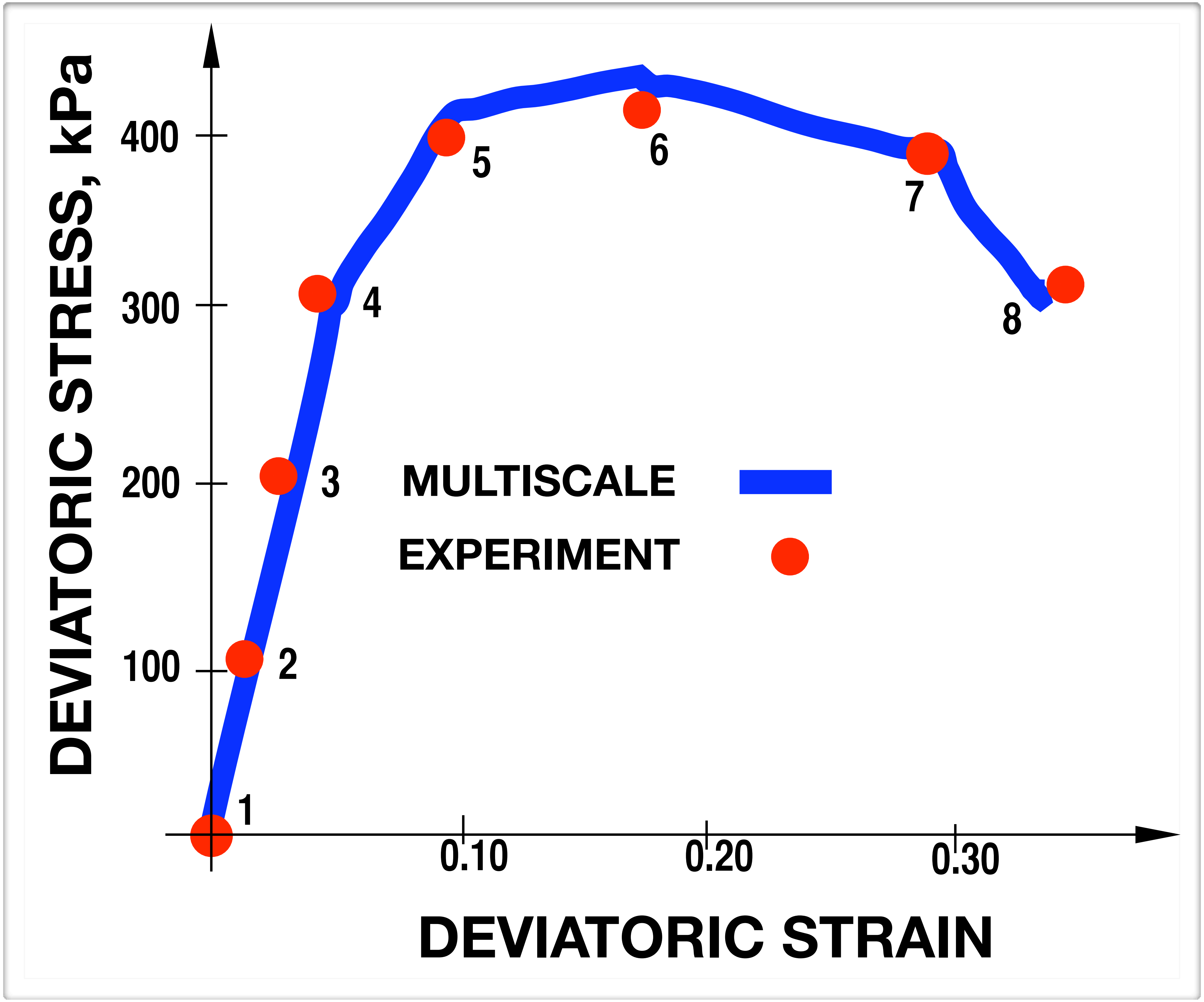


Strain fields and dilatancy

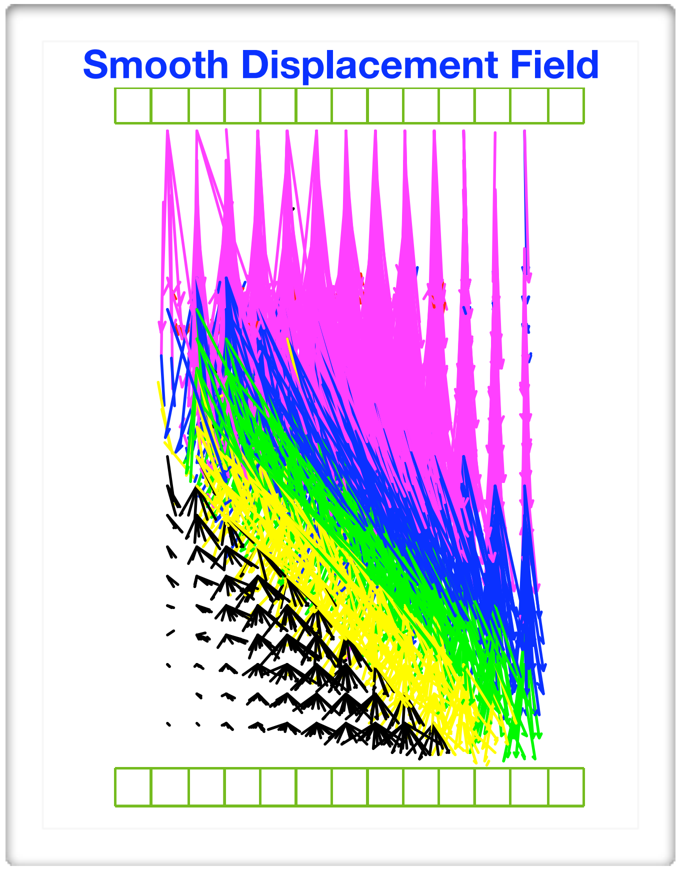


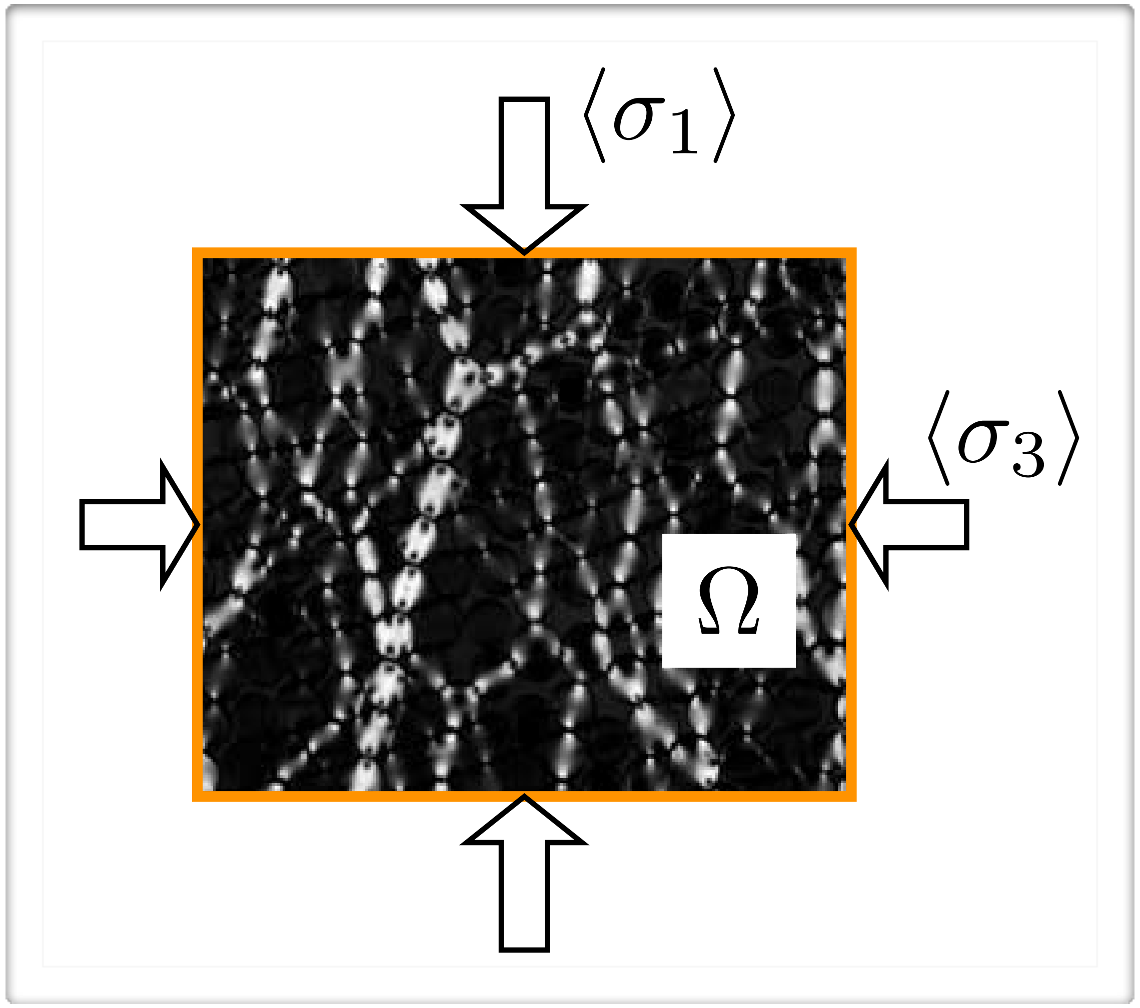


Strain prediction Vs. experiment


DEVIATORIC STRESS, kPa
400
300
200
100
1
2
3
4
5
6
7
8
MULTISCALE
EXPERIMENT
0.10
0.20
0.30
DEVIATORIC STRAIN

Kinematics Vs. Elastostatics

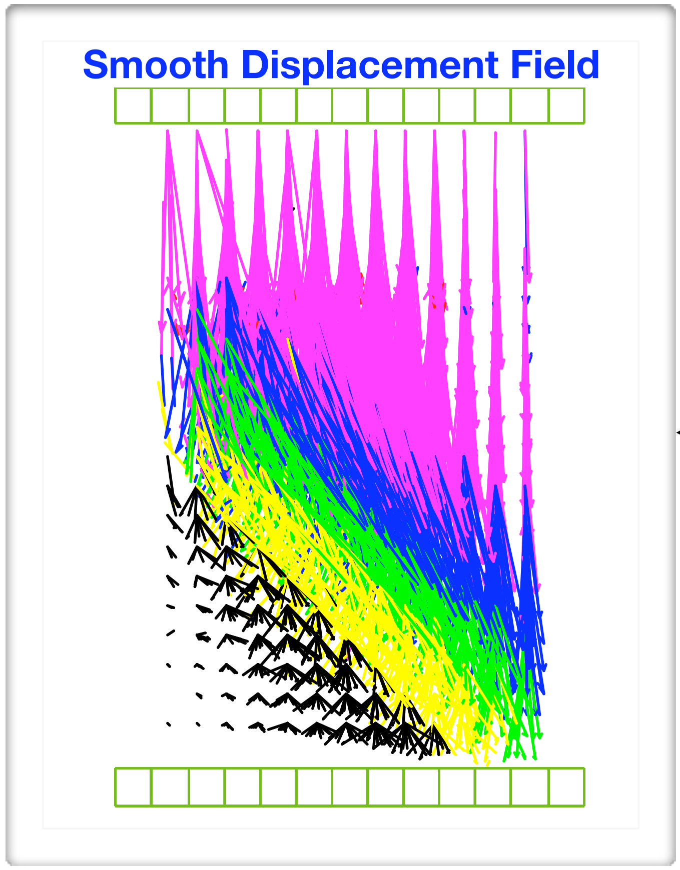




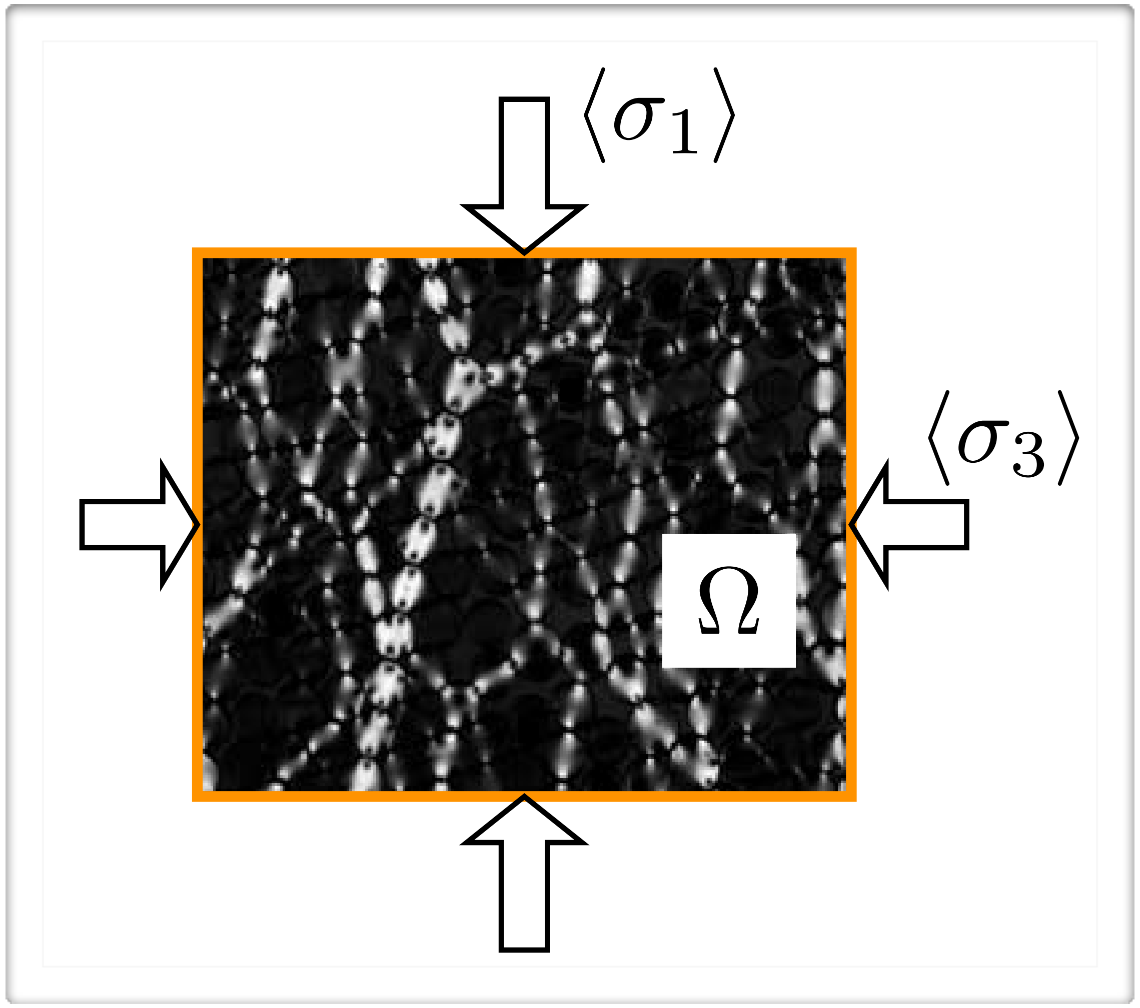
kinematics can be measured @ grain scale

stresses cannot be measured @ grain scale

Kinematics Vs. Elastostatics



need to fill this gap

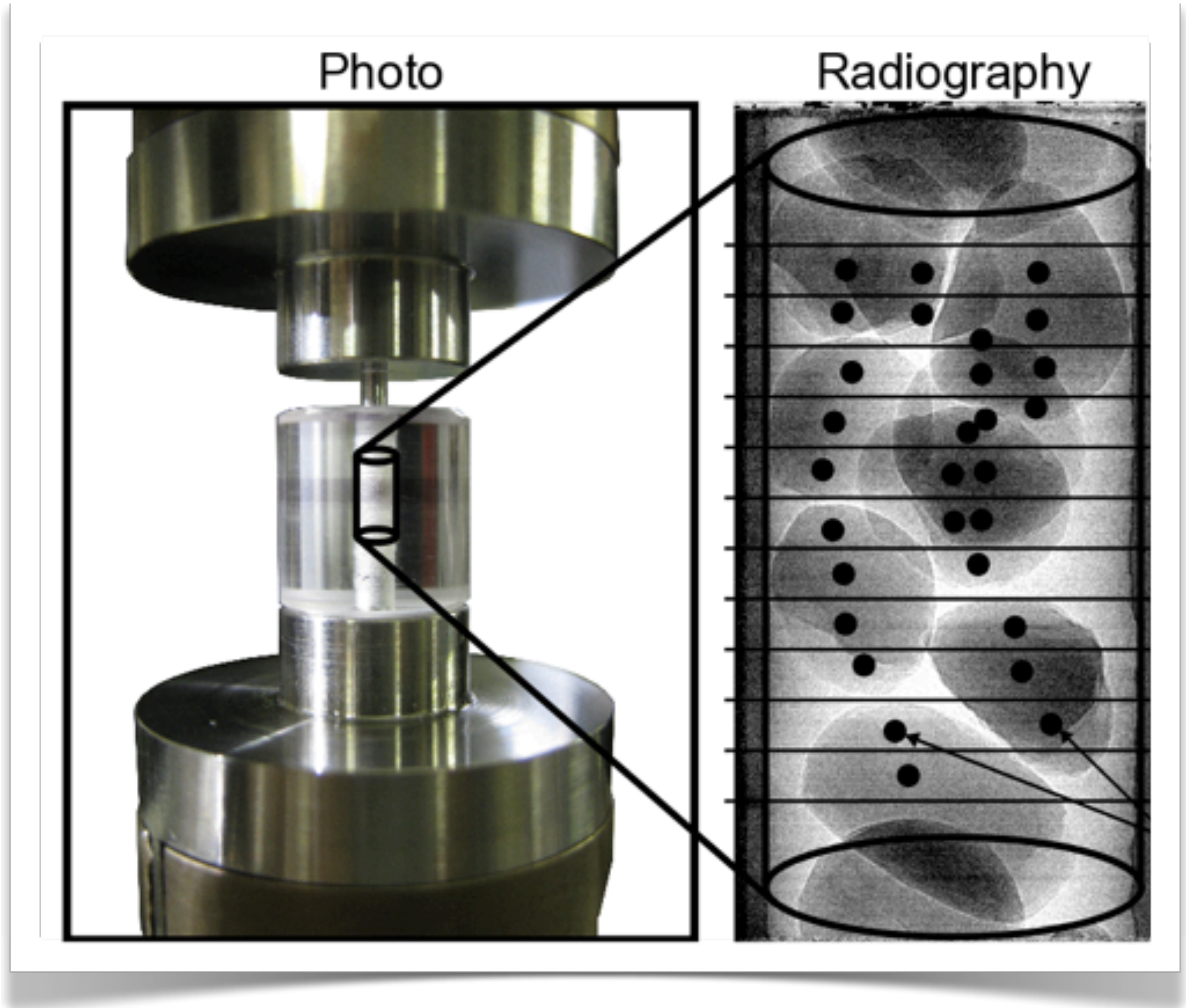


kinematics can be measured @ grain scale

stresses cannot be measured @ grain scale

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

Robert Hooke: 1635-1703

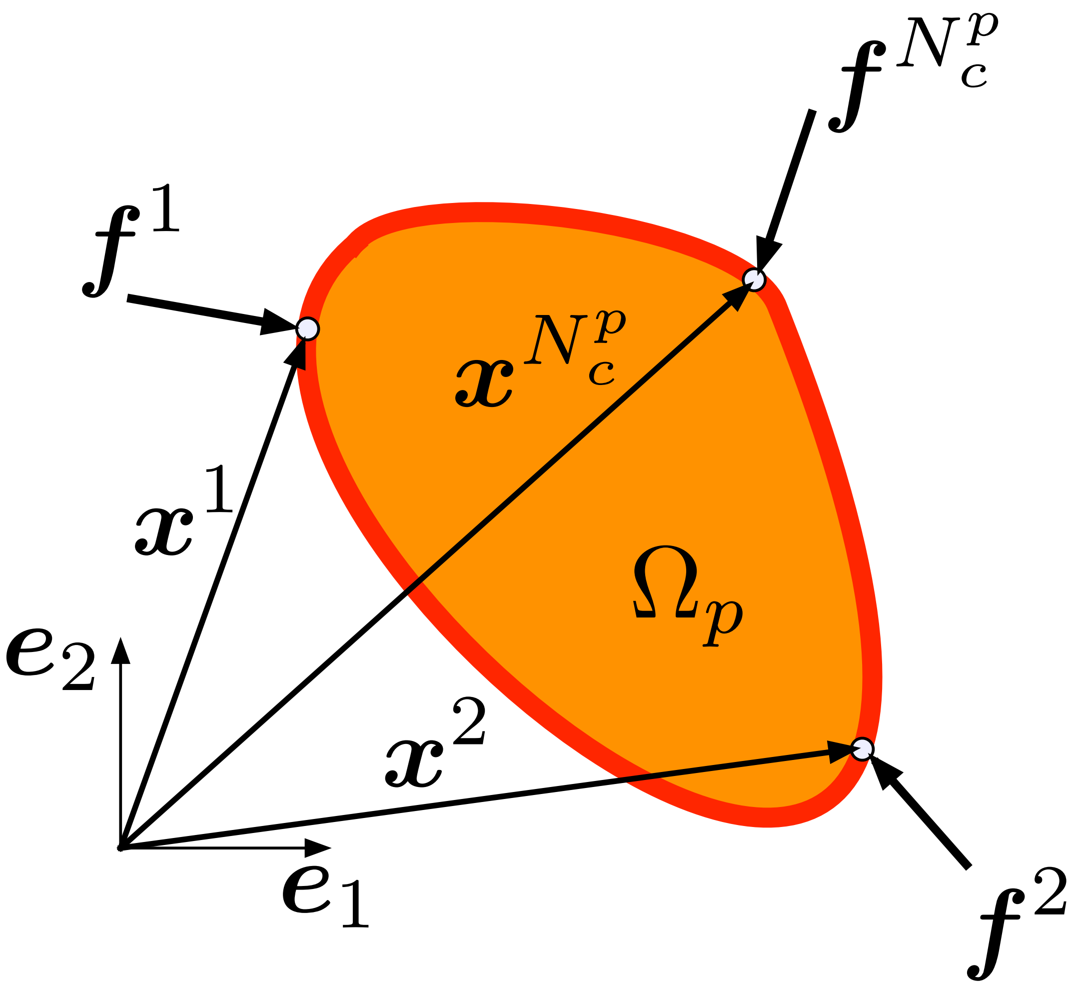
$$\boldsymbol{f} = m\boldsymbol{a}$$

force relates to momentum

$$\boldsymbol{f} = k\boldsymbol{\delta}$$

ut tensio sic vis

The concept of force



$$\sum_{\alpha=1}^{N_c^p} \boldsymbol{f}^{\alpha} = \boldsymbol{0}$$

$$\sum_{\alpha=1}^{N_c^p} \boldsymbol{f}^{\alpha} \times \boldsymbol{x}^{\alpha} = \boldsymbol{0}$$

static equilibrium

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

balance of linear momentum

fundamental relationships @ particle level

Result 1

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{\Omega} \sum_{p=1}^{N_p} \sum_{\alpha=1}^{N_c^p} \boldsymbol{f}^\alpha \otimes \boldsymbol{x}^\alpha$$

directly recovers Christoffersen et al., 1981

Linkage between grain-scale and macro-scale

Result 2

If particle elastic:

$$\bar{\boldsymbol{\sigma}}^p = \boldsymbol{c} : \bar{\boldsymbol{\epsilon}}^p$$

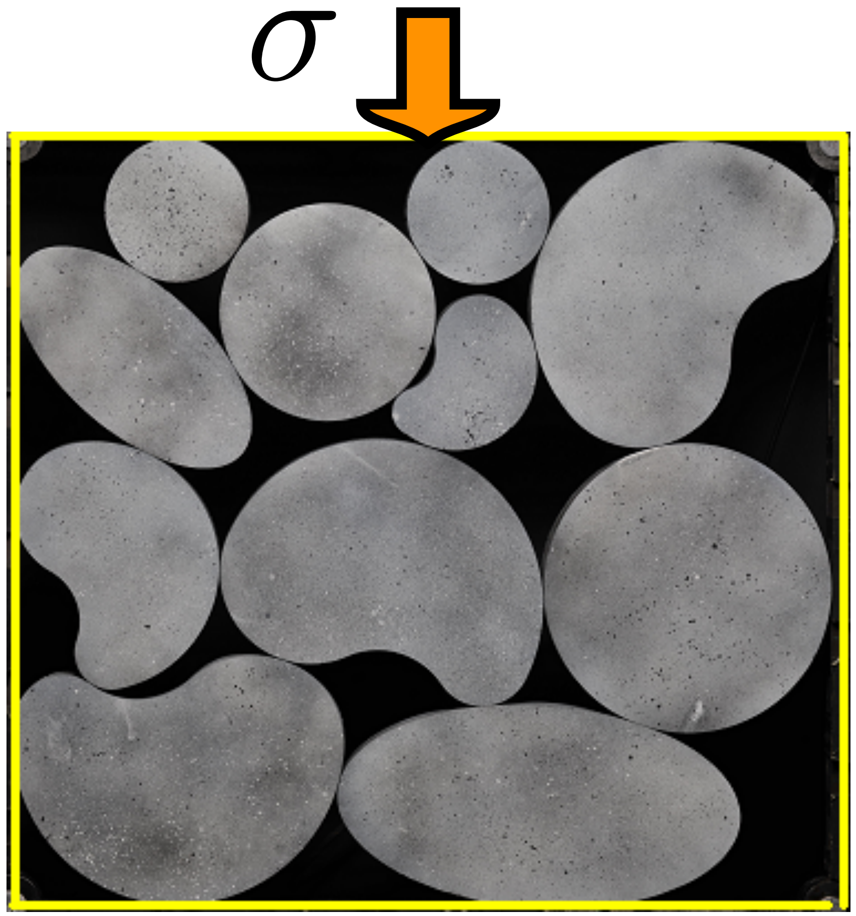
average grain strains furnish average stresses

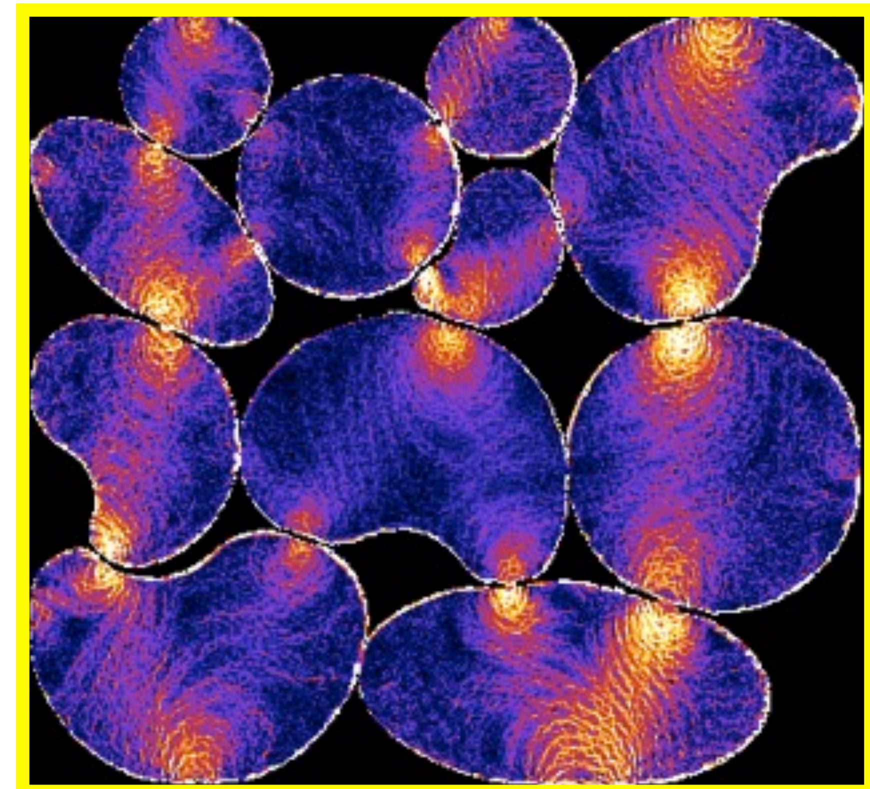
$$\bar{\boldsymbol{\sigma}}^p = \frac{1}{\Omega_p} \sum_{\alpha=1}^{N_c^p} \boldsymbol{f}^\alpha \otimes \boldsymbol{x}^\alpha$$

'known' from 3DXRD

'want' for macro stress

KEY: ut tensio sic vis



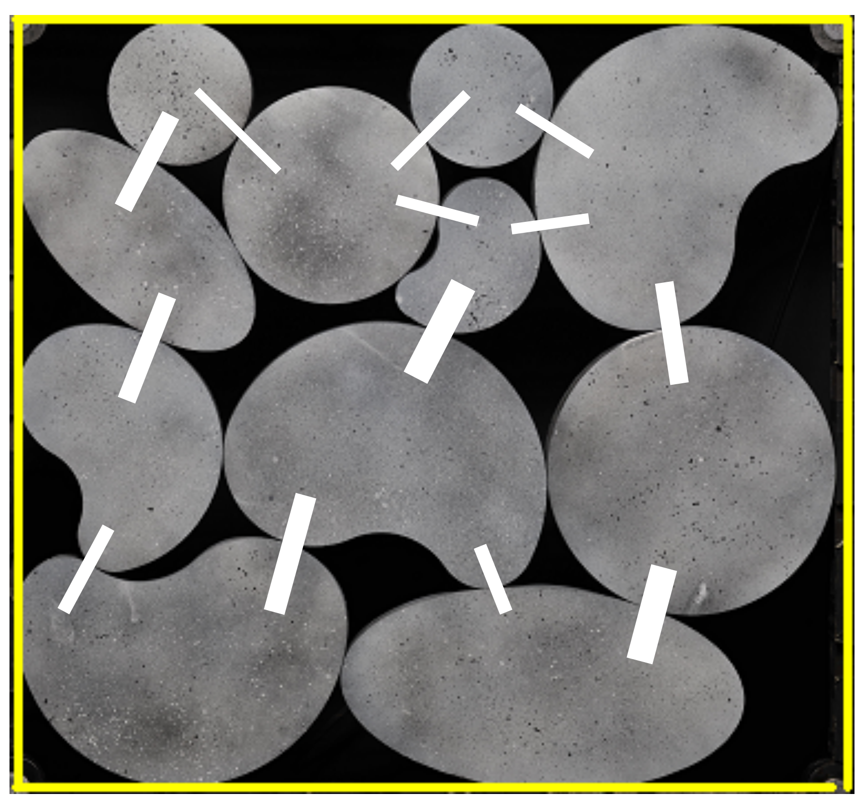


macroscopic loading → strain measurement

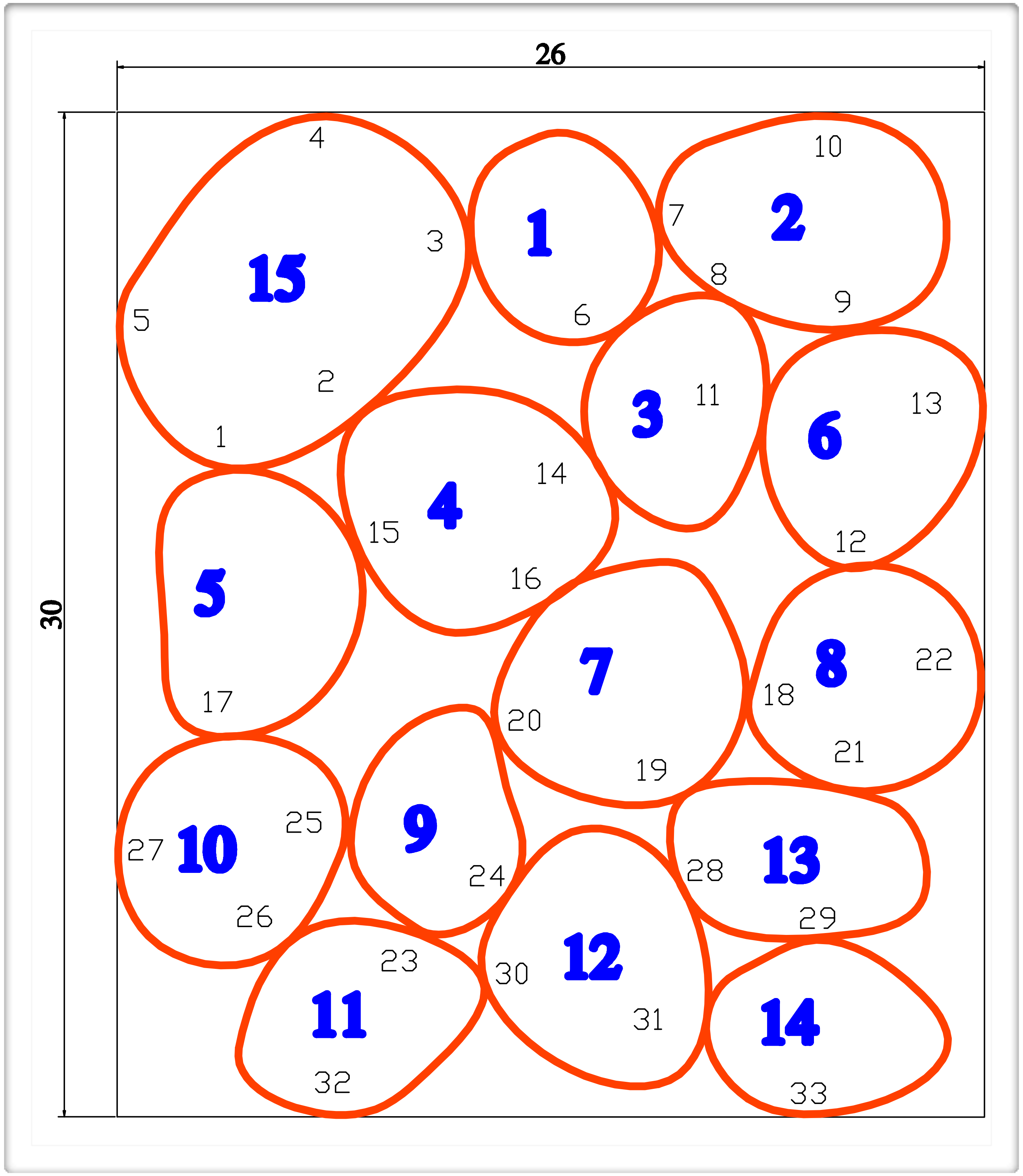
↓

use GEM to calculate contact forces

experiment
+
GEM
concept



2D array of angular particles



Array grain geometry and position is given (e.g., from 3DXRCT)

$N_p = 15$ # of particles

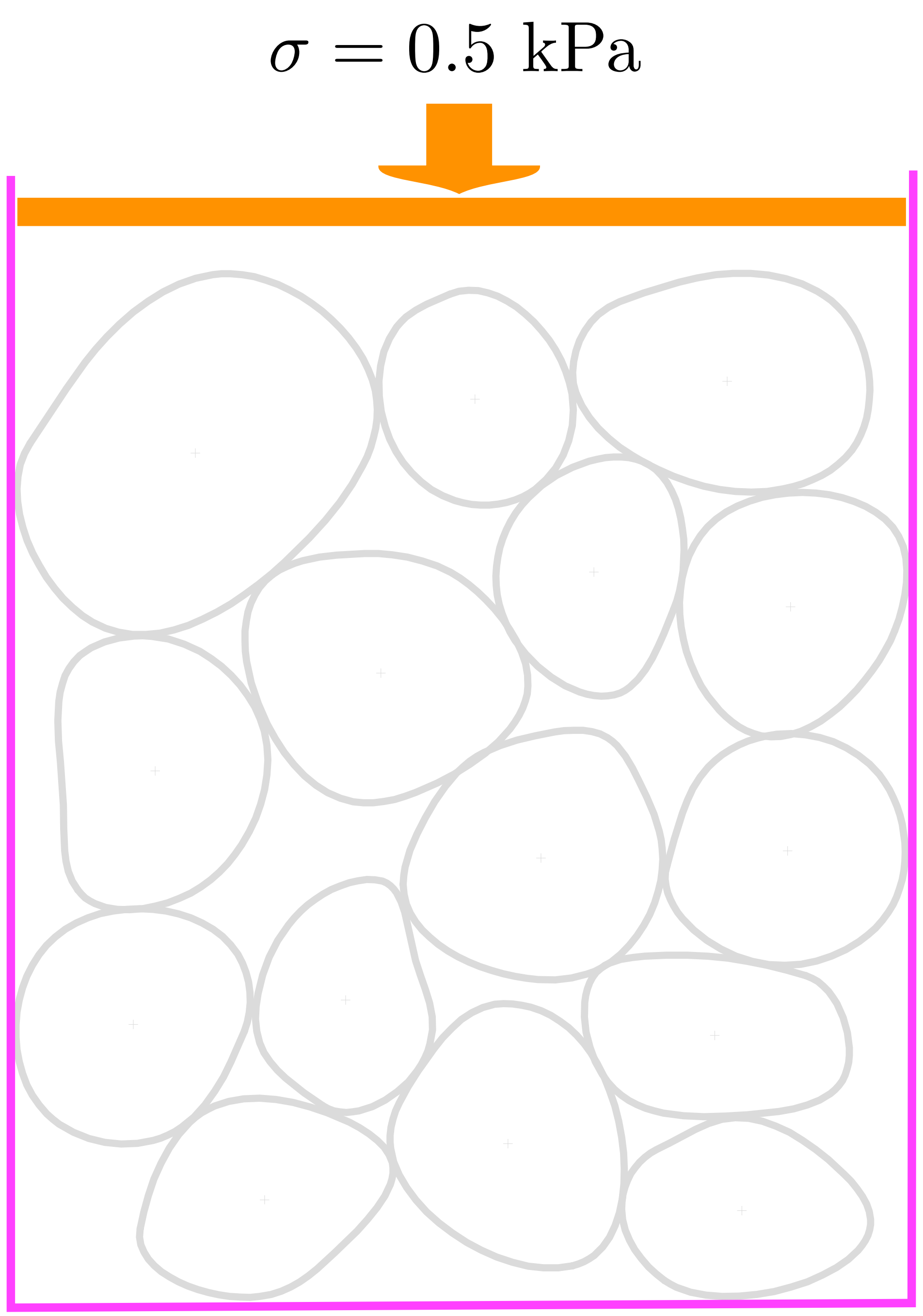
$N_c = 33$ # of contacts

Get 15x3=45 eqn from statics

Have 33x2=66 unknowns

Statically Indeterminate Problem!

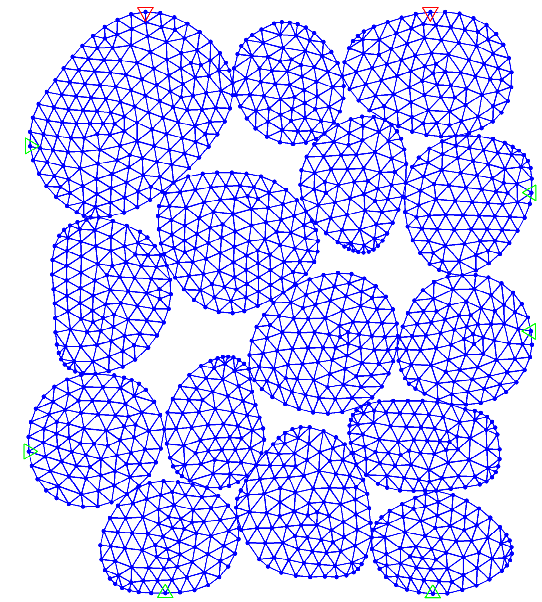
Ko compression

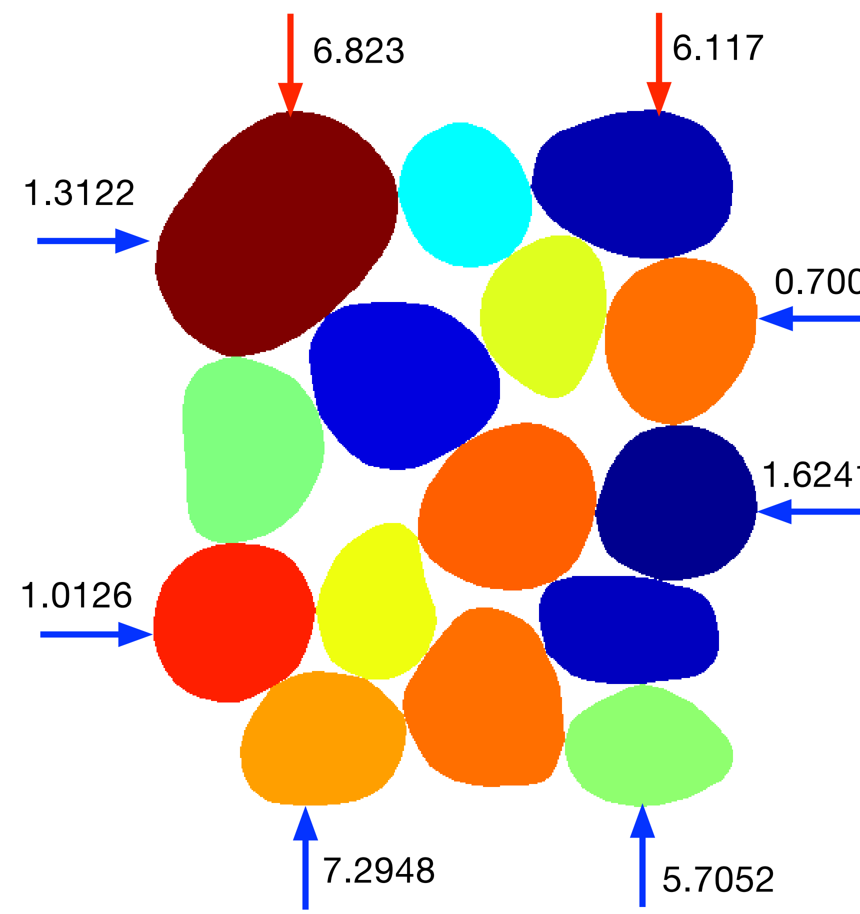


smooth walls

infinite friction

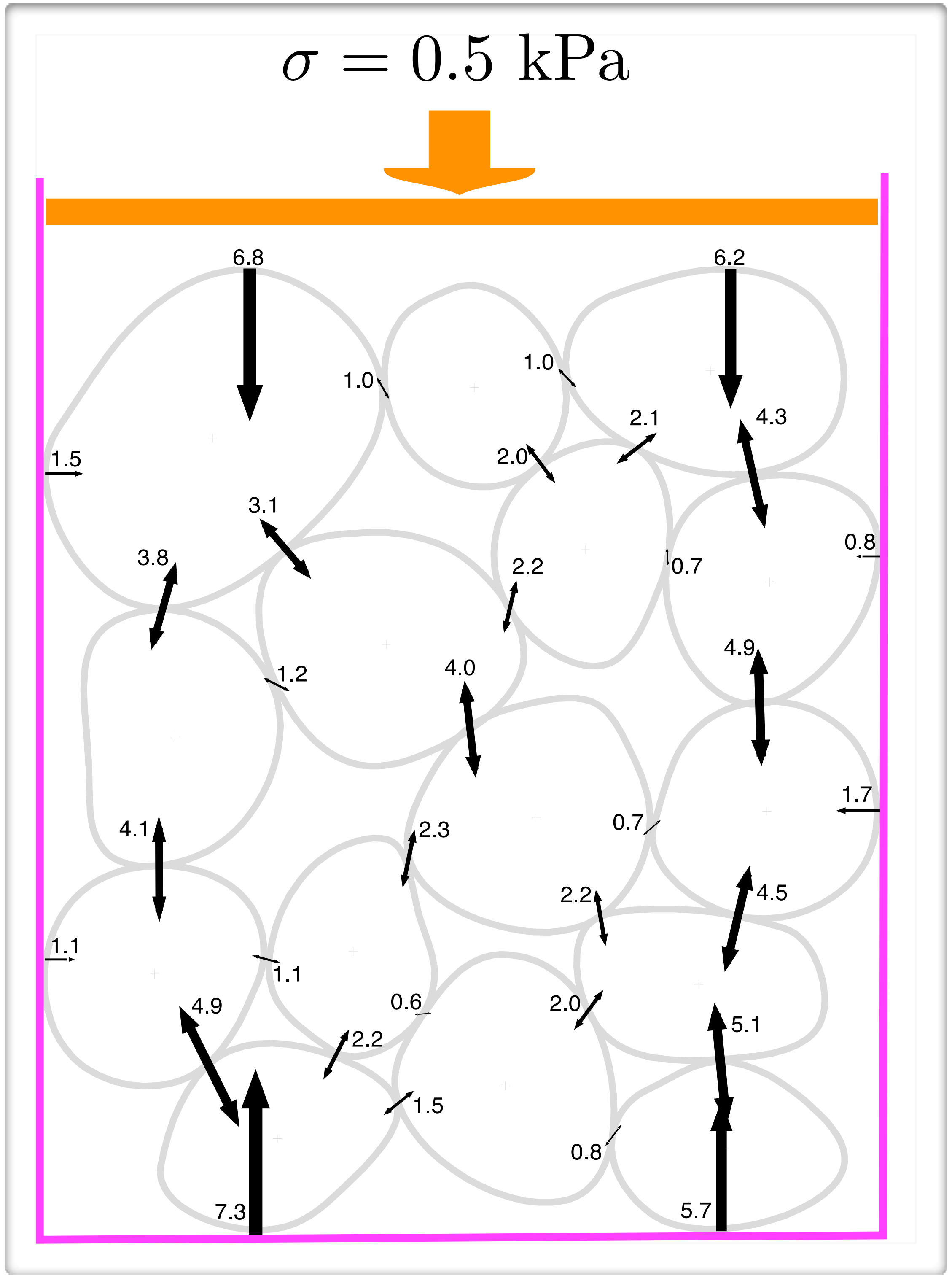
numerical experiment



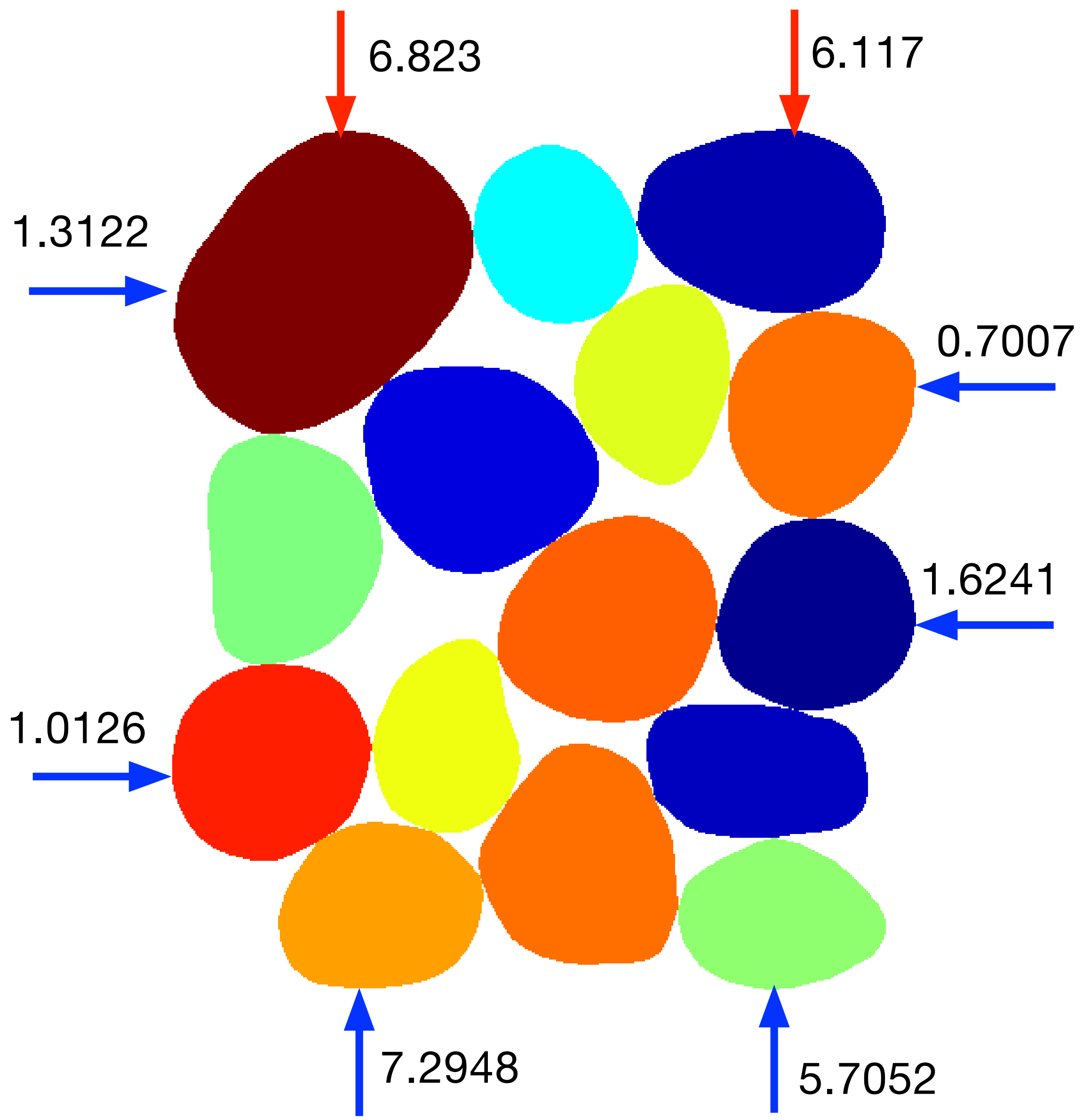


'measured' ave strains

GEM Ko compression

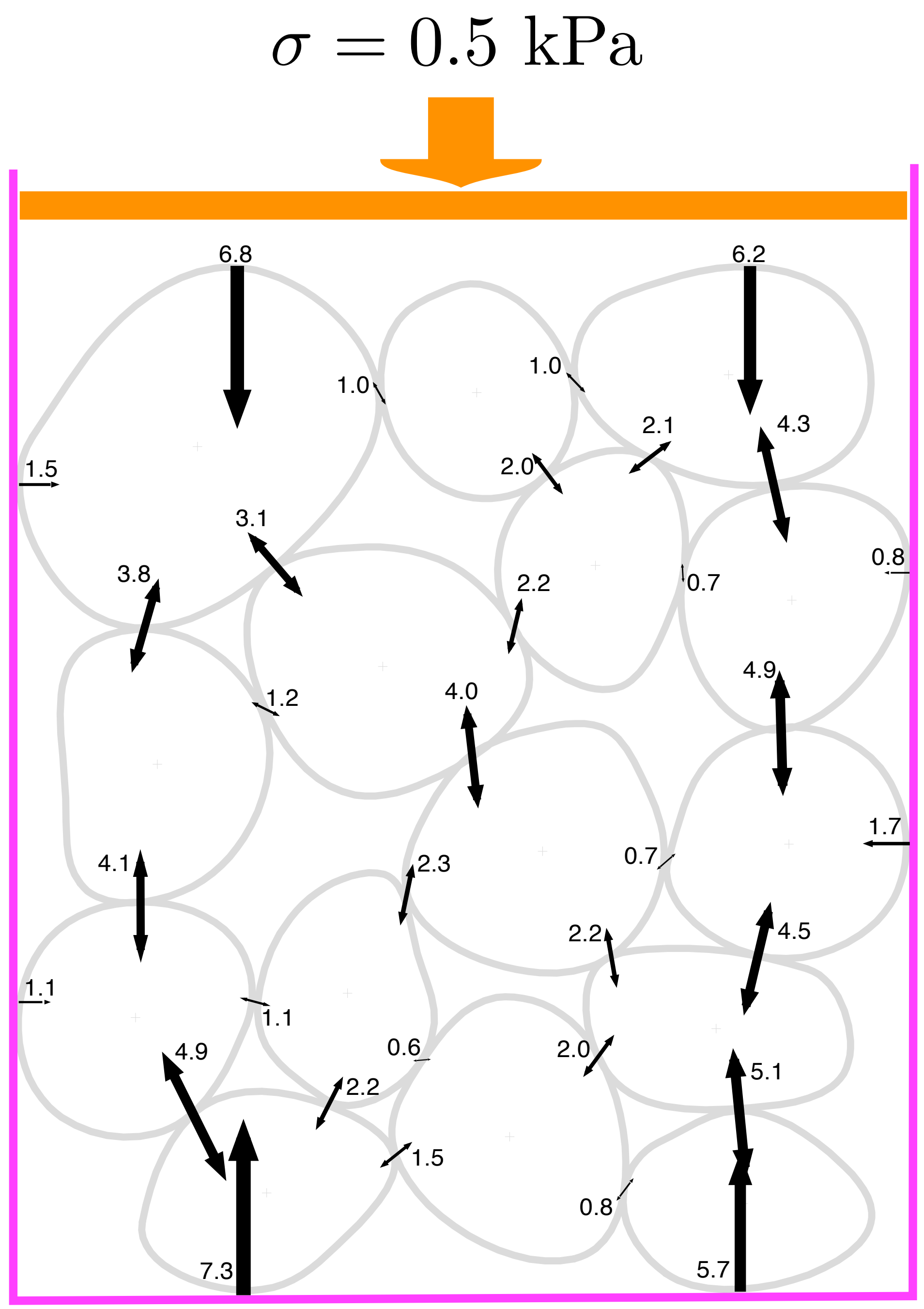


distribution of contact forces in sample

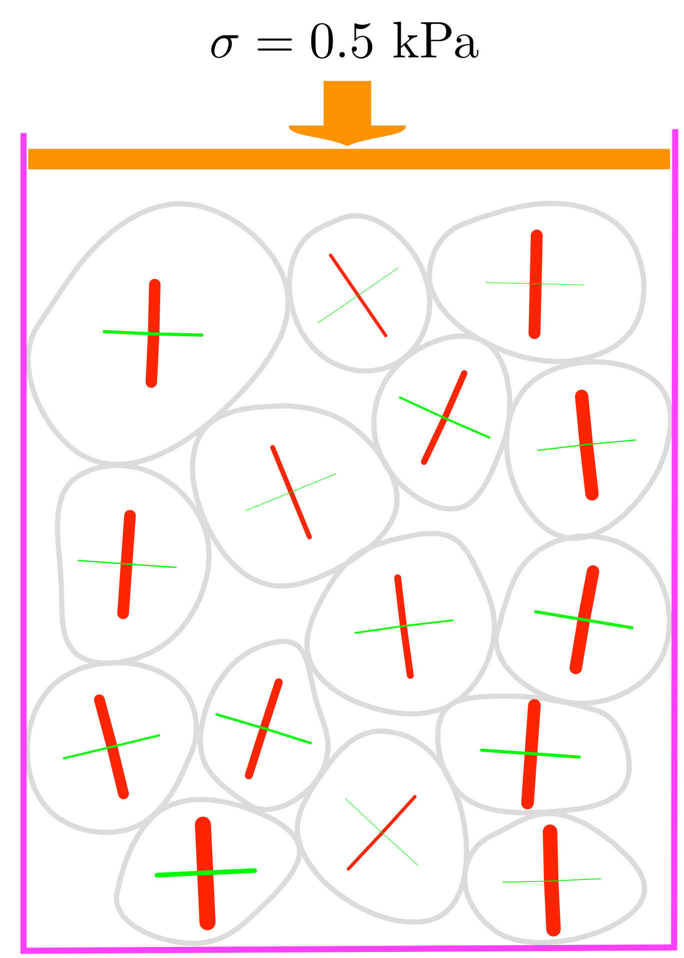


compare with FEM

GEM Ko compression



distribution of contact forces in sample



principal grain stress directions

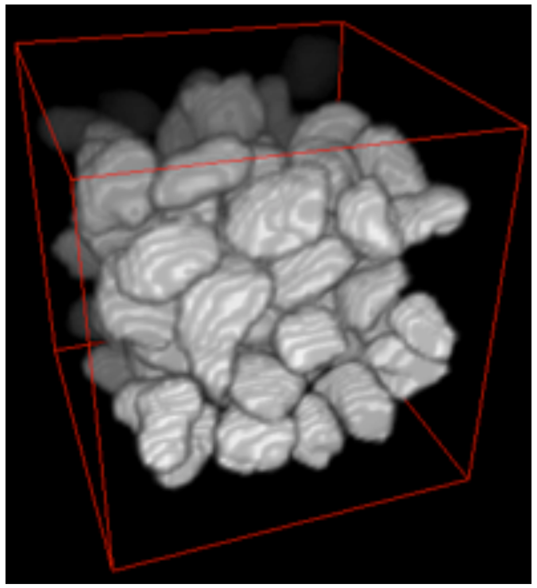
$$\langle \boldsymbol{\sigma} \rangle = \begin{bmatrix} -0.085 & 0.001 \\ 0.001 & -0.496 \end{bmatrix}$$

quasi-Ko

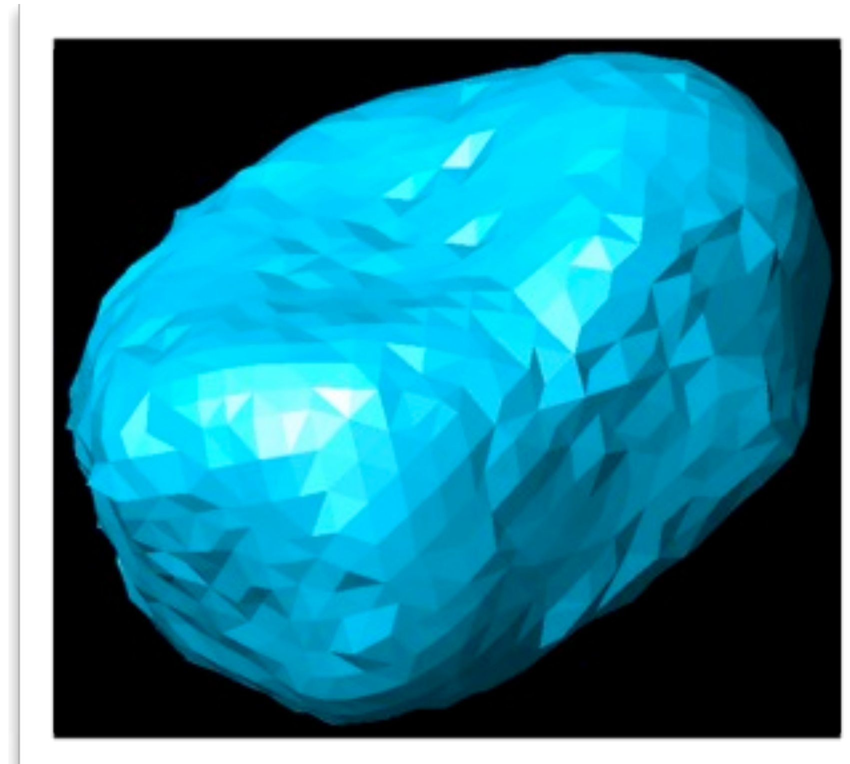
Closure

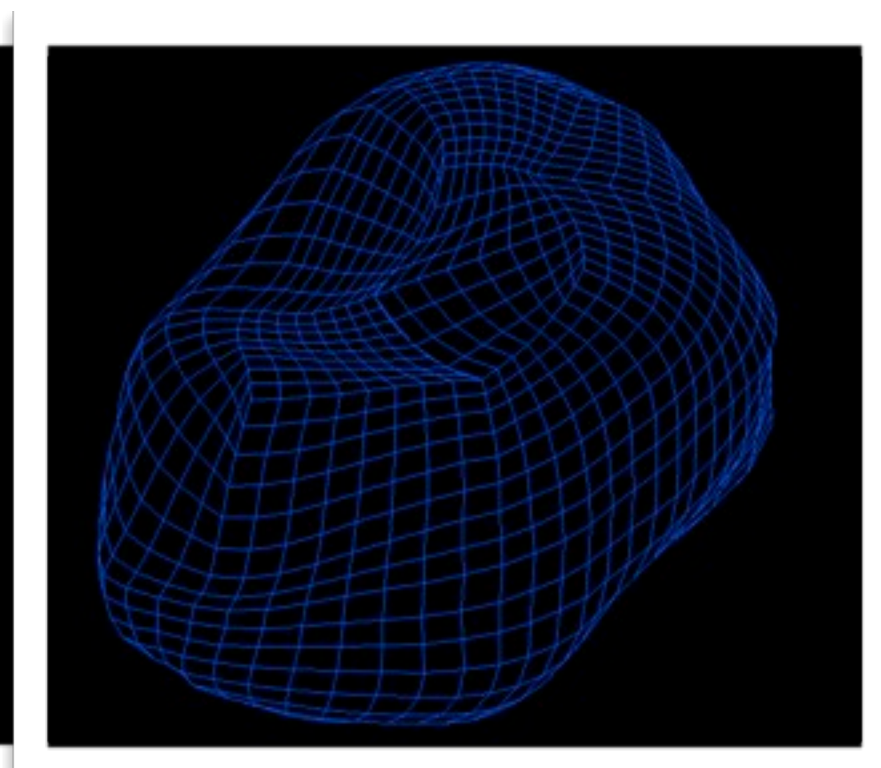
- Multiscale can bypass phenomenology
- Hierarchical works well with experiments
- Combine imaging & computing: predict
- First predictive multiscale framework
- See the unseen, measure the unmeasured

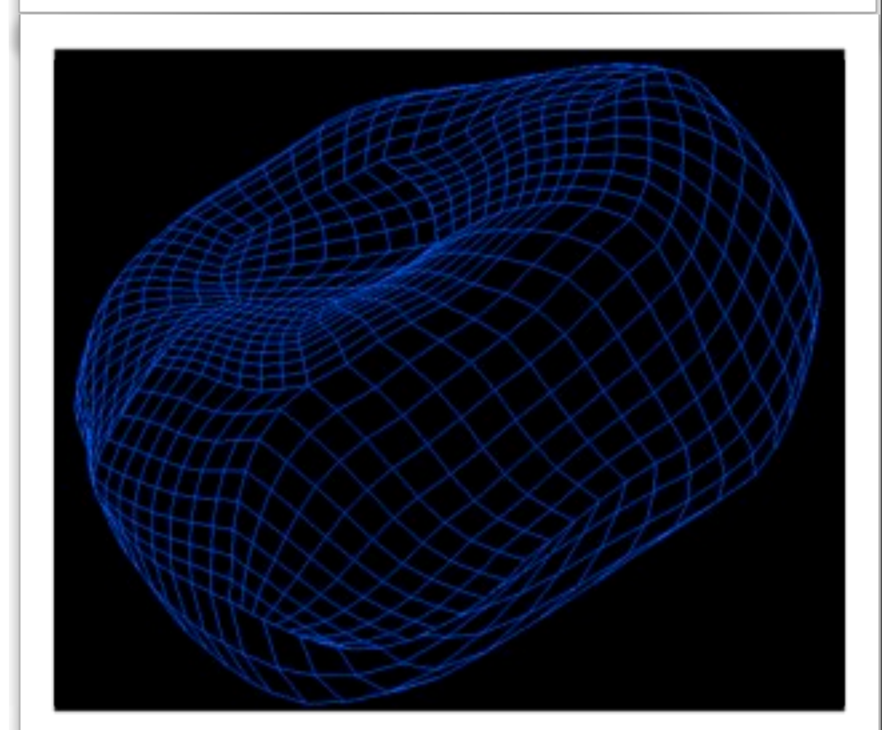
The future...



EXACT particle shape for DEM







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