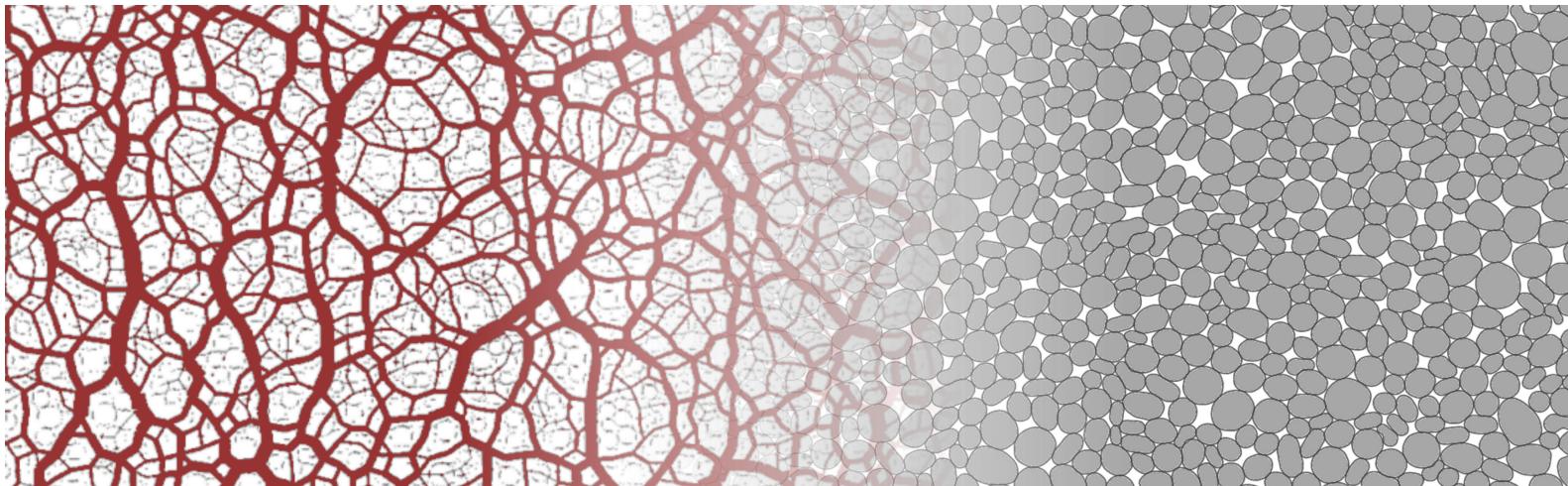


Data-Driven Modeling of Geomaterials



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Alert Doctoral School, Aussois, France
Sep. 28, 2023



Caltech


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www.mm.ethz.ch

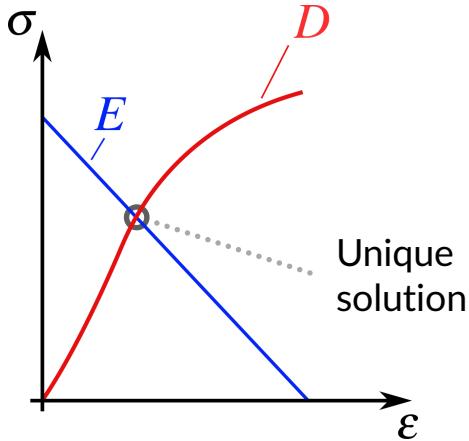
 CENTRALE
NANTES

Introduction

Conventional (+ ML-based surrogate)

$$\begin{cases} \nabla \cdot \sigma + \rho b = 0 & (1) \\ \epsilon = \text{sym}(\nabla u) & (2) \\ \sigma = \sigma(\epsilon) \end{cases}$$

e.g. learned constitutive relation (LSTM/TANN/..)

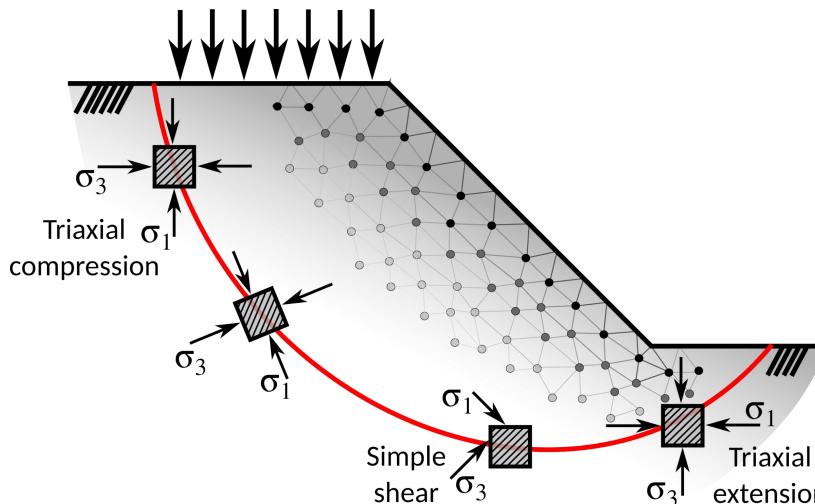


- Uncertainty in functional form
- Uncontrolled extrapolation
- Laborious training/Fast inference

Mozzafar et al., 2019

Masi et al., 2021

Fung et al., 2022



Data-Driven Computing (DD)

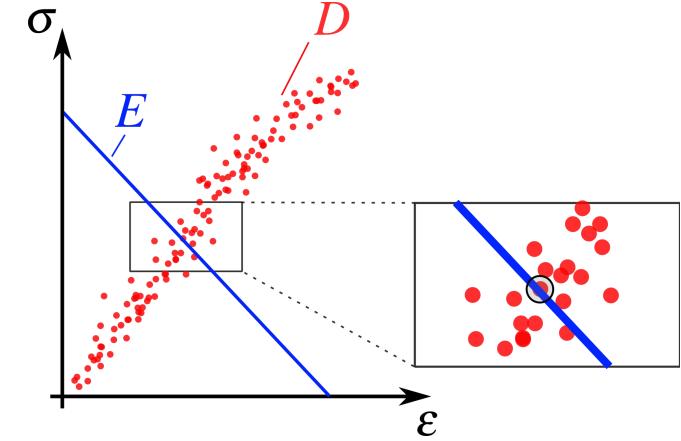
Kirchdoerfer et al., 2016

Phase Space: $Z = \{(\epsilon, \sigma)\}$

Equilibrium Set: $E = \{z \in Z \mid (1), (2)\}$

Material Data Set: $D \subset Z$

$$\min_{z \in E} \min_{y \in D} d(z, y)$$



- Pure data/No fitting/Explicit conservation laws
- Eminent physical meaning (distance)

Overview

I) Data-Driven Computational Mechanics

- a) Formulation
- b) Hands-off example
- c) Improving convergence

II) Data Mining

- a) Experiments (Identification)
- b) Simulations (Multiscale)
- c) Adaptive data sampling

III) History-dependent Formulation

IV) Multi-field Formulation

V) Advanced Applications

- a) Shear banding
- b) Breakage mechanics

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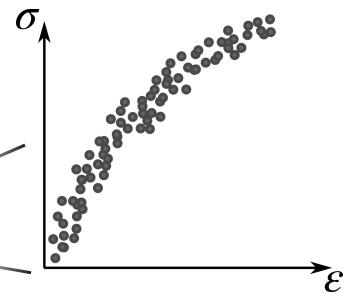
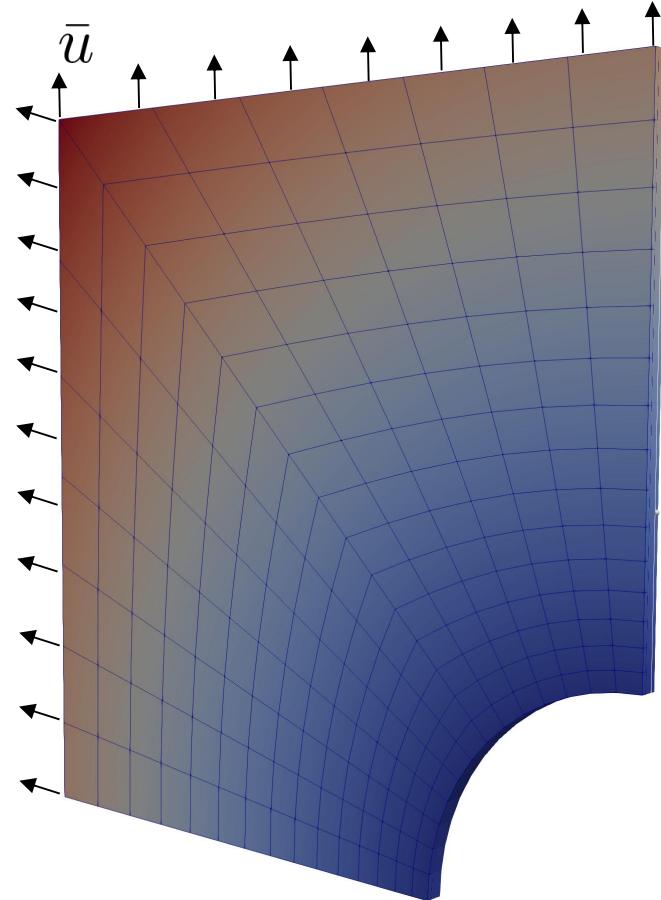
IV) Multi-field Formulation

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Data-Driven Computational Mechanics

Kirchdoerfer et al, 2016



Perform double minimization in staggered fashion

$$\min_{z \in E} \min_{y \in D} d(z, y)$$

$$\begin{aligned} & \min \sum_e w_e d_e(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e) \\ \text{s.t. } & \boldsymbol{\varepsilon}_e = \sum_i \mathbf{B}_{ei} u_i, \\ & \sum_e w_e \mathbf{B}_{ei}^T \boldsymbol{\sigma}_e = F_i \end{aligned}$$

→ Mechanical states
 $\mathbf{z} = \{(\boldsymbol{\varepsilon}^e, \boldsymbol{\sigma}^e)\}_{e=1,\dots,N}$

$$d_e(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}_e) = \min_{\boldsymbol{\varepsilon}_e^*, \boldsymbol{\sigma}_e^* \in D_e} (\boldsymbol{\varepsilon}_e - \boldsymbol{\varepsilon}_e^*)^T \mathbb{C}_e (\boldsymbol{\varepsilon}_e - \boldsymbol{\varepsilon}_e^*) + (\boldsymbol{\sigma}_e - \boldsymbol{\sigma}_e^*)^T \mathbb{C}_e^{-1} (\boldsymbol{\sigma}_e - \boldsymbol{\sigma}_e^*)$$

→ Material states
 $\mathbf{y} = \{(\boldsymbol{\varepsilon}^{e*}, \boldsymbol{\sigma}^{e*})\}_{e=1,\dots,N}$

The stiffness \mathbb{C}_e is simply a distance-inducing numerical parameter

Fixed-point algorithm

Iterative scheme, involving:

- i) Solution of two modified ‘elasticity’ problems
- ii) Database search

$$\left(\sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \mathbf{B}_e \right) \mathbf{u}^{(i)} = \sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \varepsilon_e^{*(i)} \quad (1)$$

$$\left(\sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \mathbf{B}_e \right) \boldsymbol{\eta}^{(i)} = \mathbf{f} - \sum_{e=1}^M w_e \mathbf{B}_e^T \sigma_e^{*(i)} \quad (2)$$

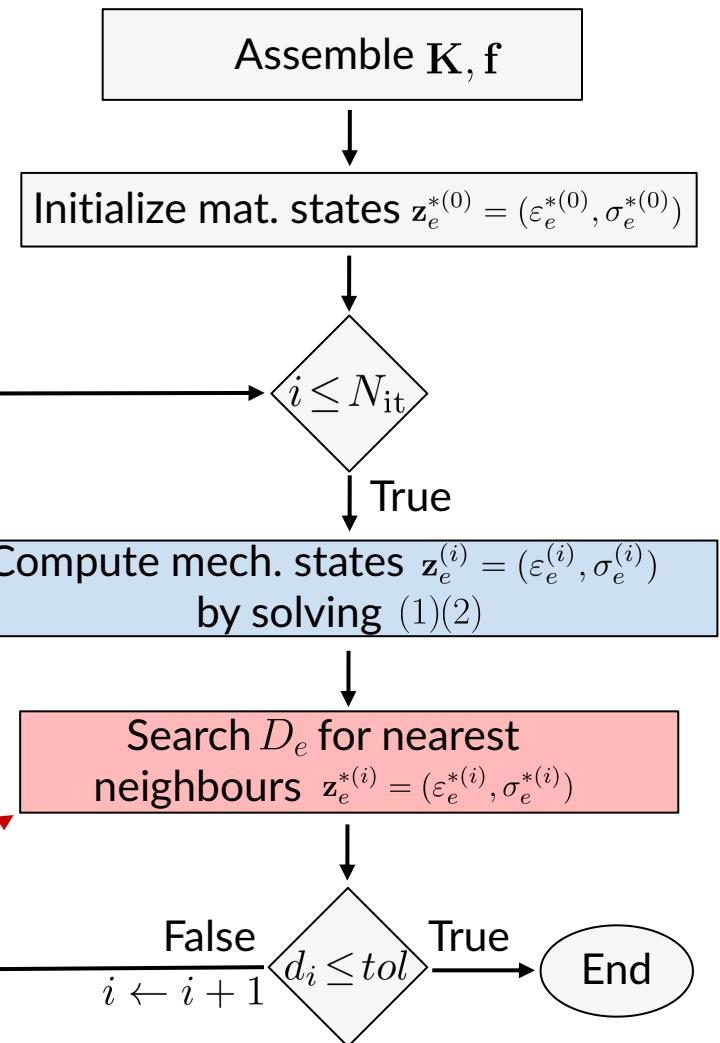
$$\sigma_e^{(i)} = \sigma_e^{*(i)} + \mathbb{C}_e \sum_{\alpha=1}^N \mathbf{B}_{ea} \eta_{\alpha}^{(i)}$$

Positive-definite
distance-
inducing tensor

$$|z^e| = \mathbb{C}^e \boldsymbol{\varepsilon}^e \cdot \boldsymbol{\varepsilon}^e + \mathbb{C}^{e^{-1}} \boldsymbol{\sigma}^e \cdot \boldsymbol{\sigma}^e$$

$$\begin{array}{c} \boxed{\mathbf{K}} \quad \boxed{\mathbf{u}} = \boxed{\mathbf{F}_{\varepsilon}} \\ \boxed{\mathbf{K}} \quad \boxed{\boldsymbol{\eta}} = \boxed{\mathbf{F}_{\sigma}} \end{array}$$

Major
computational
burden
(tree-search)



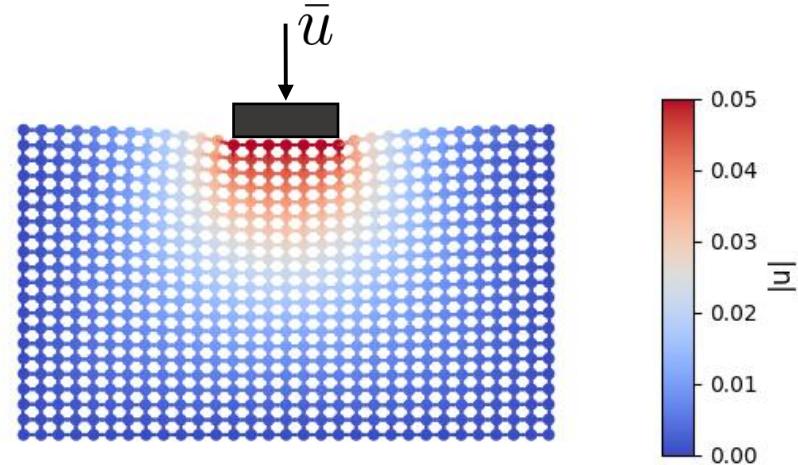
An open-source Python library

github.com/kkarapiperis/ddcm-2D

The screenshot shows the GitHub repository page for 'ddcm-2D'. It features a commit history from 'kkarapiperis' showing the addition of main example files and source code. The README.md file is titled 'Data-Driven Computational Mechanics' and describes the software for solving 2D boundary value problems. It lists prerequisites (Python 3.10, Numpy 1.21.2, Matplotlib 3.4.3) and a license (MIT). Suggested GitHub Actions workflows include 'Actions Importer', 'Publish Python Package', and 'Python package'.



A simple flat-punch
boundary value problem

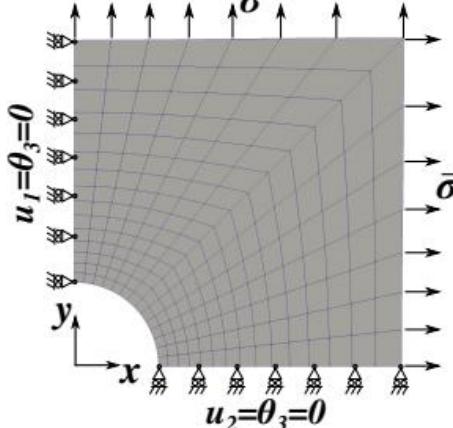


Improving accuracy

Karapiperis et. al., 2021

Can we solve for the metric-inducing tensor?

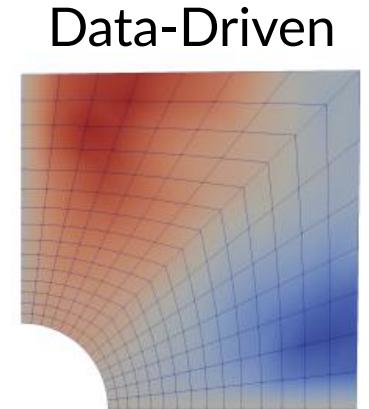
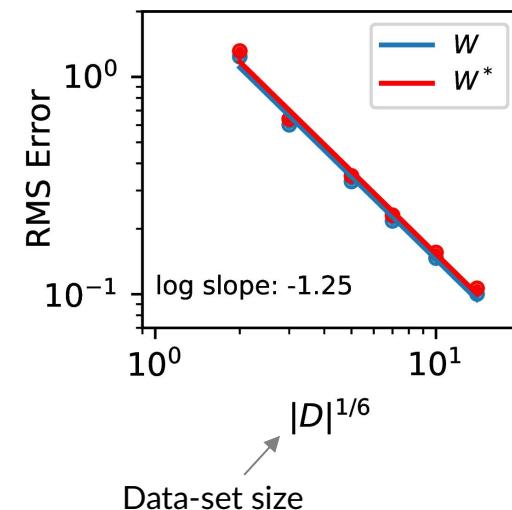
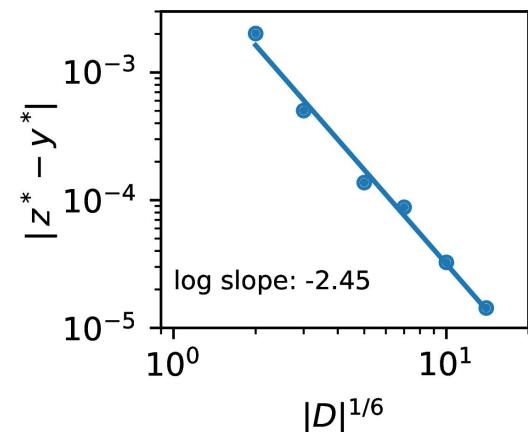
$$|z^e| = \min_{\mathbb{C}^e \succeq 0} \mathbb{C}^e \boldsymbol{\varepsilon}^e \cdot \boldsymbol{\varepsilon}^e + \mathbb{C}^{e^{-1}} \boldsymbol{\sigma}^e \cdot \boldsymbol{\sigma}^e$$



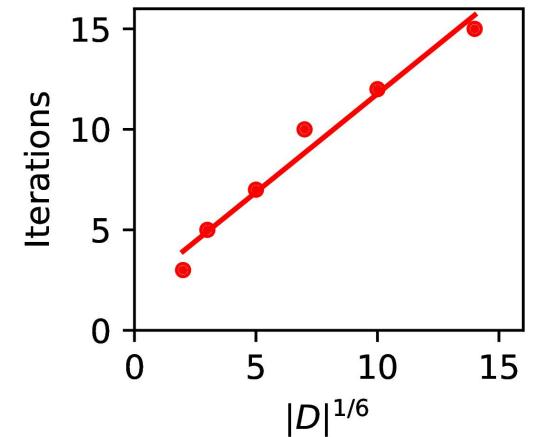
$$RMS_W = \left(\frac{\sum_e w_e W(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{ref}})}{\sum_e w_e W(\boldsymbol{\varepsilon}^{\text{ref}})} \right)^{1/2}$$

$$RMS_{W^*} = \left(\frac{\sum_e w_e W^*(\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\text{ref}})}{\sum_e w_e W^*(\boldsymbol{\sigma}^{\text{ref}})} \right)^{1/2}$$

- Truly parameter-free scheme
- Balanced error in compatibility (W^*) and equilibrium (W)

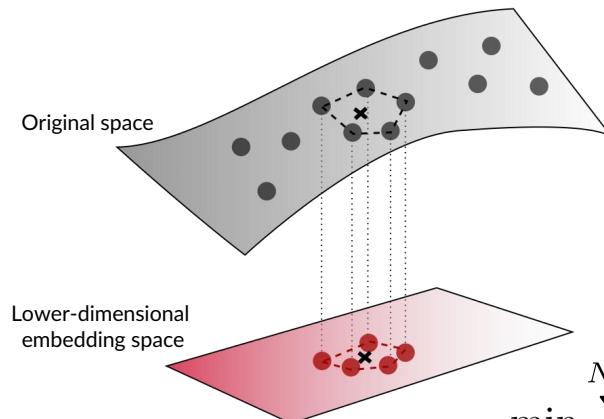


Karapiperis et. al., 2021



Tackling noise and improving convergence

Locally convex/linear embedding



Kirchdoerfer and Ortiz, 2017
Ibanez, 2018
He and Chen, 2021
Eggersmann et al, 2021

$$\min_{\mathbf{w}} \sum_i^{N_{\text{data}}} \|z_i - \sum_{j \in \mathcal{N}_i} w_{ij} z_j\|^2$$

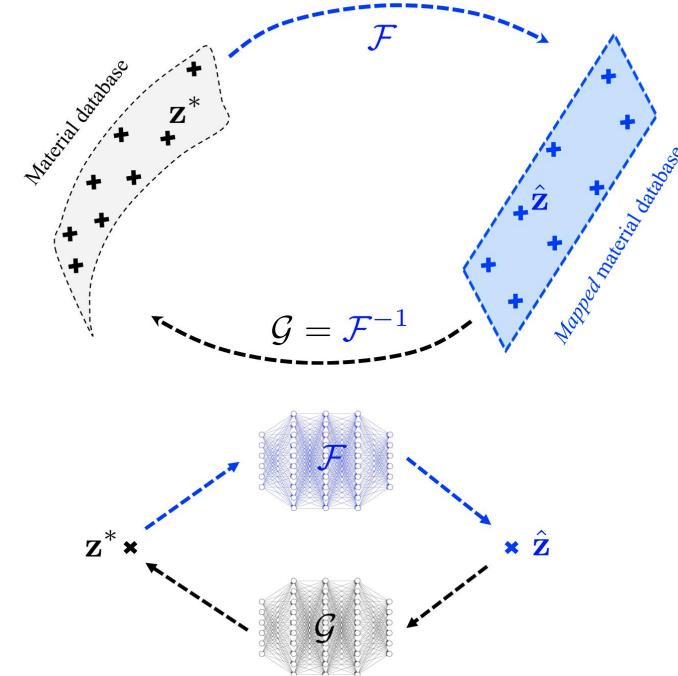
$$\text{s.t. } \sum_{j \in \mathcal{N}_i} w_{ij} = 1$$

$$w_{ij} = 0 \text{ if } j \notin \mathcal{N}_i$$

- Often noisy/high dimensional data. Live in manifolds with structure.
- Potential to improve convergence

Global embedding

Bahmani and Sun, 2021



$$\min_{\theta, \beta, \hat{\mathbb{C}}} \sum_i^{N_{\text{data}}} \|\hat{\sigma}_i - \hat{\mathbb{C}} \hat{\epsilon}_i\|^2 + \|z_i^* - \mathcal{G}(\mathcal{F}(z_i^*, \theta), \beta)\|^2$$

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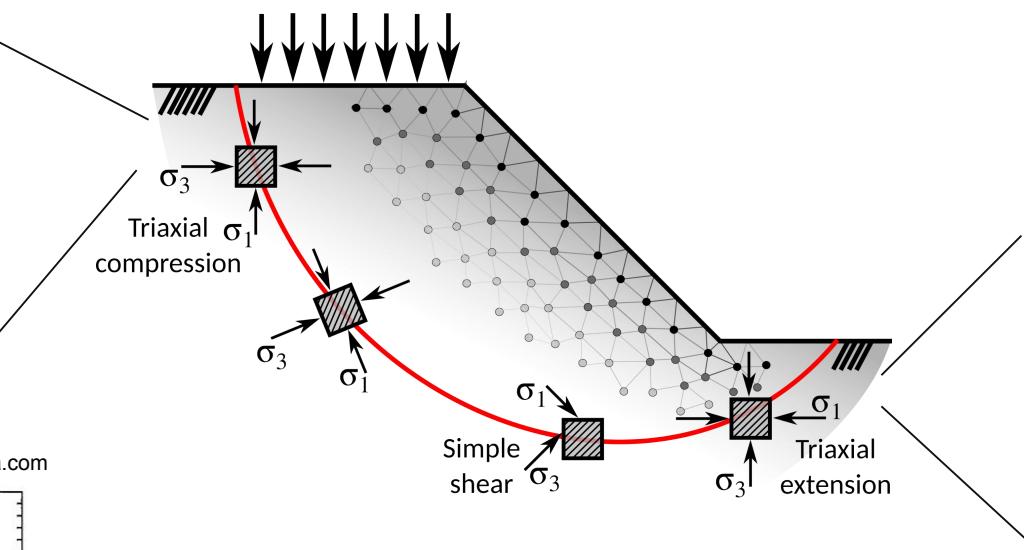
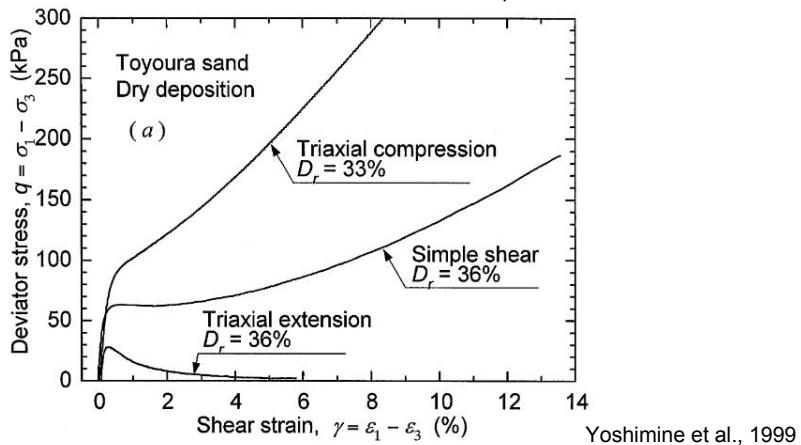
- a) Shear banding
- b) Breakage mechanics

Data mining

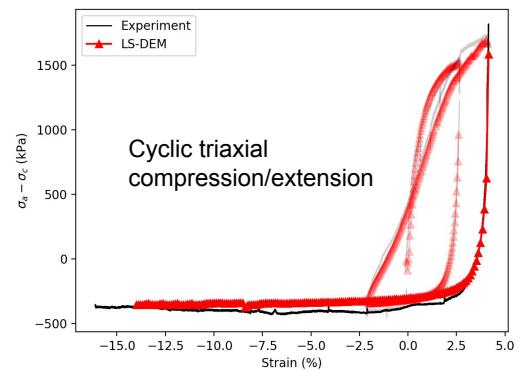
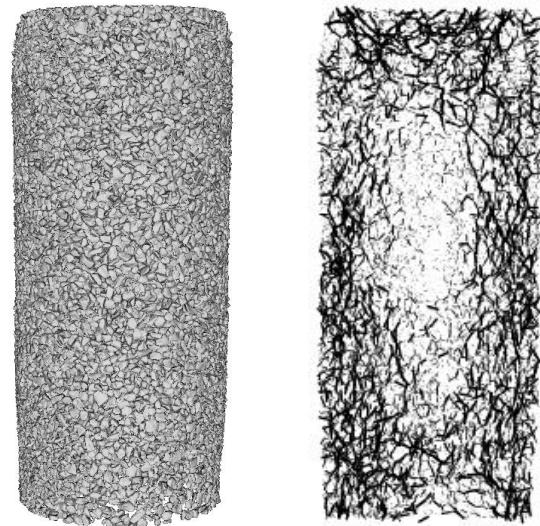
Physical Experiments



wikipedia.com



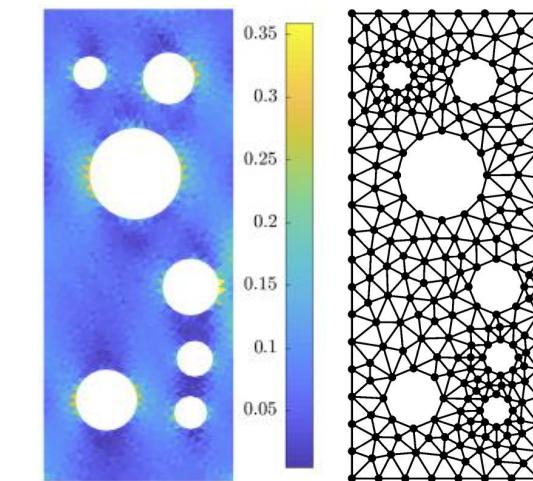
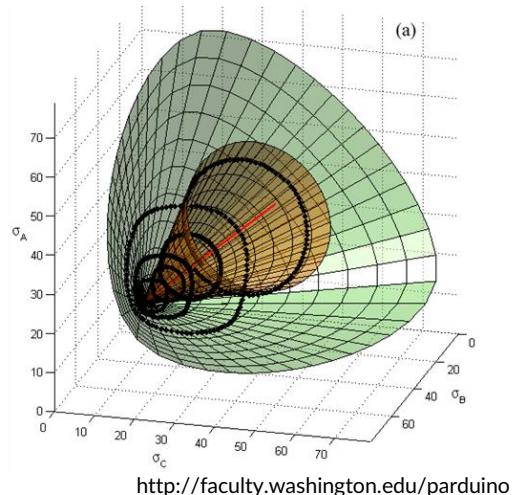
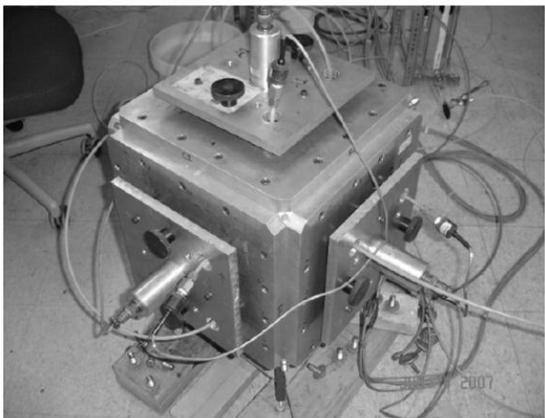
DEM simulations (Multiscale DD)



Experimental data mining

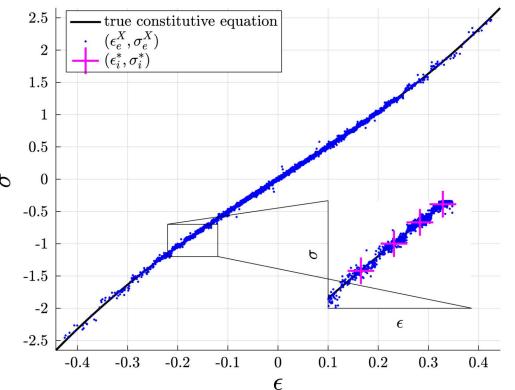
Element tests

- Boundary measurements
(e.g. from true triaxial test)



Data-Driven identification from full-field measurements

- Displacement field e.g. from DIC
- Measured reaction forces



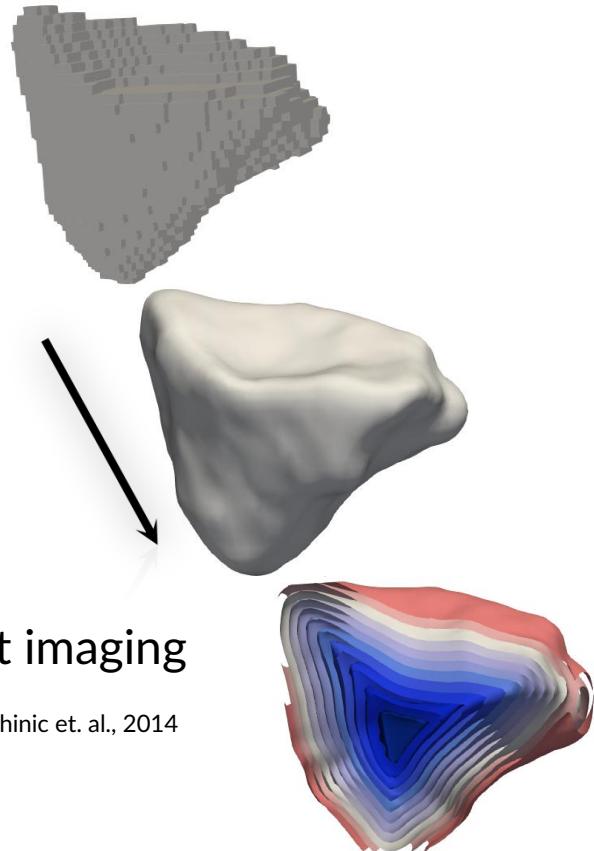
Leygue et al., 2017
Stainier et al., 2019

Find the stress-strain pairs that best satisfy equilibrium/compatibility

Level-Set DEM for granular simulations

Kawamoto et al, 2018, Karapiperis et al, 2020

Morphology

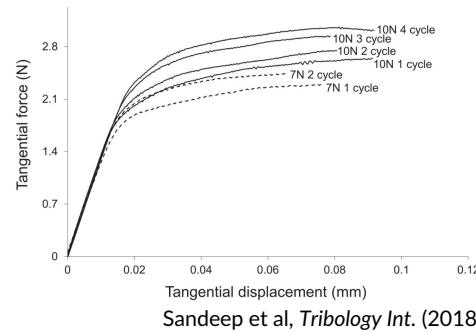
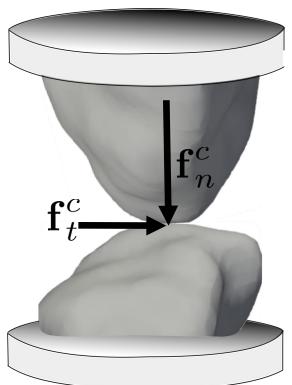


Level set imaging

Vlahinic et. al., 2014

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Interaction



$$\mathbf{f}^c = \mathbf{f}_n^c + \mathbf{f}_t^c$$

$$\mathbf{f}_n^c = k_n \delta_n \mathbf{n}$$

$$\mathbf{f}_t^c = -\frac{\Delta \mathbf{s}}{\|\Delta \mathbf{s}\|} \min(k_t \|\Delta \mathbf{s}\|, \mu \|\mathbf{f}_n^c\|)$$

Specimen generation

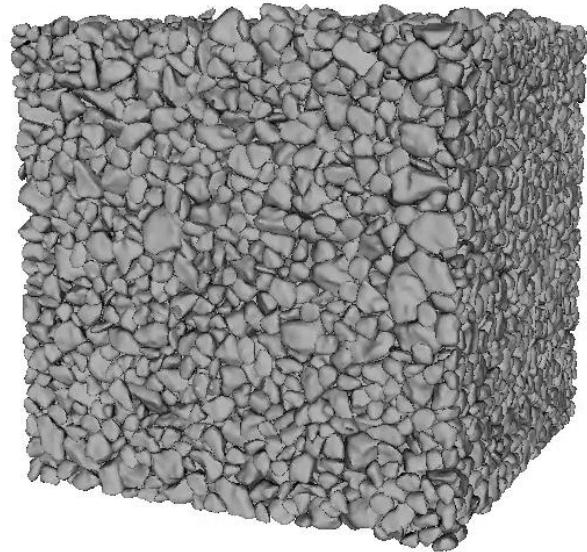
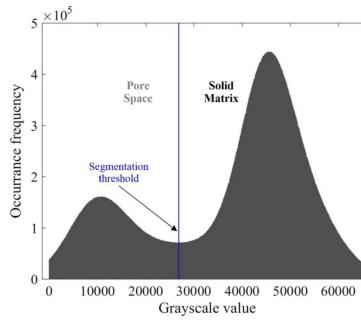


Image-based reconstruction of porous rocks/conglomerates

X-ray CT



Fu et. al., 2022

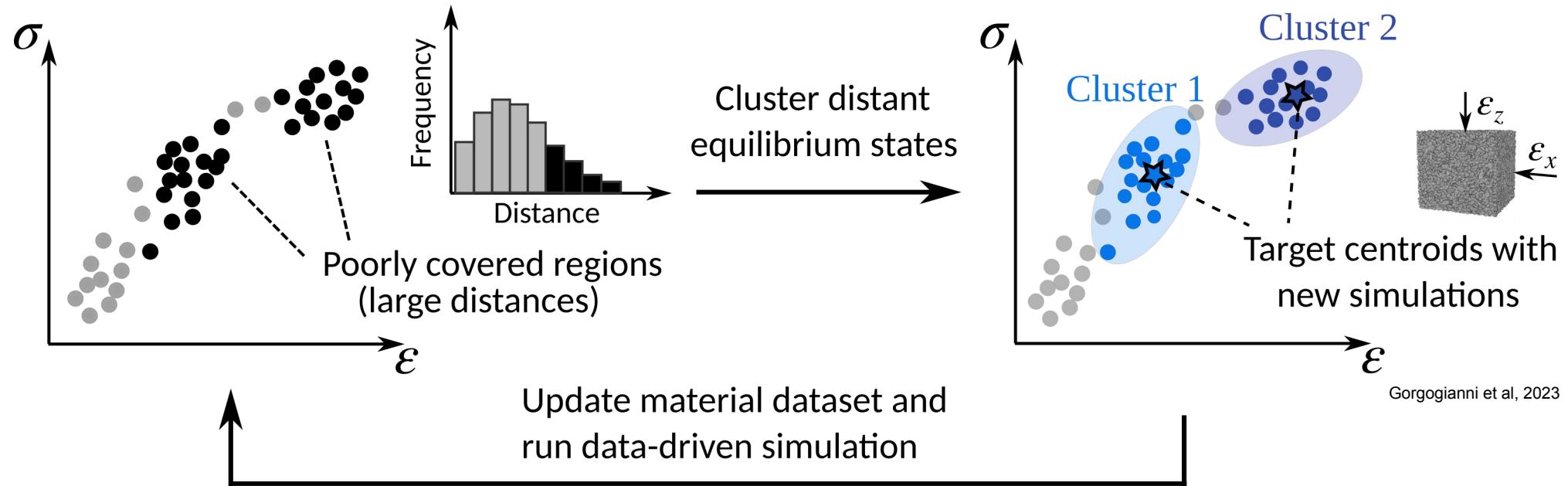


Computational specimen



What if data are still scarce?

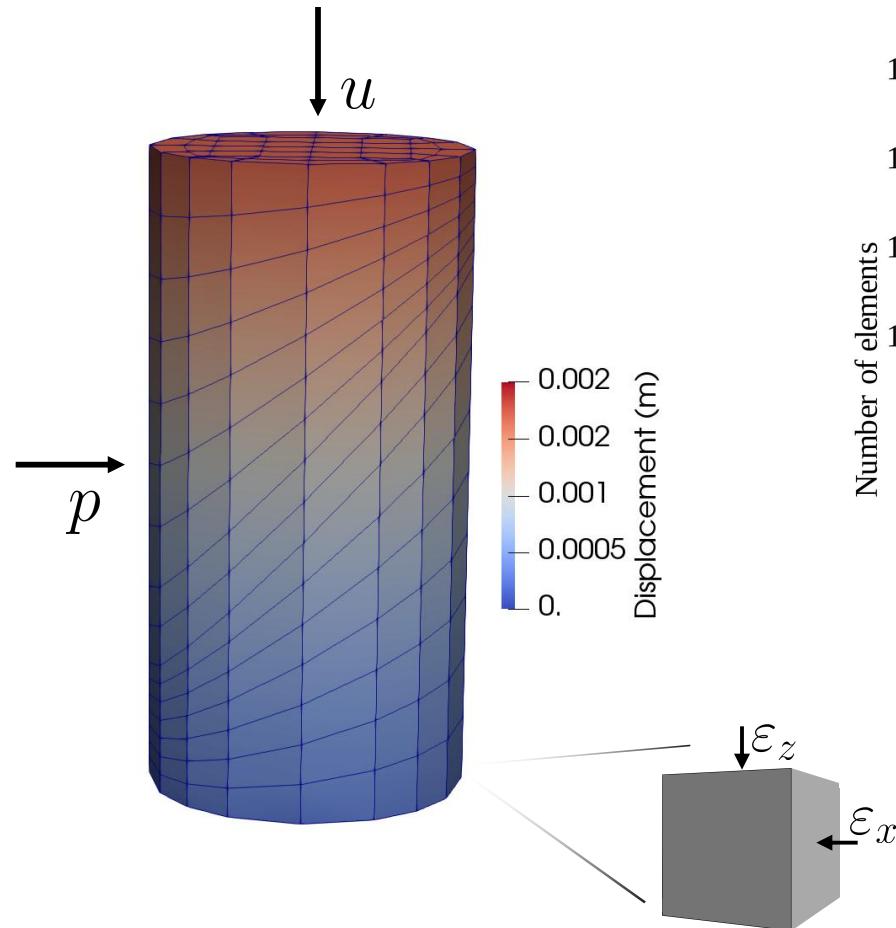
Iteratively sample poorly populated regions of the phase space



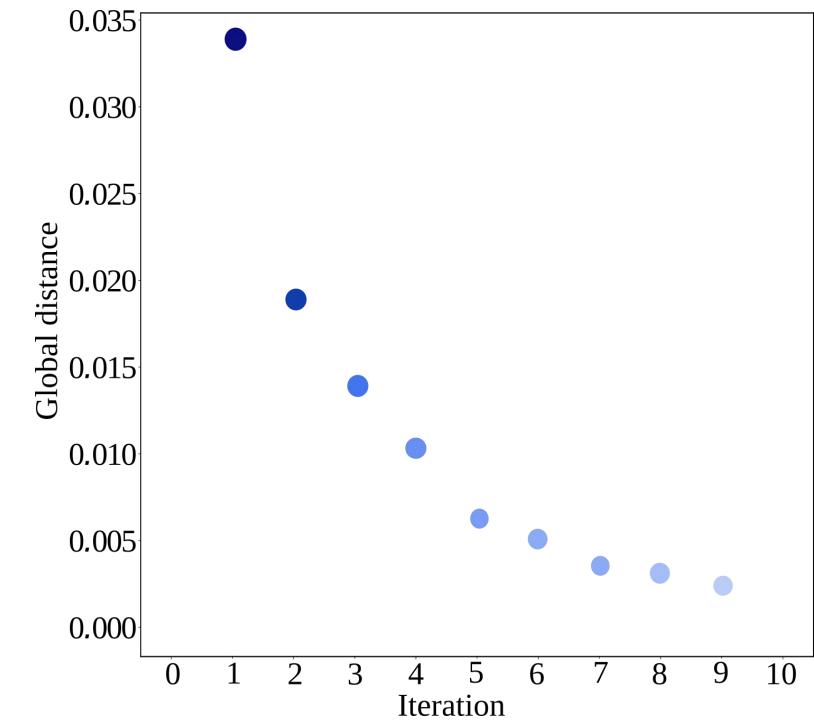
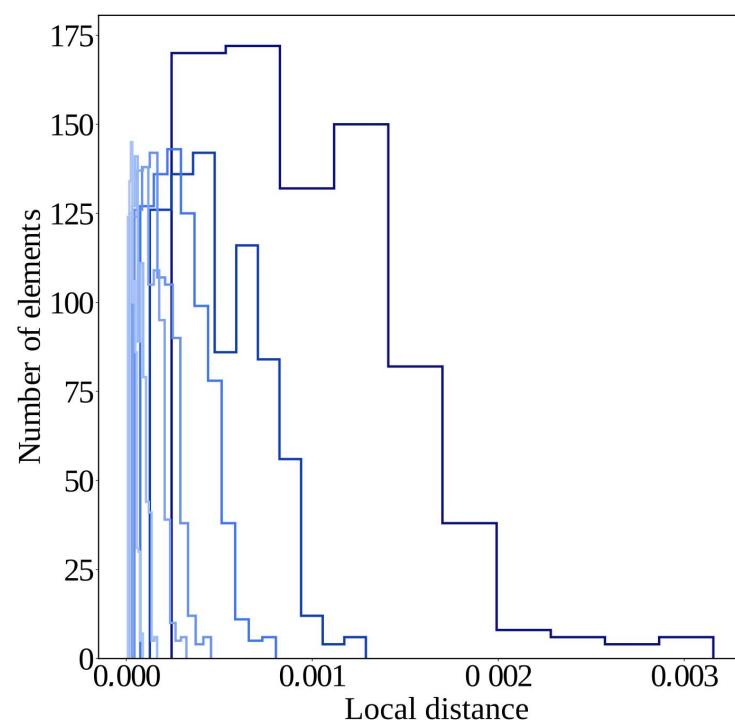
Adaptive sampling via *unsupervised learning*
Repeat until distance is small enough

Convergence study

Triaxially compressed elastic cylinder



Error decays with each iteration



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History-dependent formulation

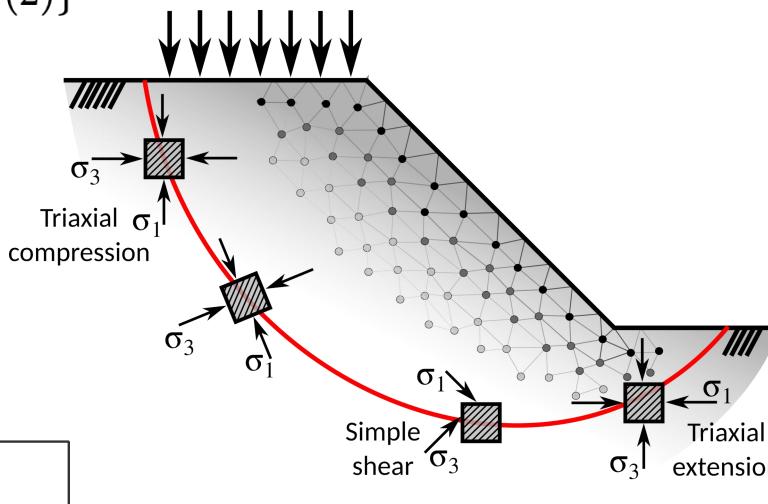
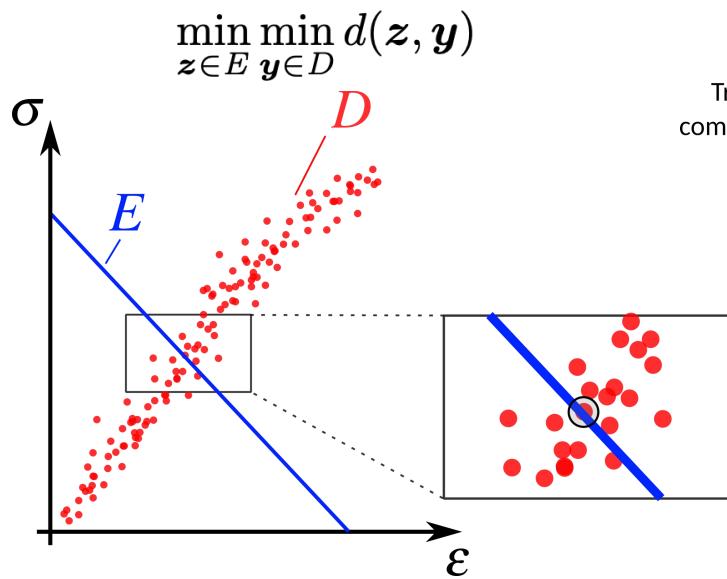
Data-Driven Computing (DD)

Kirchdoerfer et al., 2016

Phase Space: $Z = \{(\epsilon, \sigma)\}$

Equilibrium Set: $E = \{z \in Z \mid (1), (2)\}$

Material Data Set: $D \subset Z$



History-dependent DD

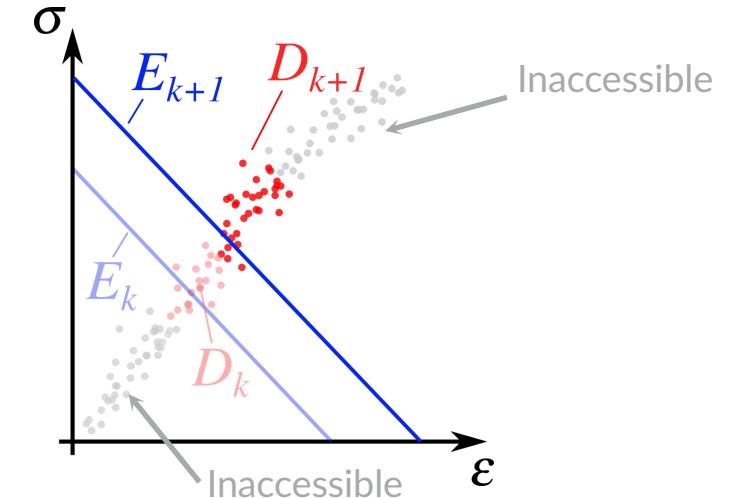
Karapiperis et al., 2020
Eggersmann et al., 2019

History-dependence \rightarrow Notion of time

Time-dependent Equilibrium Set: $E_k \subset Z$

Time-dependent Material Data Set: $D_k \subset Z$

$$\min_{z_k \in E_k} \min_{y_k \in D_k} d(z_k, y_k)$$



Modified solution algorithm

Iterative scheme, involving:

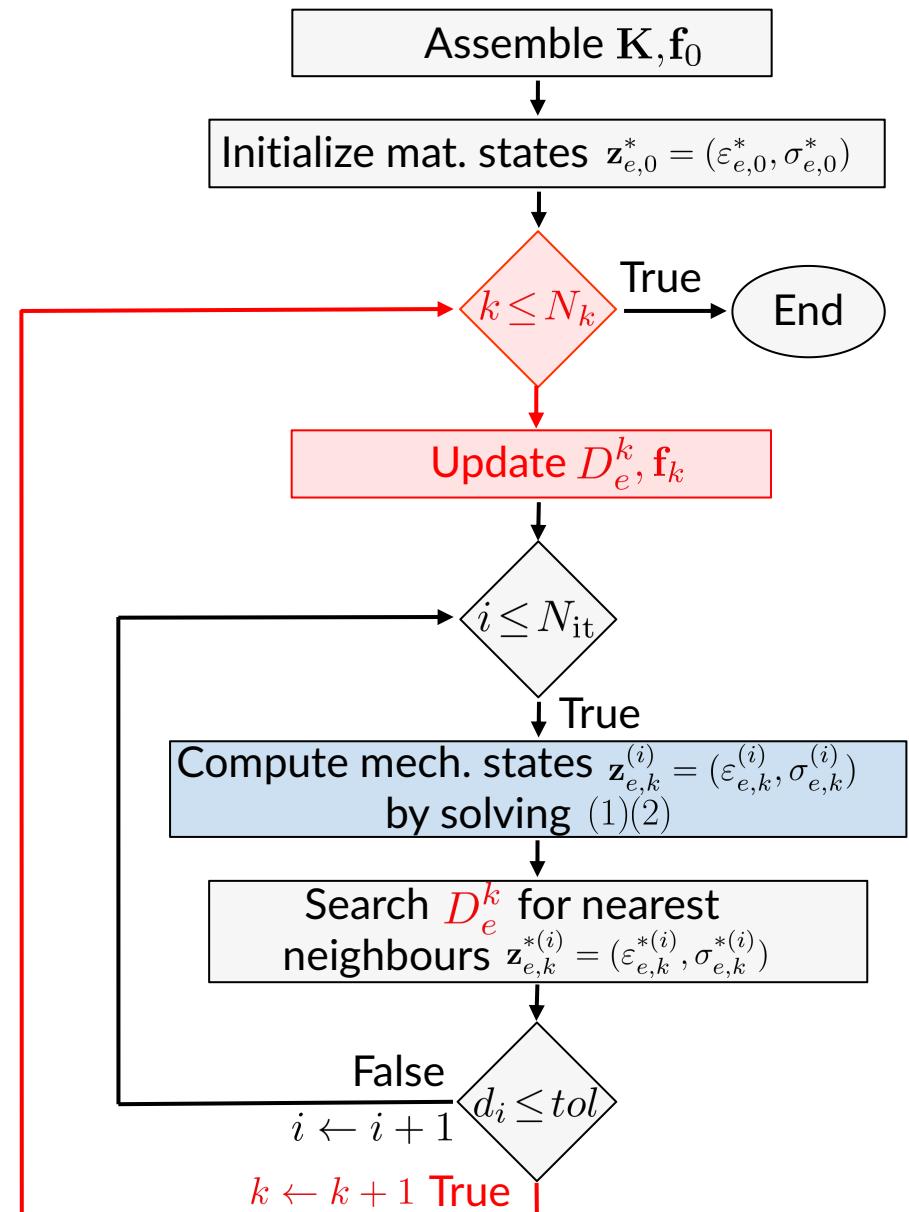
- i) Solution of two modified ‘elasticity’ problems
- ii) Database search

$$\left(\sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \mathbf{B}_e \right) \mathbf{u}_k^{(i)} = \sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \varepsilon_{e,k}^{*(i)} \quad (1)$$

$$\left(\sum_{e=1}^M w_e \mathbf{B}_e^T \mathbb{C}_e \mathbf{B}_e \right) \boldsymbol{\eta}_k^{(i)} = \mathbf{f}_k - \sum_{e=1}^M w_e \mathbf{B}_e^T \sigma_{e,k}^{*(i)} \quad (2)$$

$$\sigma_{e,k}^{(i)} = \sigma_{e,k}^{*(i)} + \mathbb{C}_e \sum_{\alpha=1}^N \mathbf{B}_{e\alpha} \eta_{\alpha,k}^{(i)}$$

$$\begin{array}{c|c|c} \mathbf{K} & \mathbf{u} & \mathbf{F}_\varepsilon \\ \hline \mathbf{K} & \boldsymbol{\eta} & \mathbf{F}_\sigma \end{array}$$

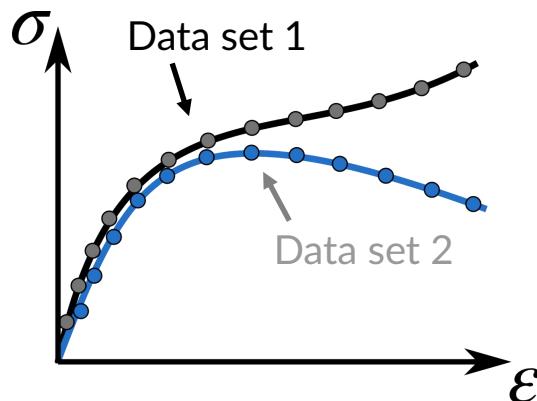


History parametrization

History-matching

Eggersmann et al., 2019

$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \mid \{\epsilon_l\}_{l \leq k}\}$$



Material-independent
Inefficient

Konstantinos Karapiperis

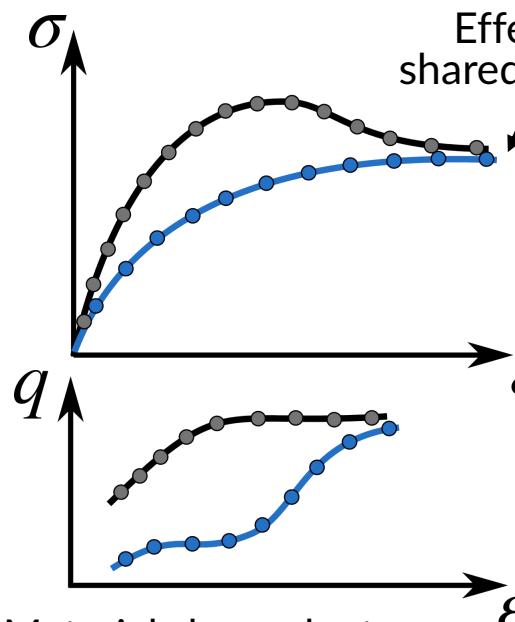
Internal variable

Eggersmann et al., 2019

Karapiperis et al., 2020

$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \mid (\epsilon_k, \sigma_k, q_k)\}$$

Internal variable: $q = \{F, \dots\}$



Material-dependent
Requires access to micromechanics
Augments space by set of int. variables

Thermodynamics

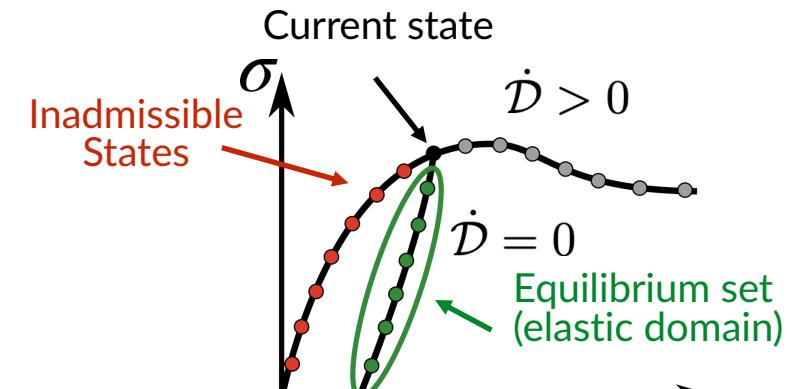
Karapiperis et al., 2020

$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \mid (\epsilon_k, \sigma_k), (1)\}$$

$$\mathcal{D}_{k+1} - \mathcal{D}_k = \frac{\sigma_k + \sigma_{k+1}}{2} : (\epsilon_{k+1} - \epsilon_k)$$

$$- (\mathcal{A}_{k+1} - \mathcal{A}_k) \geq 0 \quad (1)$$

Dissipation
Free energy



Material-independent

Alert Doctoral School, Aussois - 2023 - 20

Application to geomaterials

Free energy/Dissipation

$$\boldsymbol{\varepsilon} = \frac{1}{2V} \text{sym} \left(\sum_{p \in \partial\mathcal{P}} \mathbf{u}^p \otimes \mathbf{n}^p \right)$$

$$\boldsymbol{\sigma} = \frac{1}{V} \text{sym} \left(\sum_{c \in \mathcal{C}} \mathbf{f}^c \otimes \mathbf{l}^c \right)$$

$$\mathcal{A} = \sum_c \mathcal{A}^c = \frac{1}{2V} \sum_c \left(\frac{\|\mathbf{f}_n^c\|^2}{k_n} + \frac{\|\mathbf{f}_t^c\|^2}{k_t} \right)$$

$$d\mathcal{D} = \sum_c d\mathcal{D}^c = \frac{1}{V} \sum_c \mathbf{f}_t^c \cdot d\mathbf{u}^{c, \text{slip}}$$

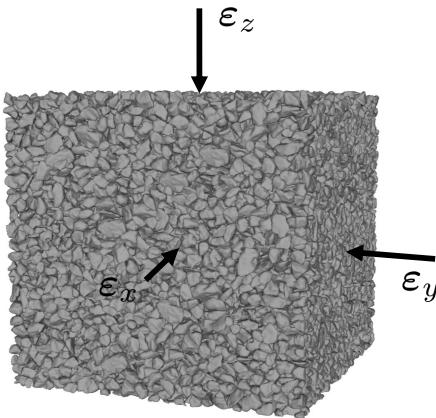
Internal variables

$$\begin{aligned} \mathbf{q} &= P_{\text{nf}}(\mathbf{n}, \mathbf{f}, \mathbf{l}) \\ &= \underbrace{P_{\mathbf{n}}(\mathbf{n})}_{\substack{\text{Contact} \\ \text{structure}}} \underbrace{P_{\mathbf{f}|\mathbf{n}}(\mathbf{f}|\mathbf{n})}_{\substack{\text{Frictional} \\ \text{history}}} \underbrace{P_{\mathbf{l}|\mathbf{f}, \mathbf{n}}(\mathbf{l}|\mathbf{f}, \mathbf{n})}_{\substack{\text{Grain} \\ \text{size/shape} \\ \downarrow \text{Second-order} \\ \text{statistics}}} \end{aligned}$$

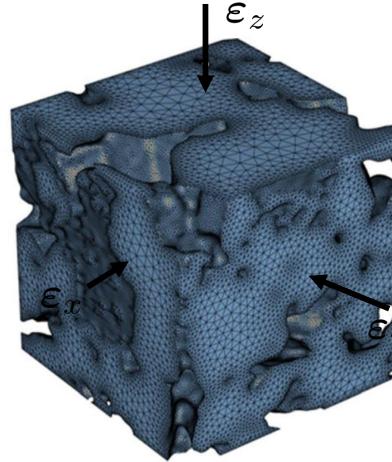
Fabric tensors

Konstantinos Karapiperis

Granular RVE



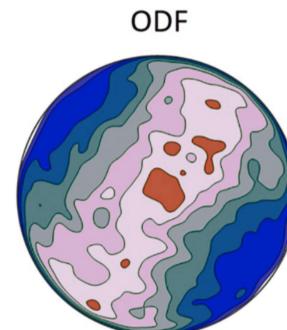
Continuum RVE



(e.g. porous rock)



Contact Fabric



Pore texture

Free energy/Dissipation

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V} \int_{\partial V} \text{sym}(\mathbf{u} \otimes \mathbf{n}) dS$$

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_{\partial V} \mathbf{t} \otimes \mathbf{x} dS$$

$$\bar{\mathcal{A}} = \frac{1}{V} \int_V \mathcal{A}(\mathbf{x}) dS$$

$$d\bar{\mathcal{D}} = \bar{\boldsymbol{\sigma}} : d\bar{\boldsymbol{\varepsilon}} - d\bar{\mathcal{A}}$$

Internal variables

$$\begin{aligned} \mathbf{q} &= \underbrace{P(s)}_{\substack{\text{Pore} \\ \text{size}}} \underbrace{P(n)}_{\substack{\text{Pore} \\ \text{orientation}}} \\ &\quad \downarrow \text{Second-order} \\ &\quad \text{statistics} \end{aligned}$$

Pore texture tensor

Application to granular materials - Material point simulations

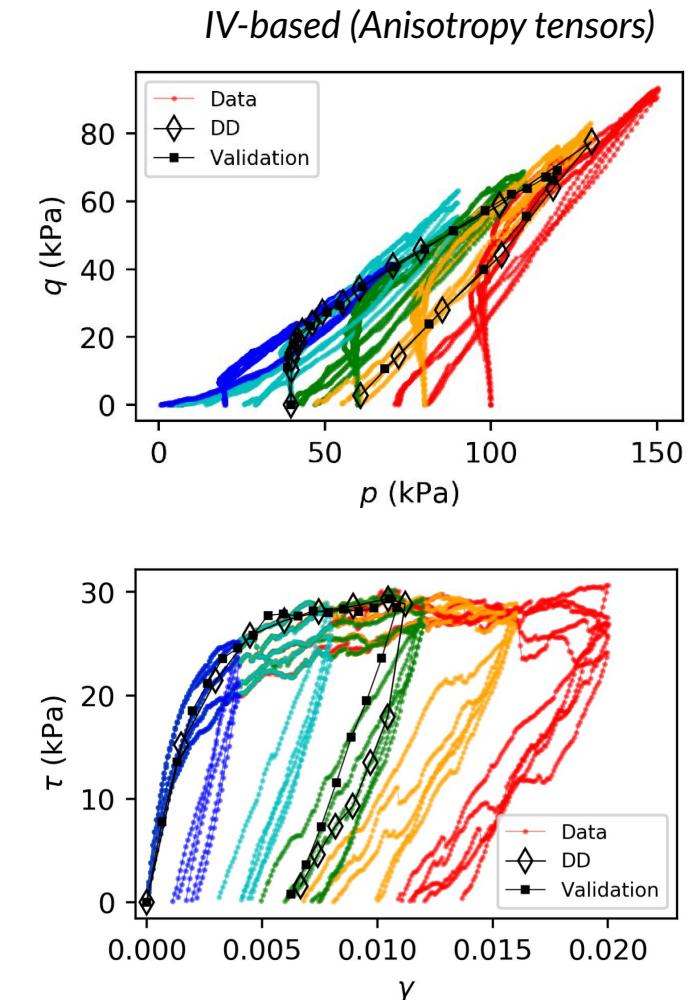
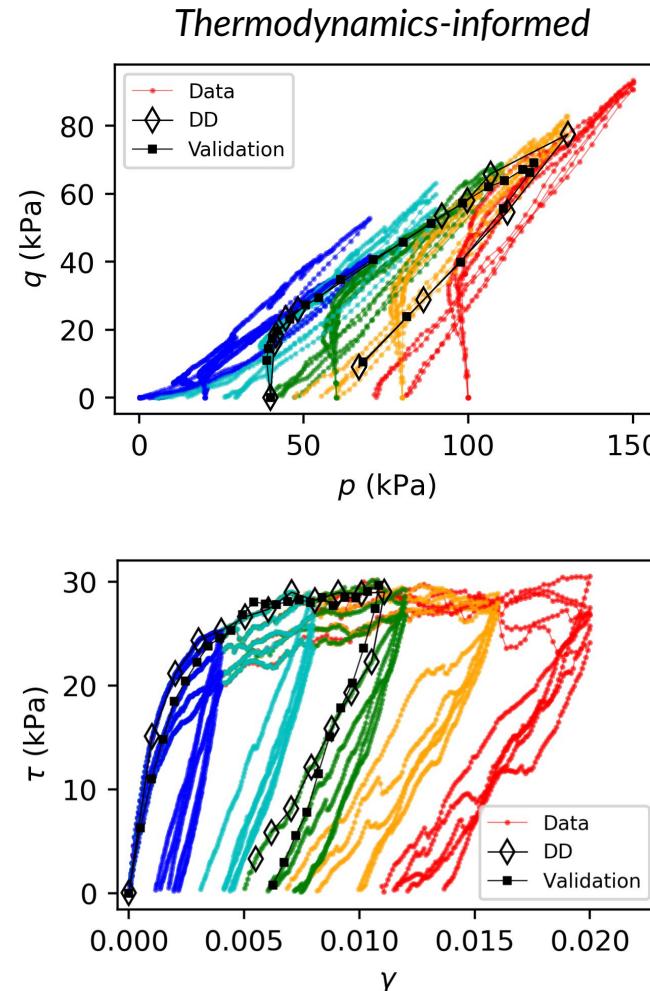
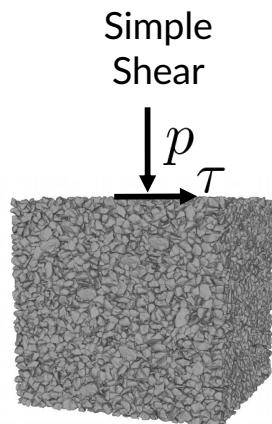
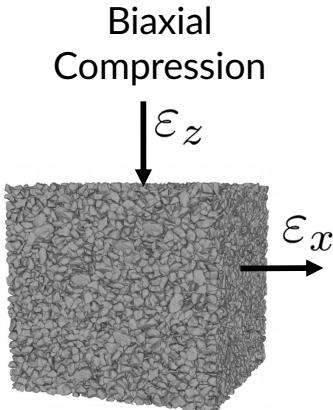
A simplified problem:

$$\min_{\mathbf{z} \in D_k} d(\mathbf{z}_k, \mathbf{y}_k)$$

Periodic unit cells

Quasistatic
conditions

$$I \leq 10^{-4}$$



Overview

I) Data-Driven Computational Mechanics

- a) Formulation
- b) Live example
- c) Improving convergence

II) Data Mining

- a) Experiments (Identification)
- b) Simulations (Multiscale)
- c) Adaptive data sampling

III) History-dependent Formulation

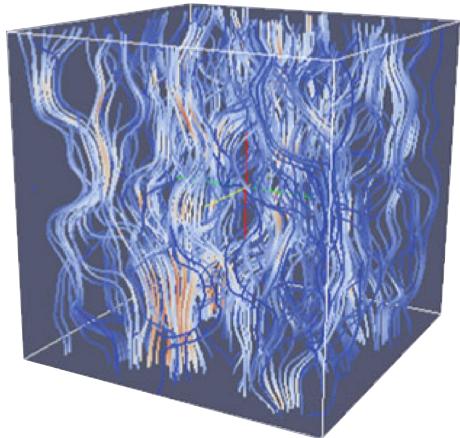
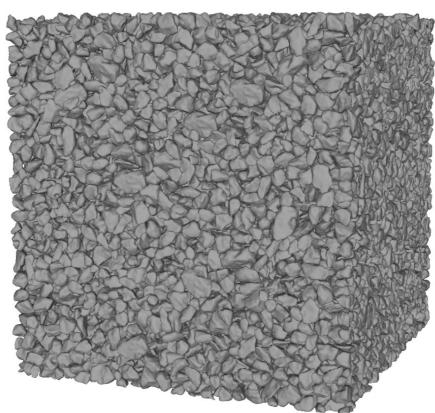
IV) Multi-field Formulation

V) Advanced Applications

- a) Shear banding
- b) Breakage mechanics

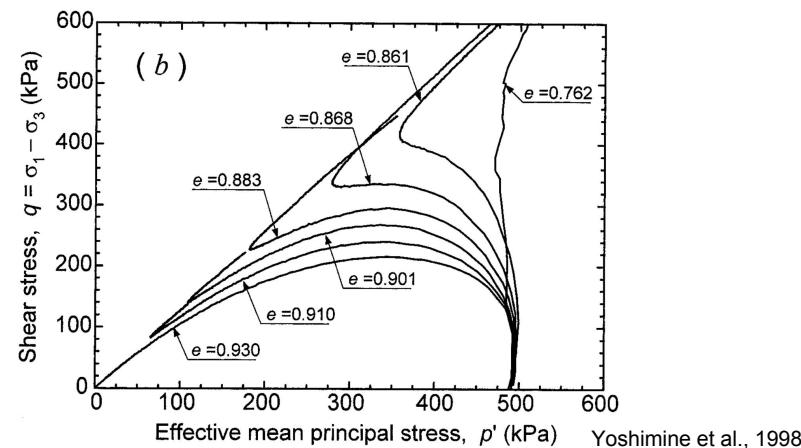
Multi-field problems

Coupled problems



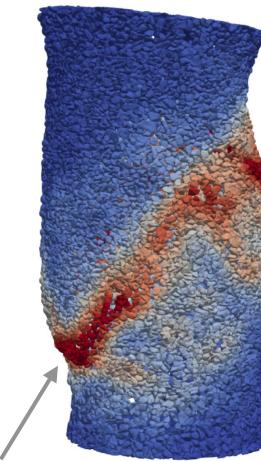
Sun et al., 2013

Porous flow



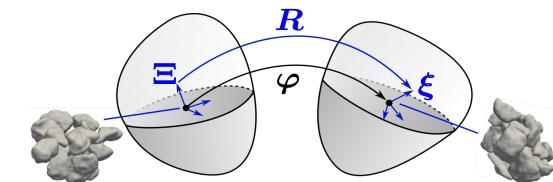
Konstantinos Karapiperis

Gradient/nonlocal theories



Characteristic width $\sim 10d$

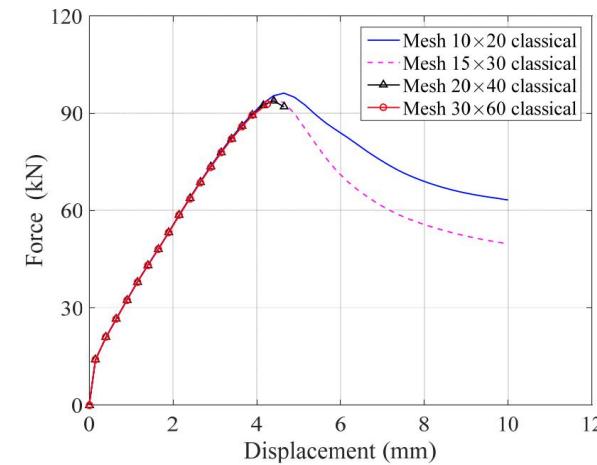
Locally nonaffine deformation



$$\mathcal{A} = \mathcal{A}(\nabla \mathbf{u}, \theta, \nabla^2 \mathbf{u}, \nabla \theta, \dots) \rightarrow \ell$$

Eringen, 1964

Muhlhaus and Vardoulakis, 1989



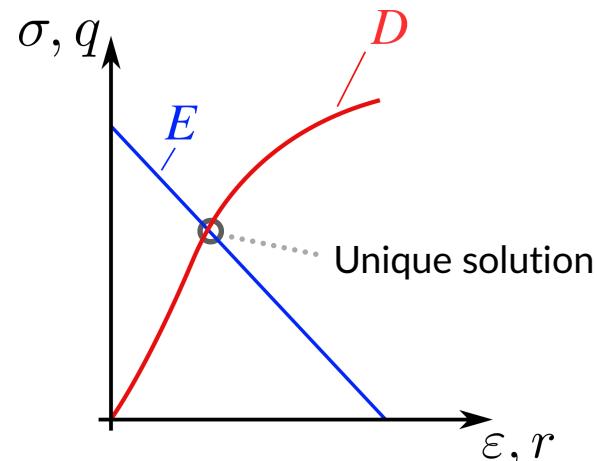
Alert Doctoral School, Aussois - 2023 -24

Poromechanical problem

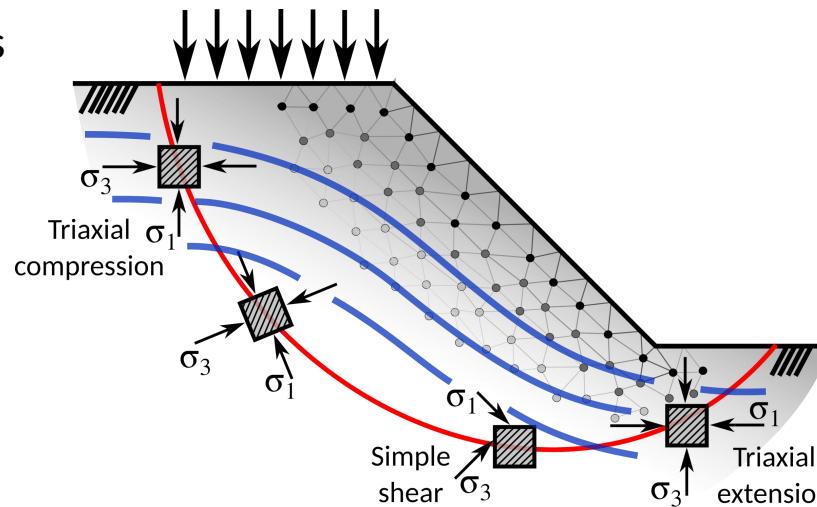
Conventional poromechanics

$$\left\{ \begin{array}{l} \nabla \cdot \sigma + \rho b = 0 \quad (1) \\ \nabla \cdot q + \dot{\varepsilon}_{\text{vol}} + s = 0 \quad (2) \\ \varepsilon = \text{sym}(\nabla u) \quad (3) + \text{B.Cs} \\ r = \nabla p \quad (4) \\ \sigma = \sigma'(\varepsilon) - pI \quad (5) \\ q = q(r) \quad (6) \end{array} \right.$$

Constitutive relations



- Incompressible fluid
- Compressible solid skeleton



Data-Driven poromechanics

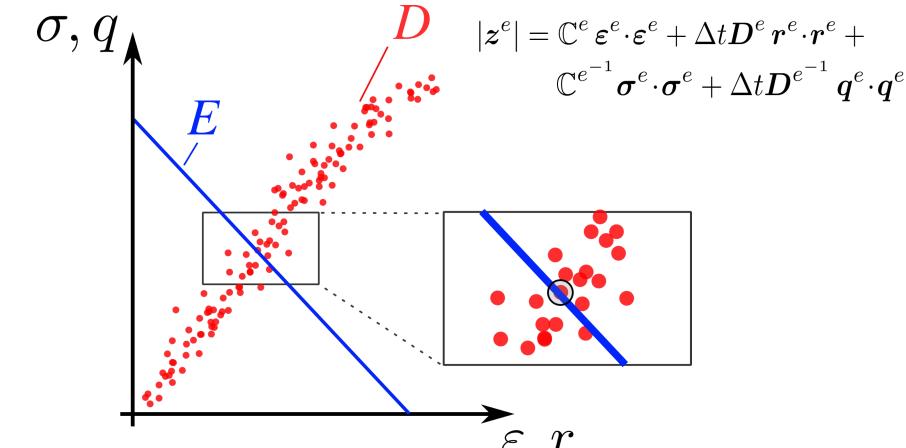
Bahmani et al., 2021

Phase Space $Z = \{(\varepsilon, r, \sigma, q)\}$

Equilibrium/Mass Balance set $E = \{z \in Z | (1)-(4)\}$

Material Data set $D \subset Z$

$$\min_{z \in E} \min_{y \in D} d(z, y)$$



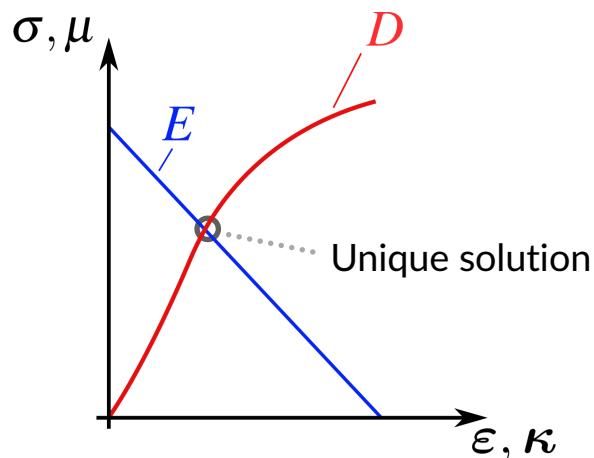
- Possible hybrid model/data-driven formulations
- Modified distance definition

Micropolar formulation

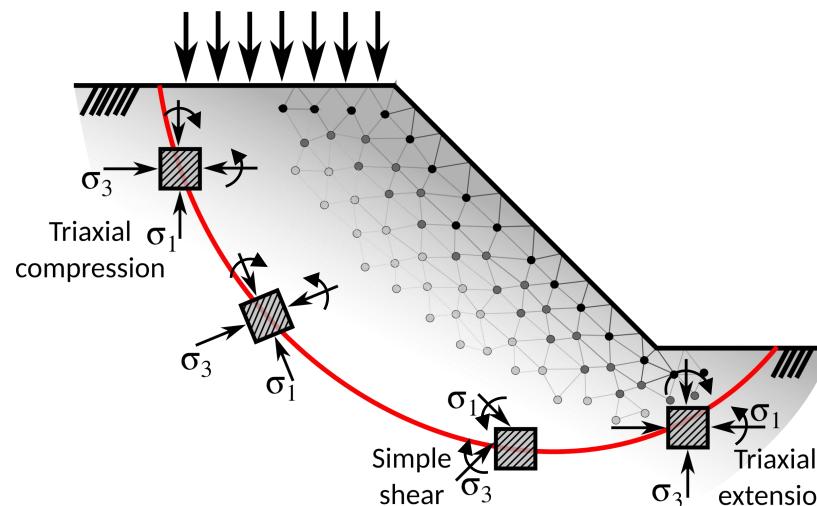
Conventional micropolar

$$\begin{cases} \nabla \cdot \sigma = 0 & (1) \\ \nabla \cdot \mu - \epsilon : \sigma = 0 & (2) \\ \epsilon = \nabla u - \epsilon : \theta & (3) \\ \kappa = \nabla \theta & (4) \\ \{\sigma, \mu\} = \{\sigma, \mu\}(\epsilon, \kappa, \ell) \end{cases} + \text{B.Cs}$$

Constitutive relation



- Complicated constitutive models
- Hard to define the internal length scale



Data-Driven micropolar

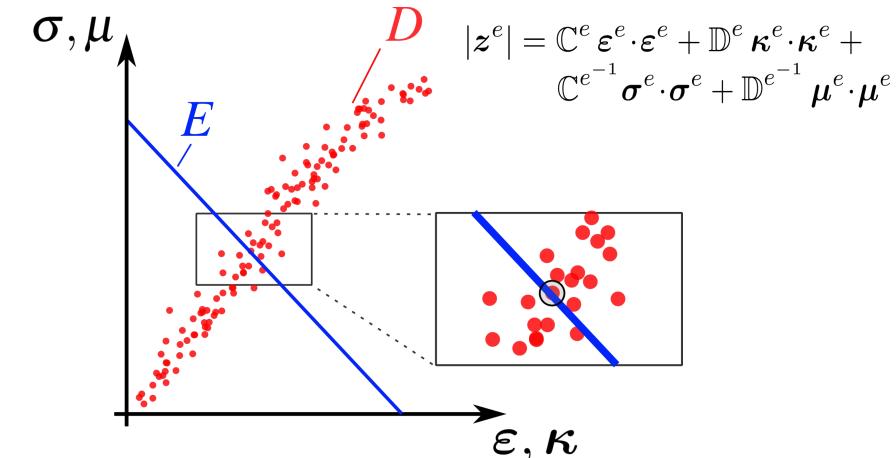
Karapiperis et al., 2021

Phase Space $Z = \{(\epsilon, \kappa, \sigma, \mu)\}$

Equilibrium set $E = \{z \in Z | (1)-(4)\}$

Material Data set $D \subset Z$

$$\min_{z \in E} \min_{y \in D} d(z, y)$$



- Discover internal length scale from the data
- Modified distance definition

Multiscale formulation and thermodynamics

Free energy/Dissipation

$$\boldsymbol{\varepsilon} = \frac{1}{V} \left(\sum_{p \in \partial\mathcal{P}} \mathbf{u}^p \otimes \mathbf{n}^p + \boldsymbol{\epsilon} \cdot \sum_{p \in \mathcal{P}} \boldsymbol{\theta}^p V^p \right)$$

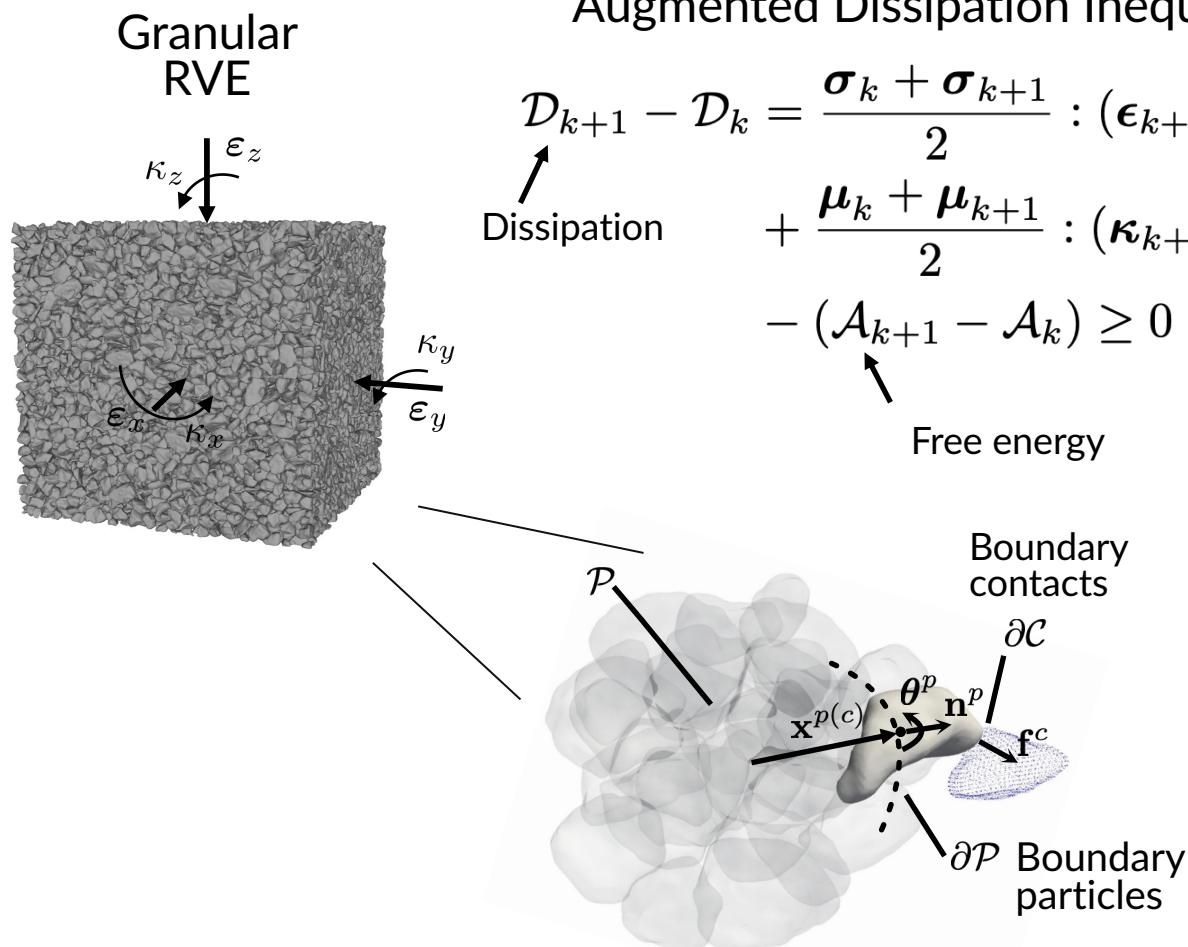
$$\boldsymbol{\kappa} = \frac{1}{V} \sum_{p \in \partial\mathcal{P}} \boldsymbol{\theta}^p \otimes \mathbf{n}^p$$

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \sum_{c \in \mathcal{C}} \mathbf{f}^c \otimes \mathbf{l}^c$$

$$\boldsymbol{\mu} = \frac{1}{V} \sum_{c \in \partial\mathcal{C}} (\mathbf{l}^c \times \mathbf{f}^c) \otimes \mathbf{x}^{p(c)}$$

$$\mathcal{A} = \sum_c \mathcal{A}^c = \frac{1}{2V} \sum_c \left(\frac{\|\mathbf{f}_n^c\|^2}{k_n} + \frac{\|\mathbf{f}_t^c\|^2}{k_t} \right)$$

$$d\mathcal{D} = \sum_c d\mathcal{D}^c = \frac{1}{V} \sum_c \mathbf{f}_t^c \cdot d\mathbf{u}^{c, \text{slip}}$$



Augmented Dissipation Inequality

$$\begin{aligned} \mathcal{D}_{k+1} - \mathcal{D}_k &= \frac{\boldsymbol{\sigma}_k + \boldsymbol{\sigma}_{k+1}}{2} : (\boldsymbol{\epsilon}_{k+1} - \boldsymbol{\epsilon}_k) \\ &\quad + \frac{\boldsymbol{\mu}_k + \boldsymbol{\mu}_{k+1}}{2} : (\boldsymbol{\kappa}_{k+1} - \boldsymbol{\kappa}_k) \\ &\quad - (\mathcal{A}_{k+1} - \mathcal{A}_k) \geq 0 \end{aligned}$$

Free energy

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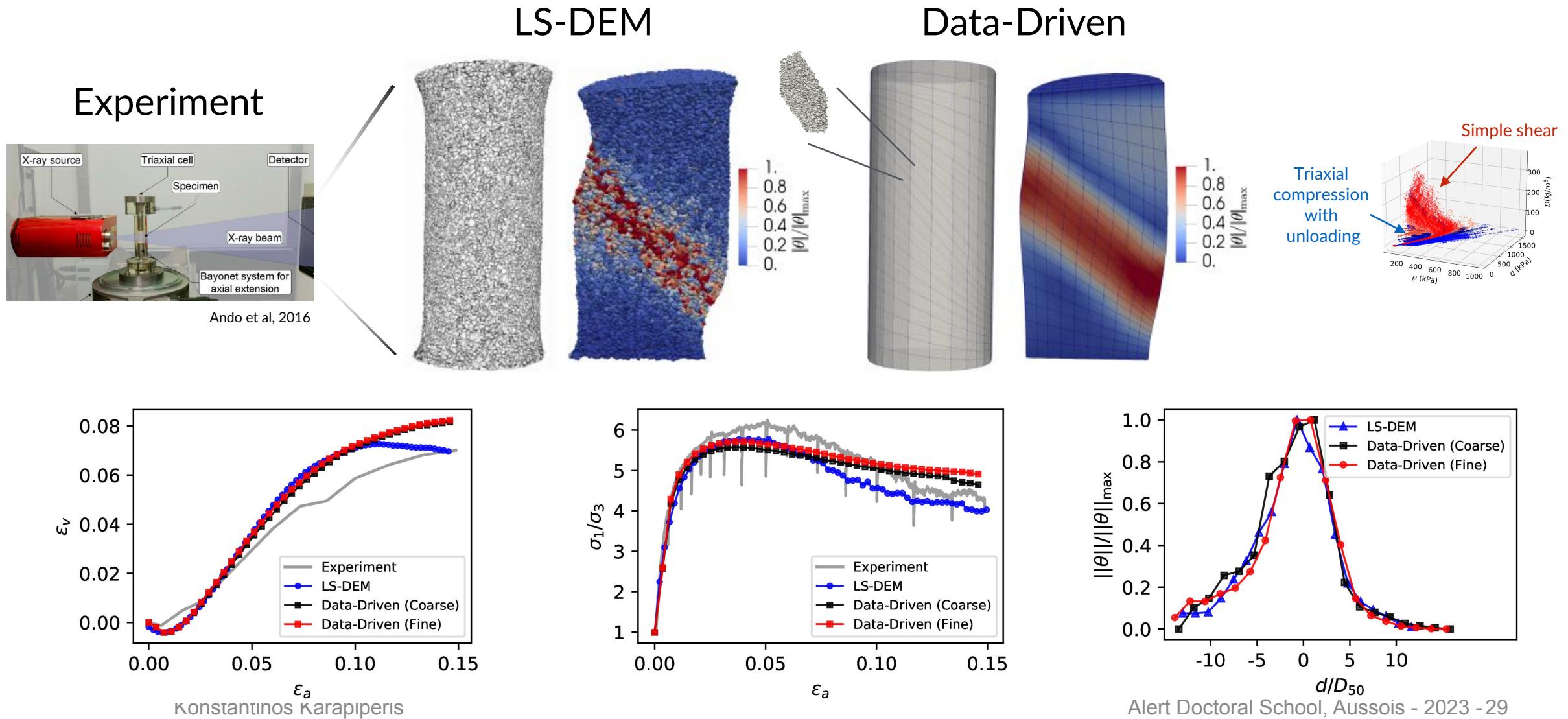
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Application I: Shear banding

Karapiperis et al, 2021



Application II: Breakage mechanics

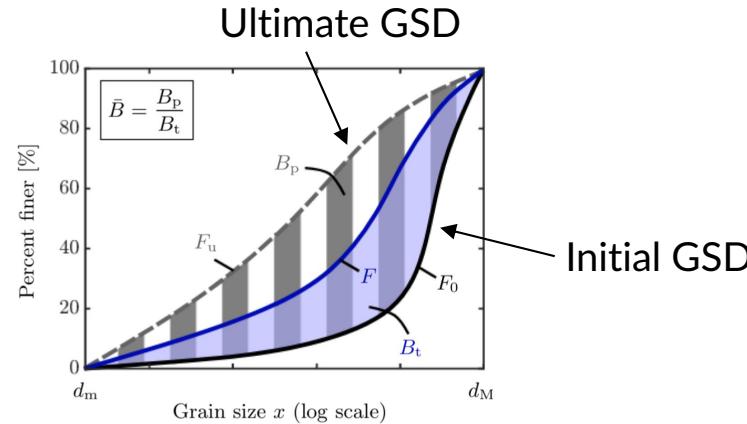
Gorgogianni et al, 2023 (CMAME)

Model-based Breakage Mechanics

Einav, J. Mech. Phys. Solids (2007)

Breakage (internal) variable:

$$B(t) = \frac{p(t) - p_0}{p_u - p_0} = \frac{F(t) - F_0}{F_u - F_0}$$



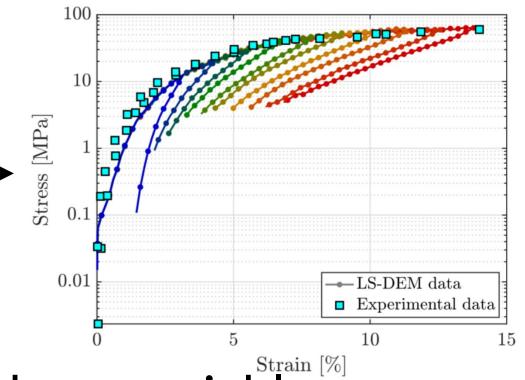
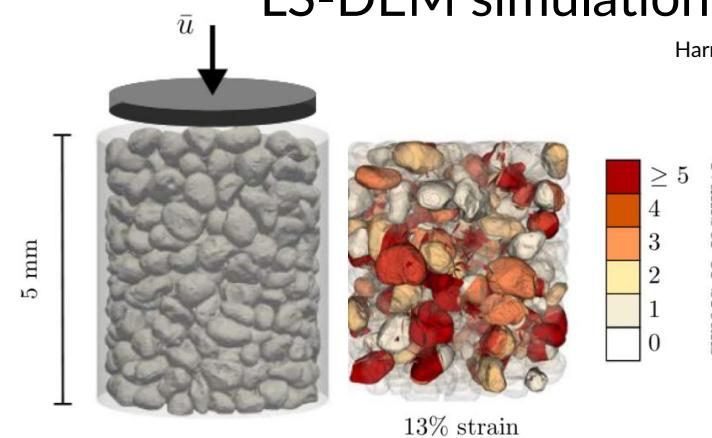
Free energy $\psi := \psi(\epsilon, B)$

Dissipation potential $\phi := \phi(\dot{B})$

Data-Driven Breakage Mechanics

LS-DEM simulations of breakable particles

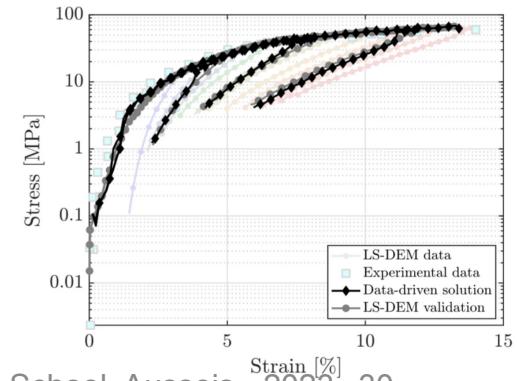
Harmon et al, Comp. Meth. Appl. Mech. Eng. (2020)



State space augmented by breakage variable

$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \mid B_{k+1} = \hat{B}(\epsilon_{k+1}, \sigma_{k+1}) \geq B_k\}$$

Data-driven
oedometric compression



Summary

- Interpretable distance-based framework
- Data from various provenances (**experiments, high-fidelity simulations**)
- Requires a lot of data → Resolved via unsupervised **adaptive sampling**,
embeddings into lower dimensional spaces
- History dependence (internal variables + **thermodynamic constraints**)
- Extension to **coupled/gradient problems**

