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Model-Free, Internal-Variable-Free, Data-Driven Plasticity

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Data-Driven Science: Taxonomy

- The emerging paradigm: *Data-Driven Science:*
  - Model-based methods: Identify model from data
  - *Model-free methods*: Make predictions from data
- *Data-Driven Computational Mechanics:*
  - Deterministic problems:
    - History-independent (elasticity, dynamics...)
    - *History-dependent* (viscoelasticity, *plasticity*...)
  - Stochastic problems
- *Data-Driven plasticity:*
  - Internal-variable formulations
  - *Internal-variable-free formulations* (path based)
- *Praxis:* Data mining, path sampling, phase space coverage, accuracy, convergence...

Computational mechanics in a data-rich world

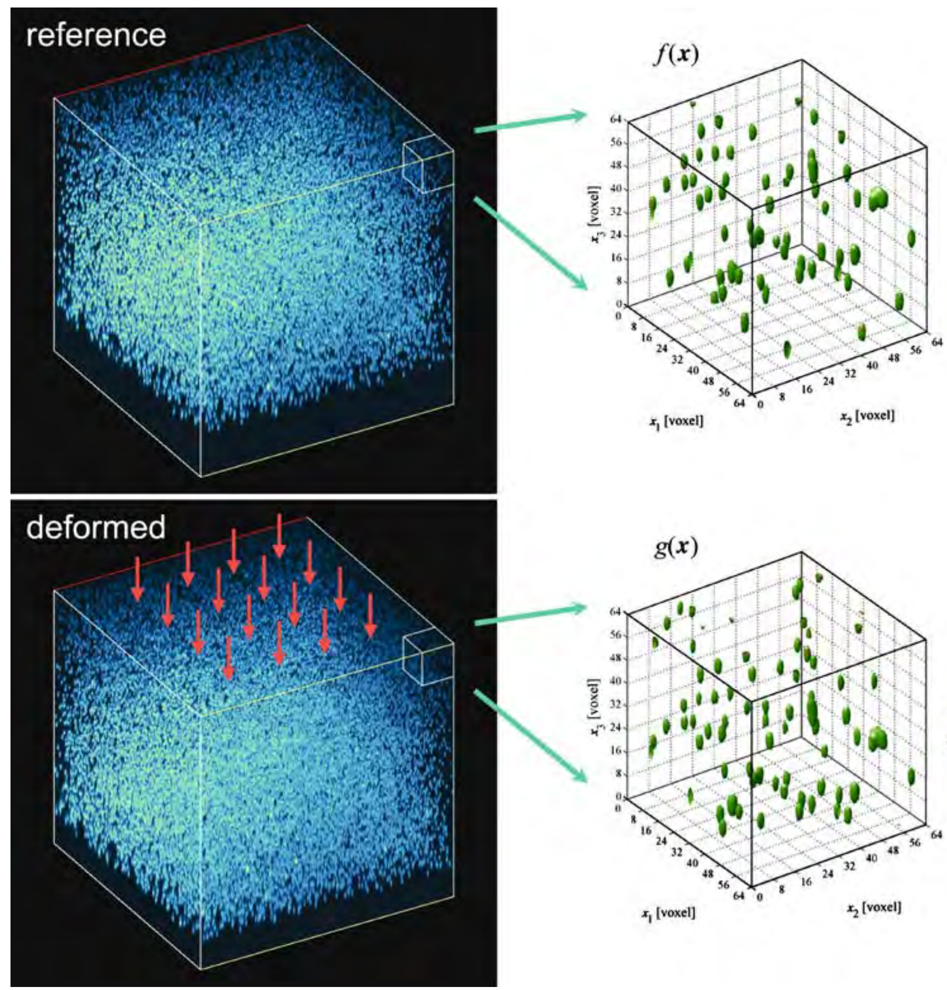
- Material data is currently plentiful due to dramatic advances in ***experimental science*** (DIC, EBSD, microscopy, tomography...) and multiscale computing (DFT → MD → DDD → SM → Hom)

Digital Volume Correlation (DVC): Two confocal volume images of an ***agarose gel*** with randomly dispersed fluorescent particles before and after mechanical loading. The ***full displacement vector field*** is measured using 3D volume correlation methods.

C. Franck, S. Hong, S.A. Maskarinec, D.A. Tirrell & G. Ravichandran, *Experimental Mechanics*, **47** (2007) 427–438.

Data-Driven Identification:

A. Leygue, M. Coret, J. Réthoré, L. Stainier & E. Verron, *IJNME*, **331** (2018) 184-196.



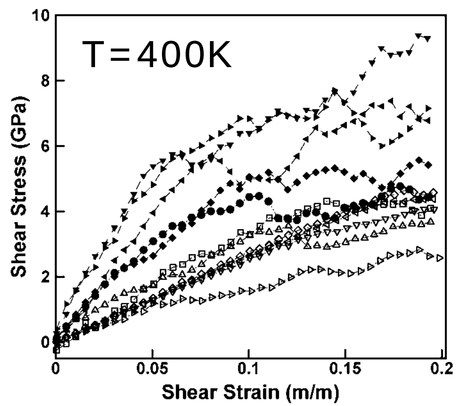
Computational mechanics in a data-rich world

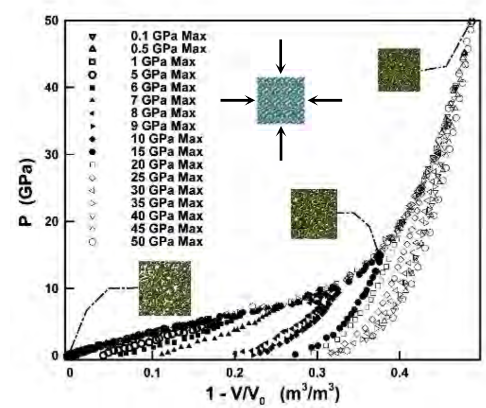
- Material data can also be generated in large volumes from high-fidelity *micromechanical calculations* (DFT, MD, DD...)
- New role for *multiscale analysis*: Data generation

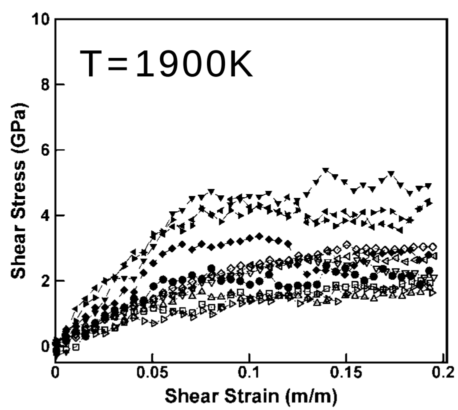
Amorphous SiO_2 glass: LAMMPS MD calculations of amorphous silica glass under *pressure-shear* loading over a range of *temperatures* and *strain rates*. RVEs are quenched from the melt, then analyzed using the BKS potential with Ewald summation.

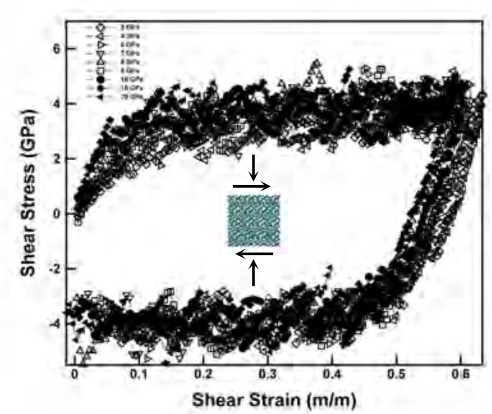
Schill, W., Heyden, S., Conti, S. & MO, *JMPS*, **113** (2018) 105-125.

Schill, W., Mendez, J.P., Stainier, L. & MO, *JMPS*, **140** (2020) 103940.









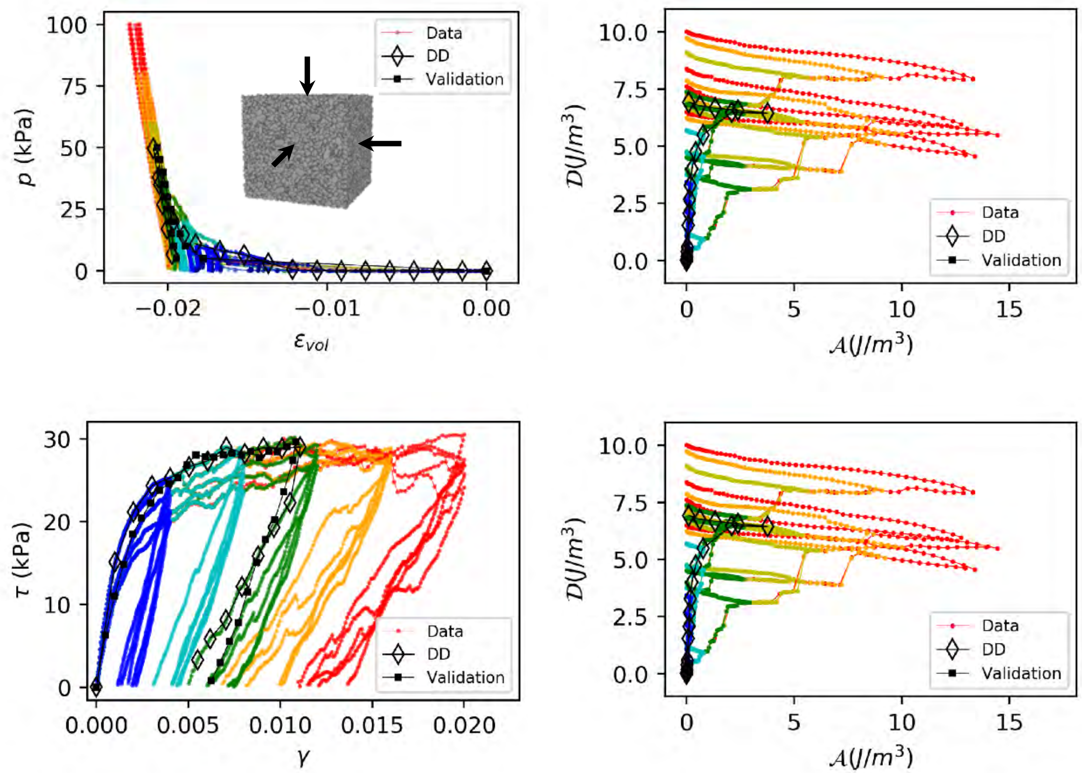
Computational mechanics in a data-rich world

- Material data can also be generated in large volumes from high-fidelity ***micromechanical calculations*** (DFT, MD, DD...)
- New role for ***multiscale analysis***: Data generation

Granular matls. (dry sand): Level-Set Discrete Element Method (LS-DEM) simulation of granular material samples. 3D irregular ***rigid particles*** interact through ***frictional contact***. Particle morphology described by level-set functions. Note calculation of ***dissipation and free energy***.

Karapiperis, K., Harmon, J., And, E., Viggiani, G. & Andrade, J.E., *JMPS*, **144** (2020) 104103.

Karapiperis, K., Stainier, L., Ortiz, M. & Andrade, J.E., *JMPS*, **147** (2021) 104239.



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Computational mechanics in a data-rich world

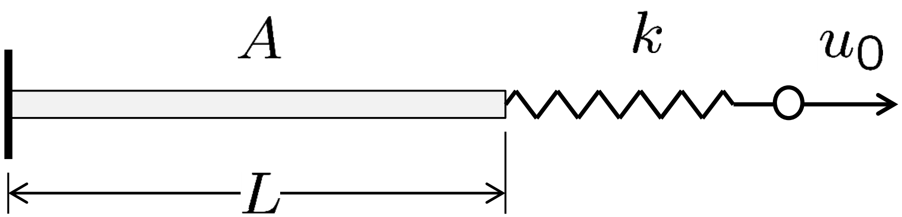
- The unprecedented *abundance of material data* presents new challenges and opportunities
- Two main strategies:
  - *Model the data, use models in BVP calculations*
  - *Embed the data directly into BVP calculations*

Model-Based:	Data	⟶	Model	⟶ Prediction
Model-Free:	Data	⟶		Prediction

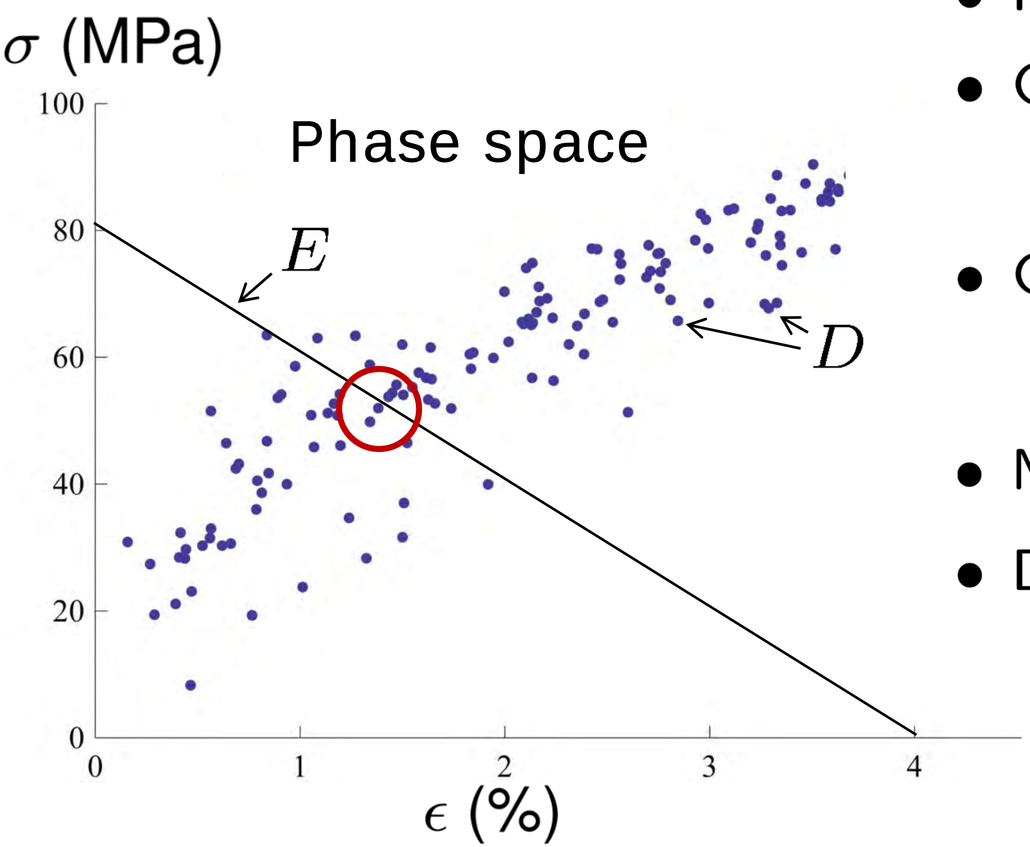
- *Critique of Model-Based computing*: Modeling results in loss of information, introduces biases, modeling error, epistemic uncertainty, is open-ended, *ad hoc*...
- Model-Free computing: *Cut out the middle man!*

The data, all the data, nothing but the data

Data-Driven history-independent problems



<u>Problem:</u> Bar actuated by loading device



- Phase space: $\{(\epsilon, \sigma)\} \equiv Z$
- Compatibility + equilibrium:

$$\sigma A = k(u_0 - \epsilon L)$$

- Constraint set:

$$E = \{\sigma A = k(u_0 - \epsilon L)\}$$

- Material data set: $D \subset Z$
- Data-Driven solution:

$$\min_{z \in E} \text{dist}(z, D)$$

T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

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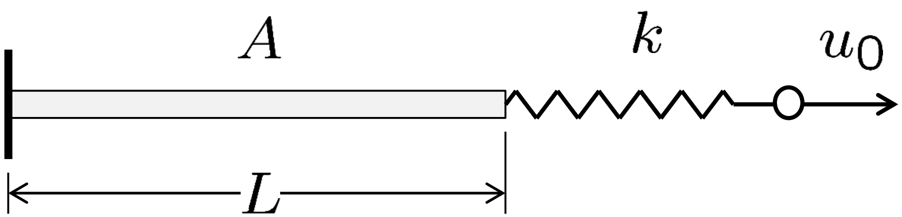
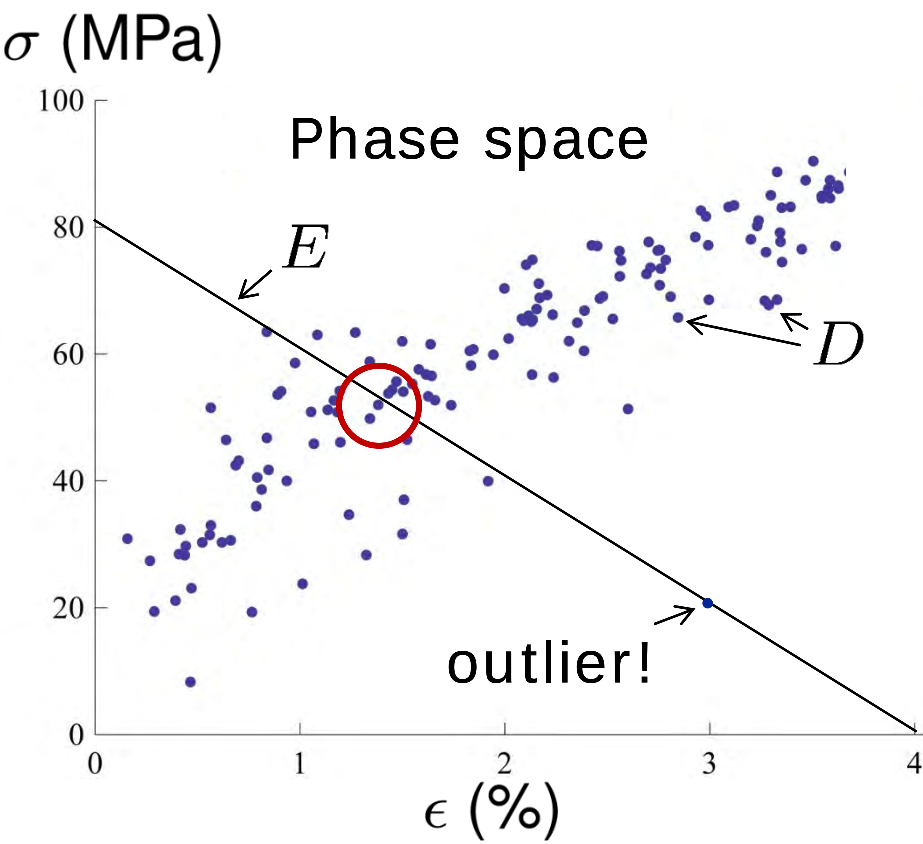
Data-Driven history-independent problems



Problem: Bar actuated by loading device



- Phase space: $\{(\epsilon, \sigma)\} \equiv Z$
- Compatibility + equilibrium:

$$\sigma A = k(u_0 - \epsilon L)$$

- Constraint set:

$$E = \{\sigma A = k(u_0 - \epsilon L)\}$$

- Material data set: $D \subset Z$
- With outliers (k-means):

$$\min_{z \in E} \left(-\frac{1}{\beta} \log \sum_{i=1}^{N} e^{-\beta \, \mathrm{dist}^2(y_i, z)} \right)$$

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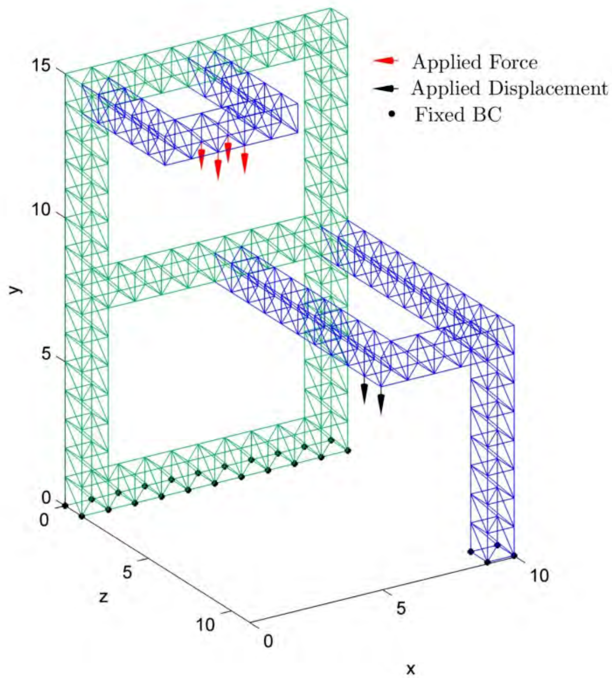
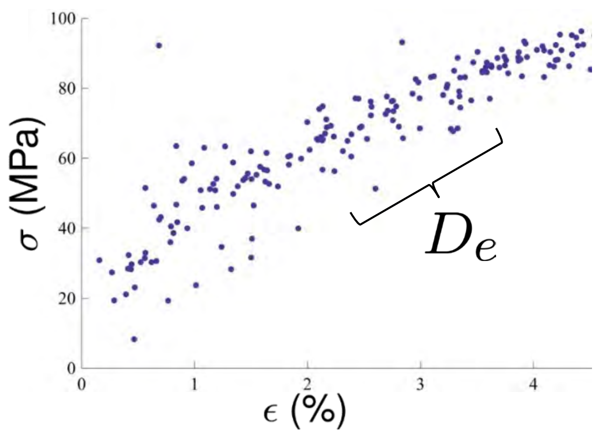
T. Kirchdoerfer and M. Ortiz, *CMAME*, **326** (2017) 622–641

Data-Driven history-independent problems





<u>Problem:</u> Structure under applied loads and displacements

- Phase space: $\{(\epsilon_e, \sigma_e)_{e=1}^m\} \equiv Z$
- Compatibility + equilibrium:

$$\epsilon = Bu, \quad B^T \sigma = f$$

- Constraint set:

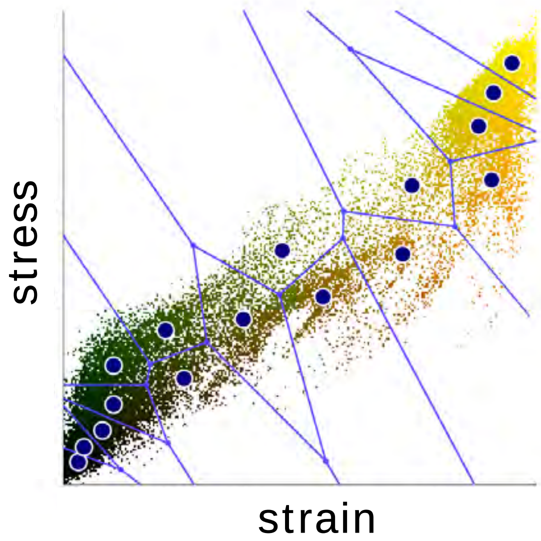
$$E = \{(\epsilon, \sigma) : \epsilon = Bu, \ B^T \sigma = f\}$$

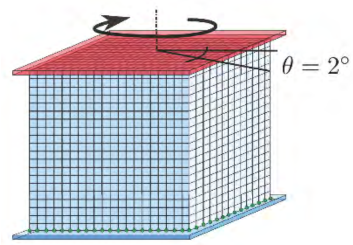
- Material data set: $D \subset Z$
- Data-Driven solution:

$$\min_{z \in E} \text{dist}(z, D)$$

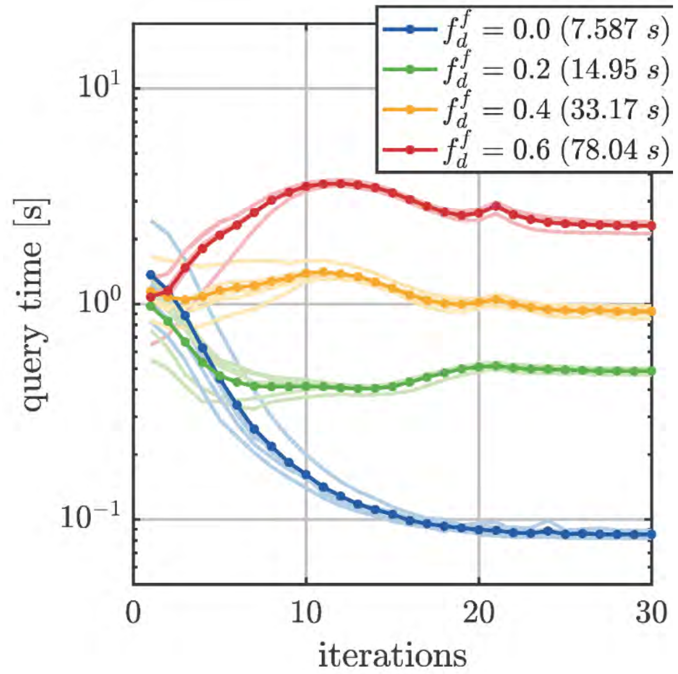
T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

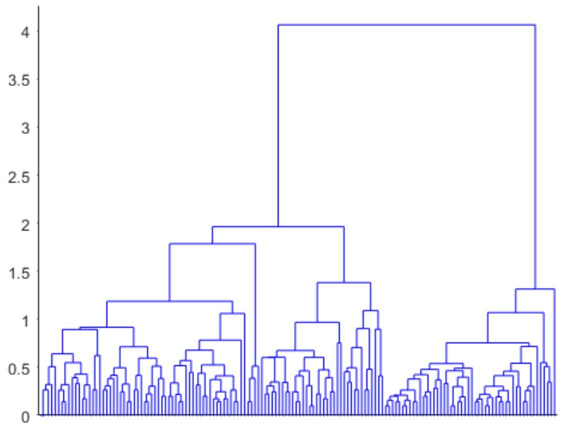
Data-Driven history-independent problems





Test problem:
Torsion of
20x20x20 cube
64000 matl pts





K-means hierarchical structure

- Test problem: Torsion of cube
- Mesh: 20x20x20, 64000 matl pts
- Material data set: ***1 billion points***
- Approx ***k-means*** search, 0.1 secs
- ***Set-oriented machine learning!***
- We learn the ***structure of the data set***
- No regression, ***no loss of information!***

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Eggersmann, R. Stainier, L., Reese, S. and Ortiz, M., *CMAME*, **382** (2021) 113855.

Data-Driven history-independent problems

- History-independent Data-Driven problems can be extended to the *PDE* (*infinite-dimensional*) setting: Linear elasticity[1], finite elasticity[2,3]...
- Well-established *existence and uniqueness* properties[1,2] of solutions of Data-Driven BVPs
- *Relaxation, approximation*, Γ-convergence[1,2]
- *Convergence with respect to data*, deterministic[1,2] or stochastic (maximum likelihood[4], inference[5])
- *History-independent Data-Driven problems are in good shape. History-dependent materials?*

[1]Conti, S., Müller, S. & Ortiz, M., *ARMA*, **229** (2018) 79-123.
[2]S. Conti, S. Müller and M. Ortiz, *ARMA*, **237** (2020) 1–33.
[3]A. Platzer, A. Leygue, L. Stainier and M. Ortiz, CMAME, 379 (2021) 113756.
[4]T. Kirchdoerfer and M. Ortiz, *CMAME*, **326** (2017) 622-41.
[5]S. Conti, F. Hoffmann and M. Ortiz, *arXiv* (2021) 2106 02728.

History-dependent materials

- Goal: Extend the Data-Driven paradigm to inelastic materials whose response is *history dependent*.

"The characteristic property of inelastic solids which distinguishes them from elastic solids is the fact that the stress measured at time t depends not only on the instantaneous value of the deformation but also on the entire history of deformation[1]."

- The theory of *materials with memory* furnishes the most general representation of inelastic materials.
- Alternative: Replace history by the effects of history, the current *microstructure* (internal state)
- Variables used to describe that microstructure, within a *continuum thermodynamics* framework, are referred to as *internal variables*

[1] R. S. Rivlin, "Materials with memory." *Tech. Rep. AD-753 460*, ONR, 1972.

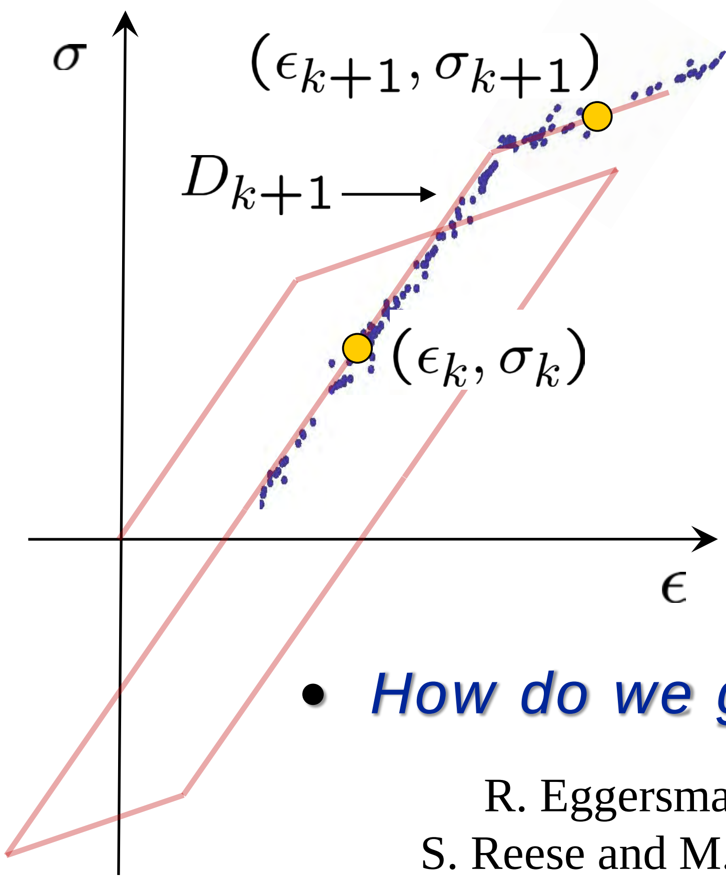
A critique of internal variables

- The concept of *internal variables* was introduced into thermodynamics by Onsager (1931), applied to continuum mechanics by Eckart (1948), others...
- Kestin and Rice (1967): The internal variable formalism cannot represent materials with *continuous relaxation spectrum* (e.g., polymers)
- Phenomenological models: The *choice of internal variables* is often *ad hoc,* no notion of *convergence*
- Internal variables can be redundant and defined up to *reparametrizations* only (no intrinsic meaning)
- *Instead: Develop Data-Driven representations that are internal-variable-free (path-based)! How?*

Data-Driven history-dependent problems

- ***Incremental material set***: Set of points in phase space ***accessible*** from (ϵ_k, σ_k) given prior history:

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



- Data-driven problem:

$$\min_{z \in E_{k+1}} d(z, D_{k+1})$$

- Need ***material history data***! (from material testing along selected loading paths...)
- History data must provide adequate ***path coverage***...
- ***How do we generate, store, structure, path data?***

R. Eggersmann, T. Kirchdoerfer, L. Stainier, S. Reese and M. Ortiz, *CMAME*, **350** (2019) 81-99.

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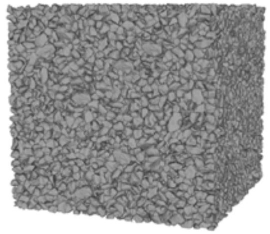
Data-Driven history-dependent problems

- How do we generate, store, structure, *path data?*
- *What is the intrinsic structure* of history-dependent (path) data for plastic materials?
- Need to revisit the *differential geometry* of incremental plasticity in phase space:
  - *Non-integrable differential or Pfaffian forms...*
  - *Maximum-dissipation connections...*
  - *History data: Directed graphs in phase space!*
- How do we provide adequate path coverage? Object-oriented path sampling, accuracy control, feedback...

Incremental plasticity in phase space



- Geometry of *phase-space trajectories*?
- What neighboring points can be *accessed* incrementally along trajectories?
- Assume *continuum thermodynamics* with fully resolved internal state (micromechanical system)
- Free energy $A(\epsilon, \theta, q)$ convex, dual $A^*(\sigma, \eta, p)$

ϵ → strain, θ → temperature, q → internal variables

σ → stress, η → entropy, p → driving forces

- By convexity and the Fenchel-Young theorem, the Coleman-Noll equilibrium relations are equivalent to

$$A + A^* - \sigma \cdot \epsilon + \eta \theta + p \cdot q = 0$$

Incremental plasticity in phase space

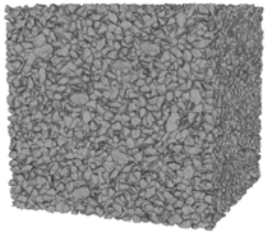
- Geometry of *phase-space trajectories*?
- By convexity and the Fenchel-Young theorem, the Coleman-Noll equilibrium relations are equivalent to

$$A + A^* - \sigma \cdot \epsilon + \eta \theta + p \cdot q = 0$$

- Assume *rate-independent* Onsager kinetics:
  - *Elastic domain* C, *convex (by second law)*
  - *Dual dissipation potential:* $\psi(\xi) = \sup \{ p \cdot \xi \, : \, p \in C \}$
- By convexity and the Fenchel-Young theorem, the *flow rule* and *yield condition* are equivalent to:

$$\psi(dq) - p \cdot dq = 0 \qquad \text{and} \qquad p + dp \in C$$

Incremental plasticity in phase space



- Summary of governing equations:
  - *Coleman-Noll equilibrium relations,*

$$d(A + A^* - \sigma \cdot \epsilon + \eta \theta + p \cdot q) = 0$$

  - *Incremental kinetic relations,*

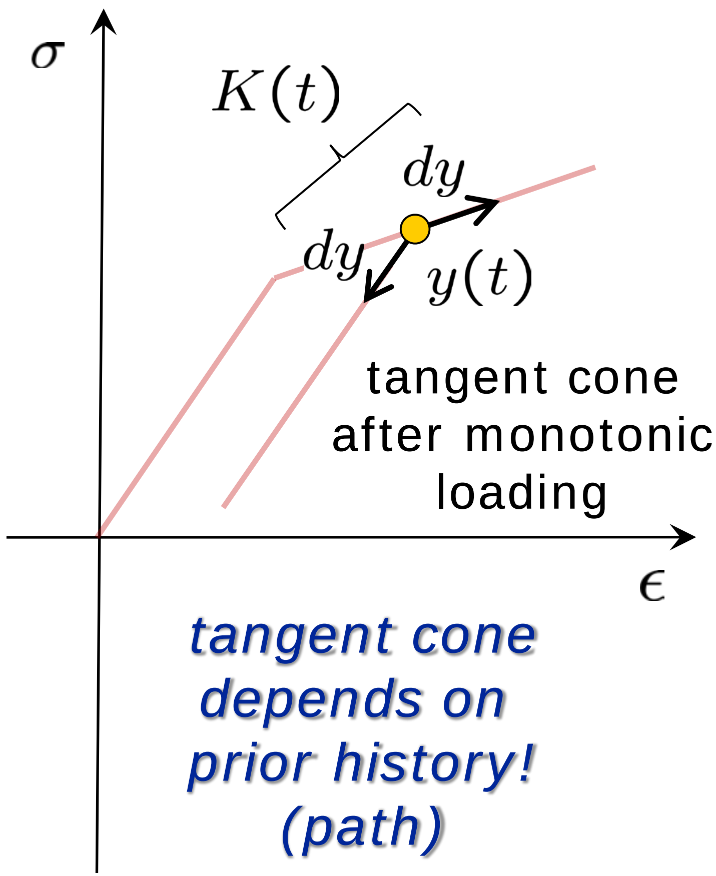
$$\psi(dq) - p \cdot dq = 0 \quad \text{and} \quad p + dp \in C$$

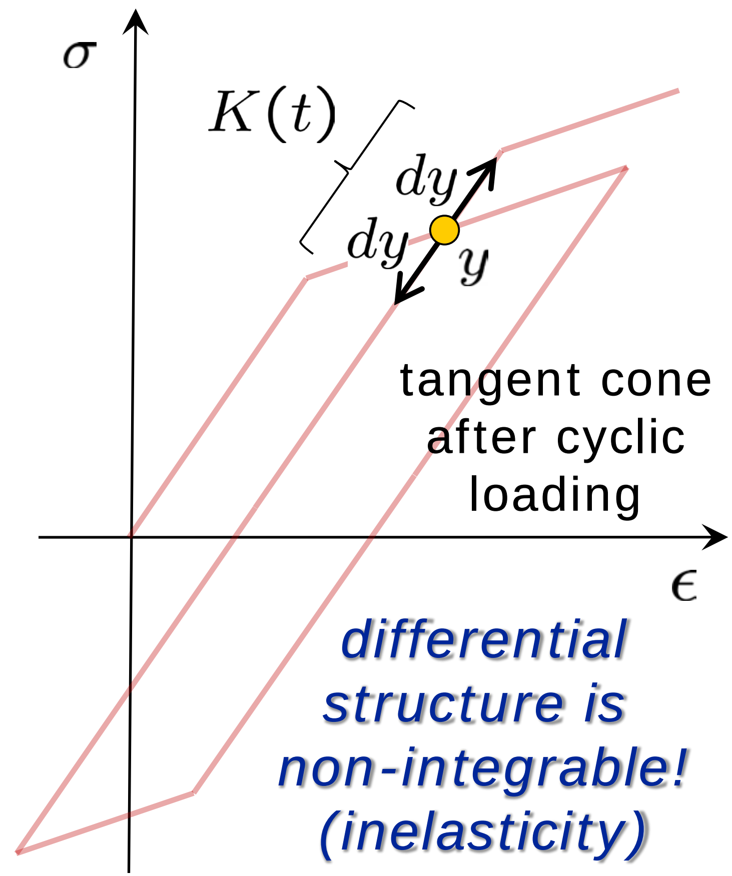
- *Eliminate* $(dq, dp) \Rightarrow$ *tangent cone*

$$K(t) = \{ \, dy = (d\epsilon, d\theta; d\sigma, d\eta) \ \text{'out of } y(t)\text{'} \ \}$$

- *Tangent cone:* Collection of possible *connections* between neighboring points in phase space
- Defines a (non-integrable) *differential form*
- Solutions are the *integral curves* (trajectories)

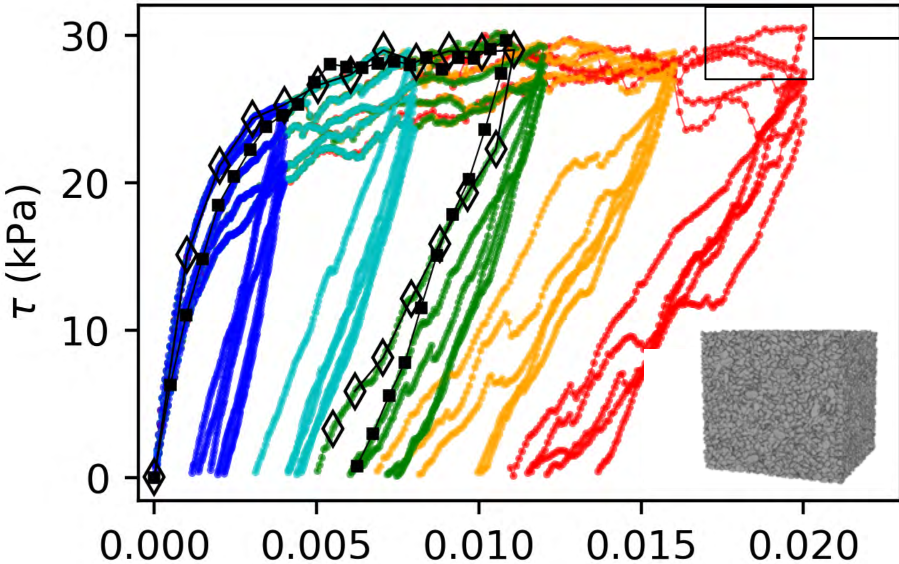
Incremental plasticity in phase space

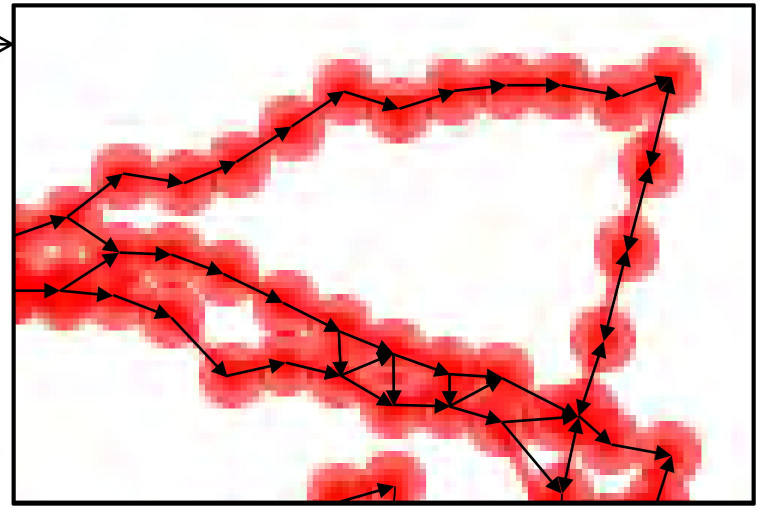




- ***Differential view of plasticity***: Points in phase space and '***connections***' between neighboring points defining possible incremental moves...

Building path data from micromechanics





Data points and connections

i) Evaluate RVE for selected loading paths

ii) Record $(\epsilon_i, \theta_i; \sigma_i, \eta_i)$, connect points i and j if

$$\psi(q_j - q_i) - \langle \frac{p_i + p_j}{2}, q_j - q_i \rangle \leq \text{TOL}$$

iii) Discard internal state (q_i, p_i) (*int. var. free!*)

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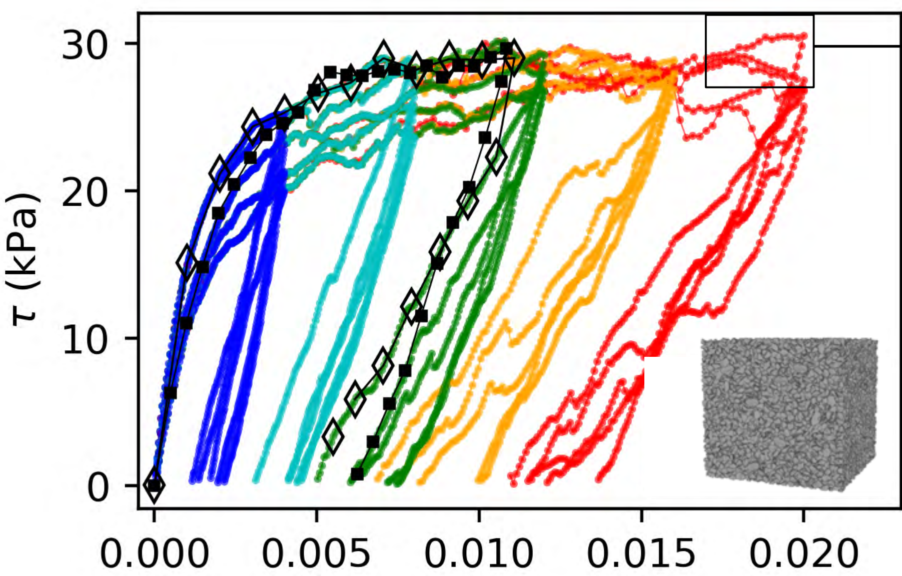
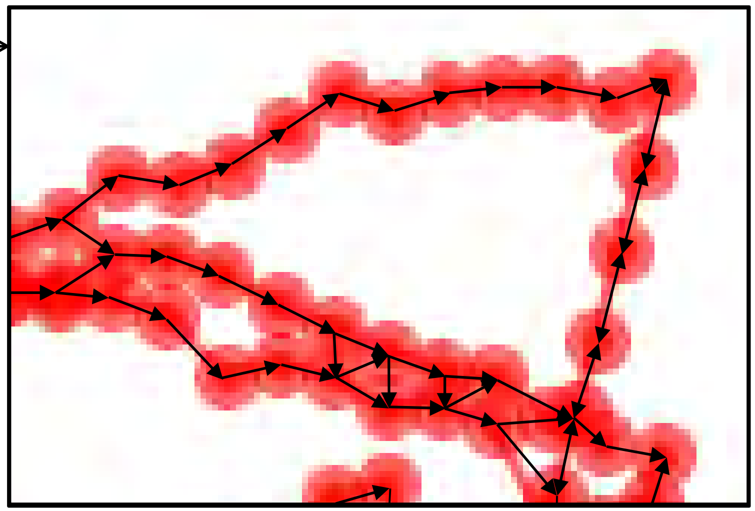
Karapiperis, K., Stainier, L., MO & Andrade, J.E., *JMPS*, **147** (2021) 104239.

Building path data from micromechanics





Data points and connections

i) Evaluate RVE for selected loading paths

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$$Diss_{i\rightarrow j} + A_j - A_i - \langle \frac{\sigma_i + \sigma_j}{2}, \epsilon_j - \epsilon_i \rangle \leq \text{TOL}$$

iii) Discard internal state (q_i, p_i) (*int. var. free!*)

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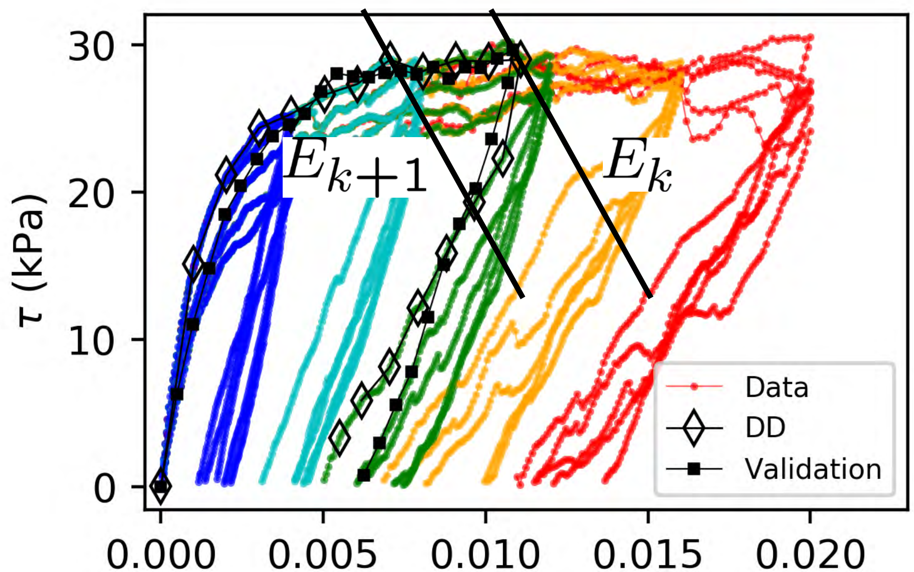
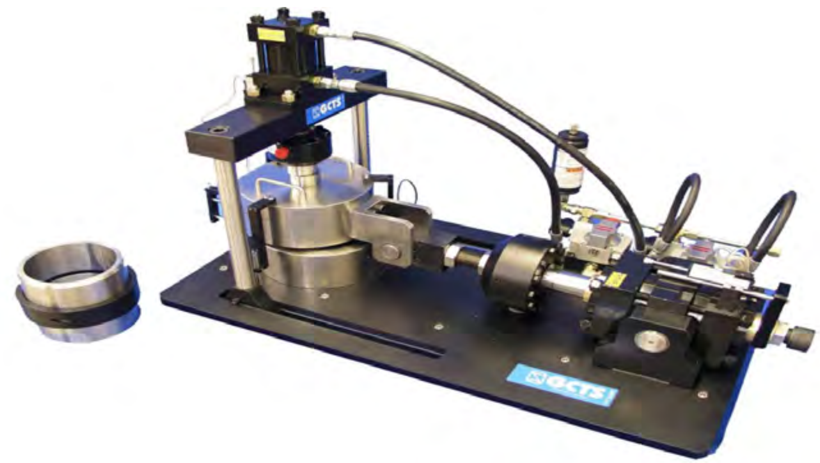
Incremental Data-Driven plasticity problem





Direct shear test device

- ***Material data set: Directed graphs in phase space!***
- Incremental material data set:

$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \ : \ \text{accessible from } (\epsilon_k, \sigma_k)\}$$

- Data-driven problem: $\min_{z \in E_{k+1}} d(z, D_{k+1})$
- ***Path dependence, loading/unloading irreversibility!***

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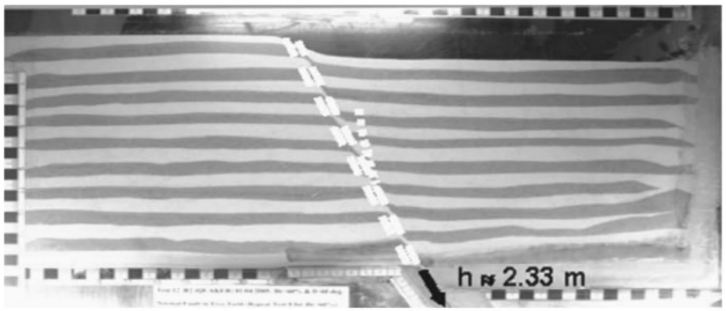
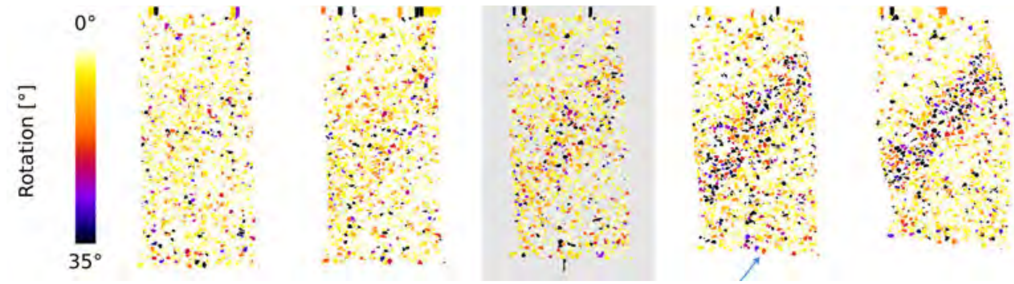
Test case – Data-Driven sand mechanics





Fault rupture experiment in sandbox configuration.[1] Sand is pluviated into a 10m x 30m container. A piston forces right half to subside, inducing fault rupture at 30° to horizontal

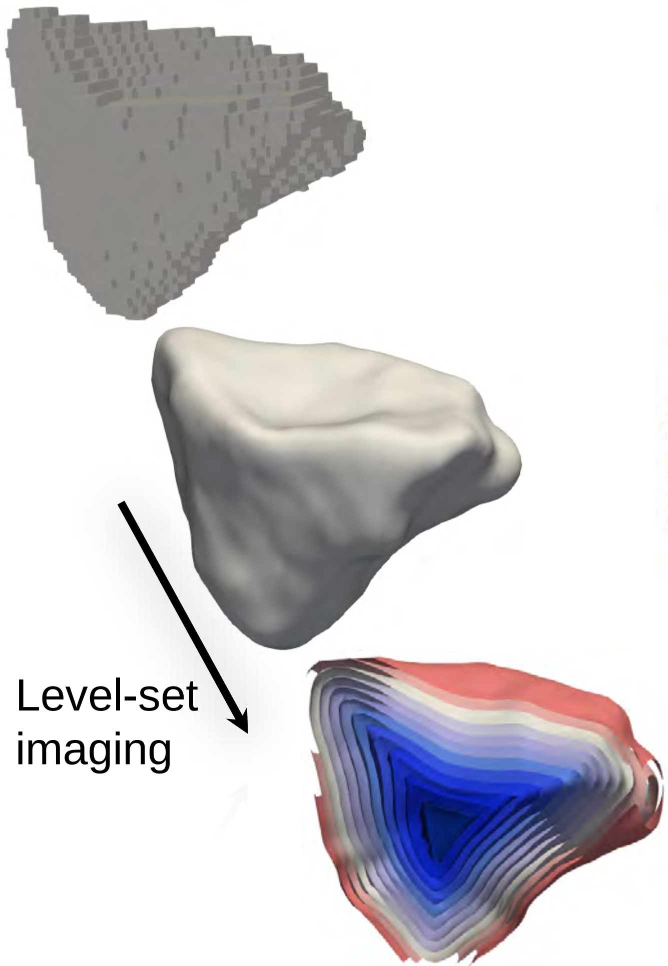
Triaxial compression test,[2] angular Hostun sand, 100 kPa confining pressure, 11 mm x 22 mm samples in latex membrane. Particles tracked by XRMT. Failure occurs by shear banding

[1]Anastasopoulos, I., *et al.*, *J. Geotech. Geoenviron. Eng.*, **133** (2007) 943–958.

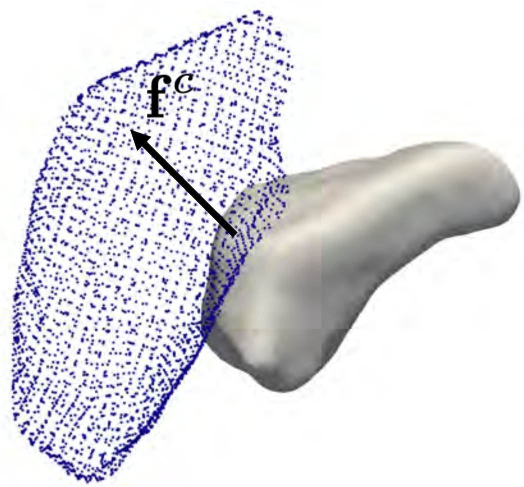
[2]Andò, E., *et al.*, *Acta Geotech.*, **7** (2012) 1-13.

Virtual experiments with LS-DEM

Morphology



Grain-grain interaction

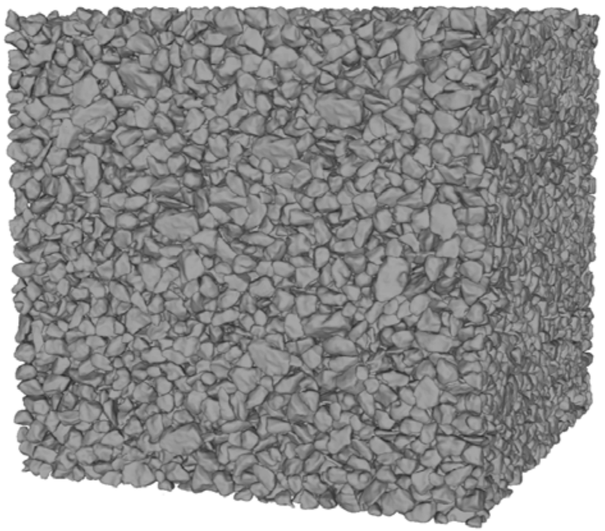


$$f^c = f_n^c + f_t^c$$

f_n^c : Hertzian

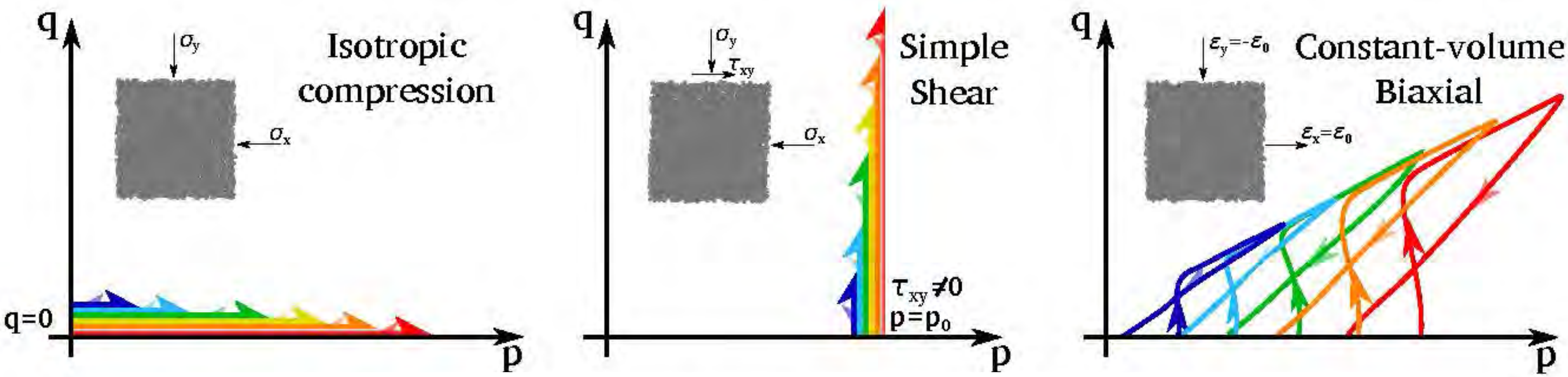
f_t^c : Coulomb

RVE generation

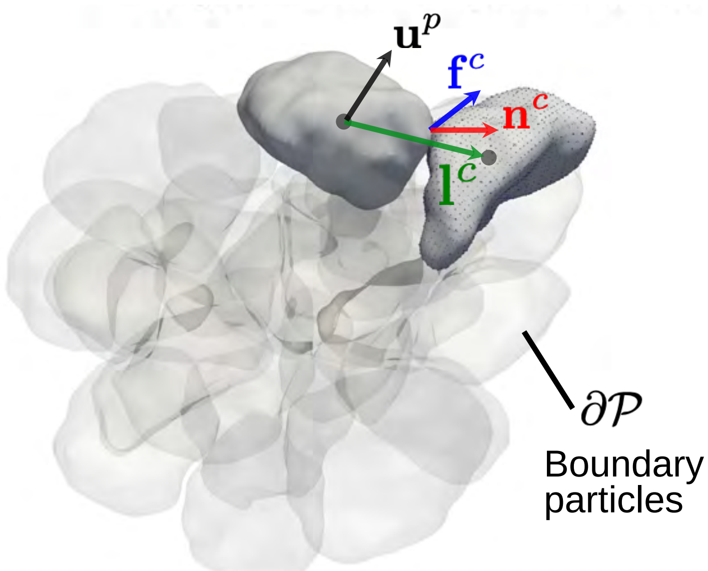


Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E., *JMPS*, **91** (2016) 1-13.

Hastun angular sand – Path sampling



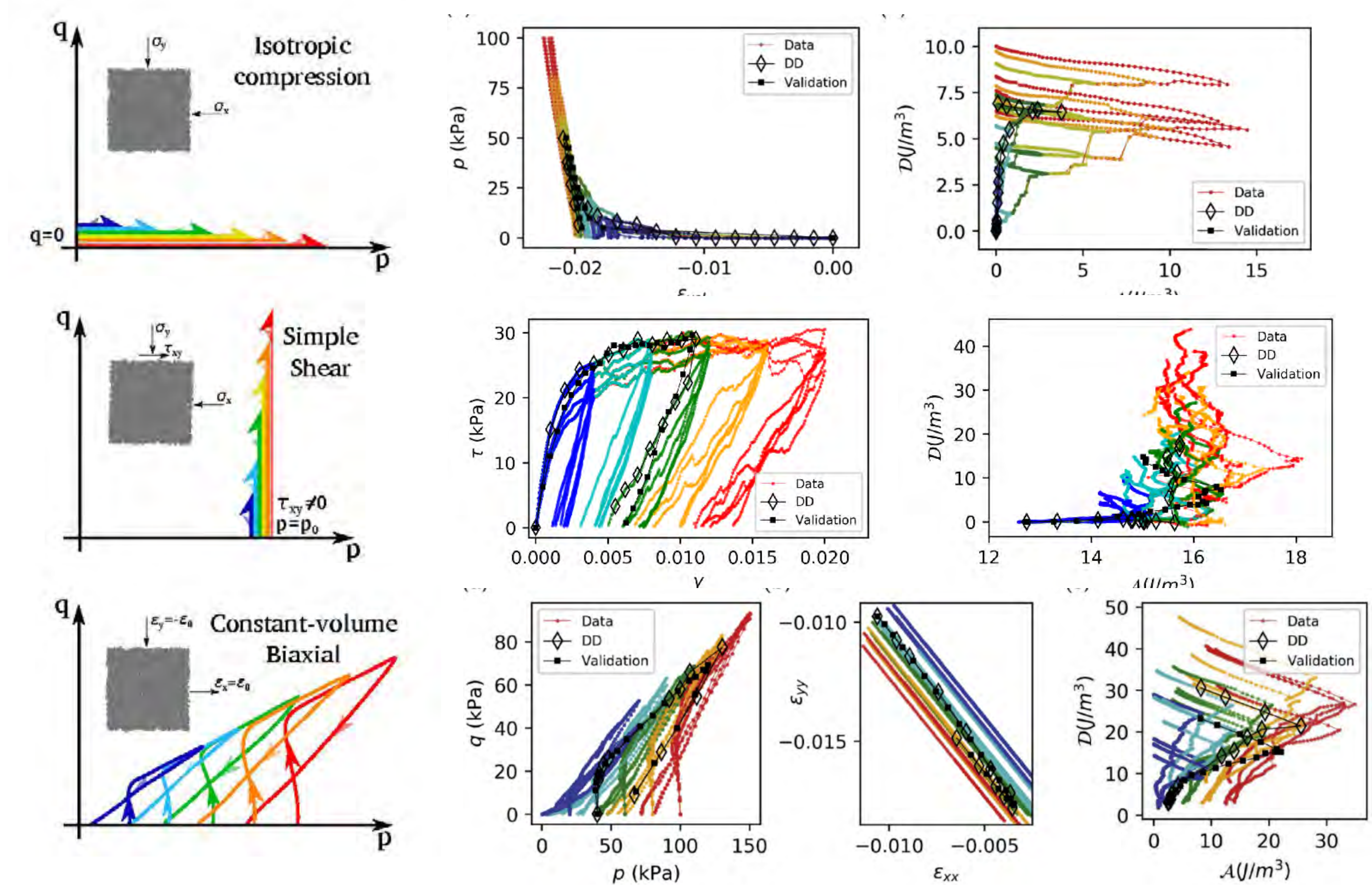
Selected paths for building the material data repository



$$
\begin{cases}
\boldsymbol{\varepsilon} = \dfrac{1}{2V}\mathrm{sym}\Big(\sum_{p\in\partial\mathcal{P}} \mathbf{u}^p \otimes \mathbf{n}^p\Big) \\
\boldsymbol{\sigma} = \dfrac{1}{V}\mathrm{sym}\Big(\sum_{c\in\mathcal{C}} \mathbf{f}^c \otimes \mathbf{l}^c\Big) \\
\mathcal{A} = \sum_c \mathcal{A}^c = \dfrac{1}{2V}\sum_c \Big(\dfrac{\|\mathbf{f}^{\mathbf{c}}_{\mathbf{n}}\|^2}{k_n} + \dfrac{\|\mathbf{f}^{\mathbf{c}}_{\mathbf{t}}\|^2}{k_t}\Big) \\
d\mathcal{D} = \sum_c d\mathcal{D}^c = \dfrac{1}{V}\sum_c \mathbf{f}^c_t \cdot d\mathbf{u}^{c,slip}
\end{cases}
$$

K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

Hastun angular sand – Path sampling

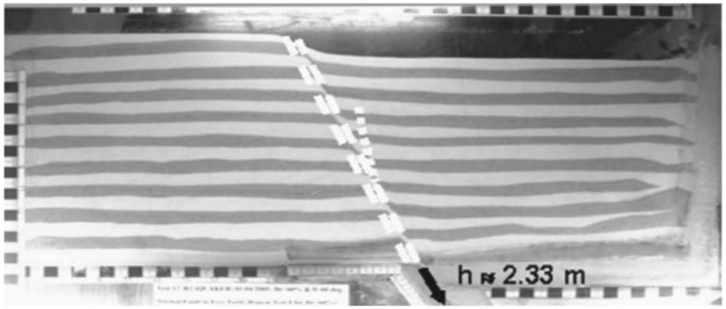


path stress-strain energy-dissipation

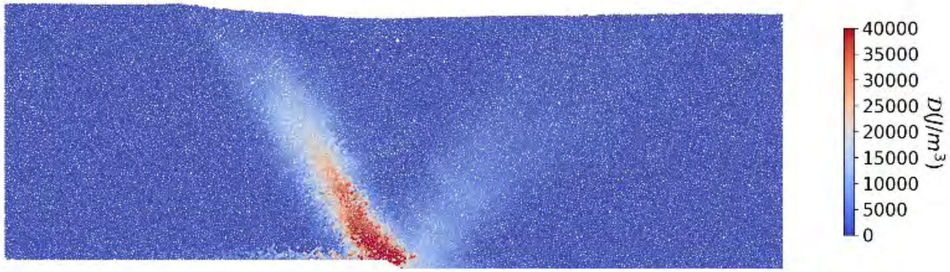
Compilation of path data for Hatsun angular sand computed from RVEs using LS-DEM

K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

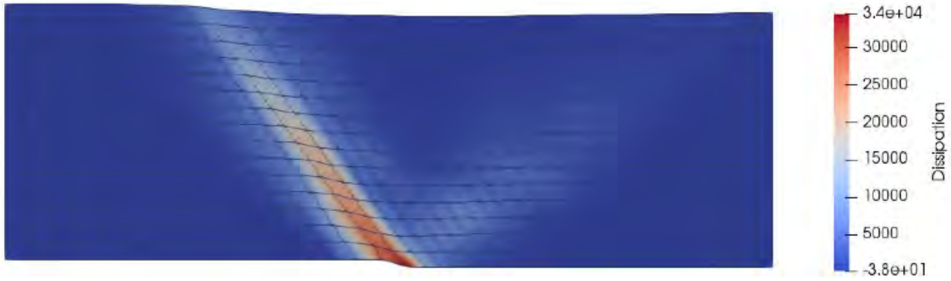
Sand mechanics – Fault rupture experiment



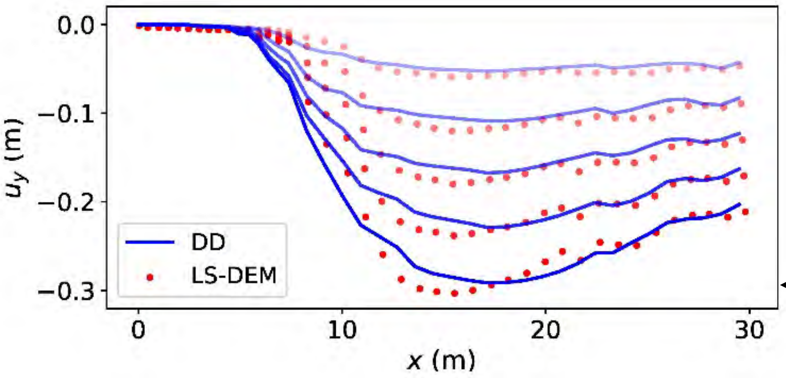
Experimental fault rupture experiment



LS-DEM simulation



Data-Driven simulation

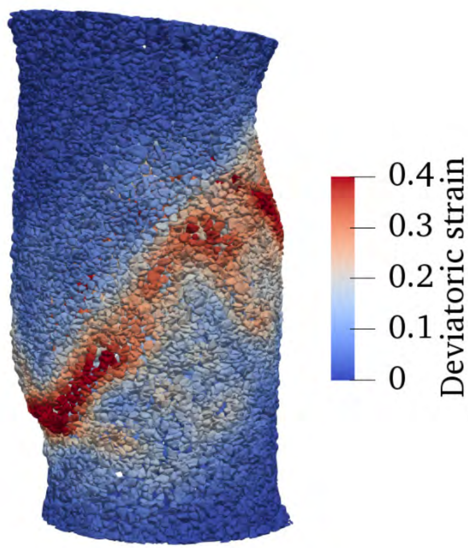


Evolution of surface settlement LS-DEM *vs*. DD simulations

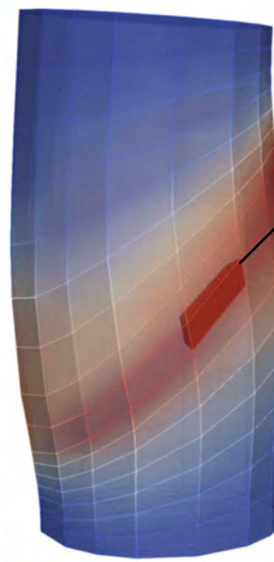
Anastasopoulos, I., *et al*., *J. Geotech. Geoenviron. Eng*., **133** (2007) 943–958.
K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

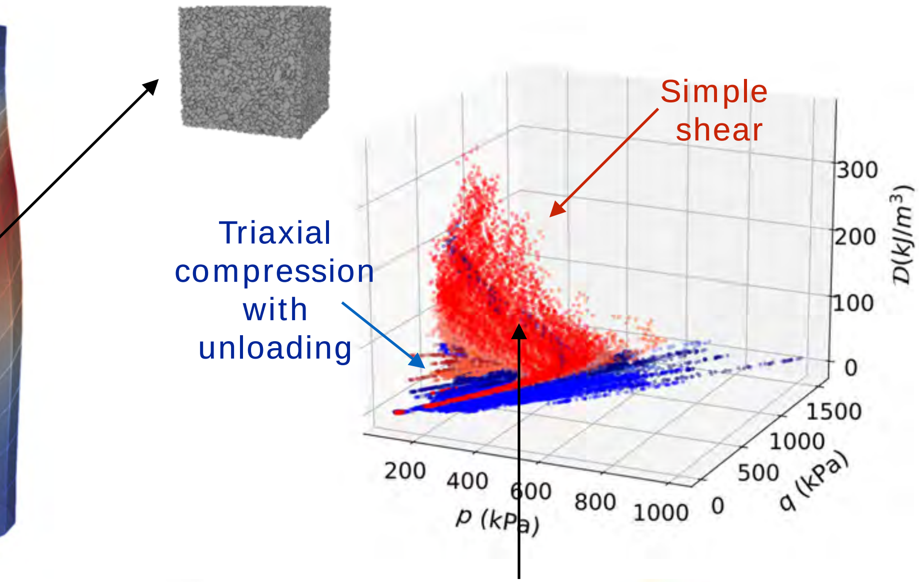
Data-Driven – Fault rupture experiment

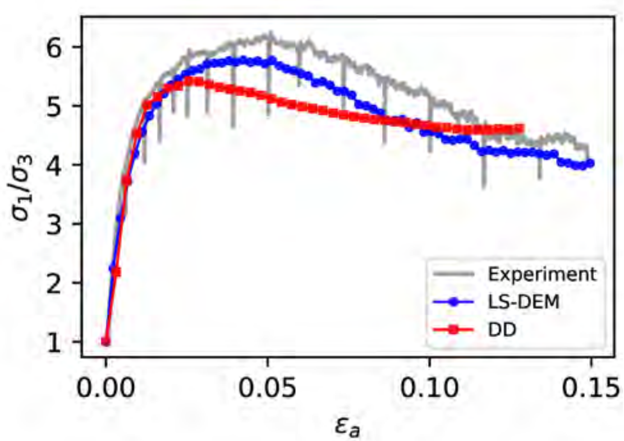
LS-DEM

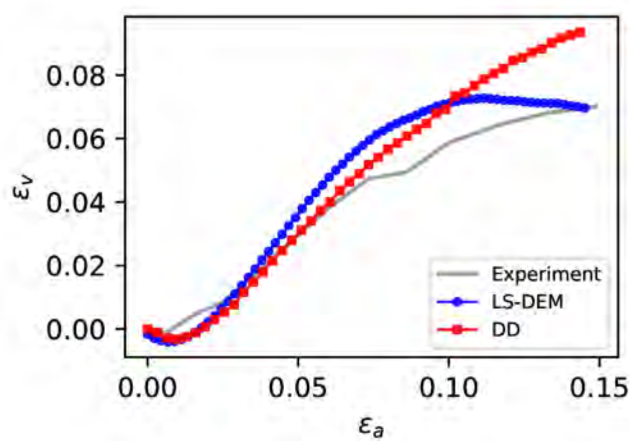


DD









K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

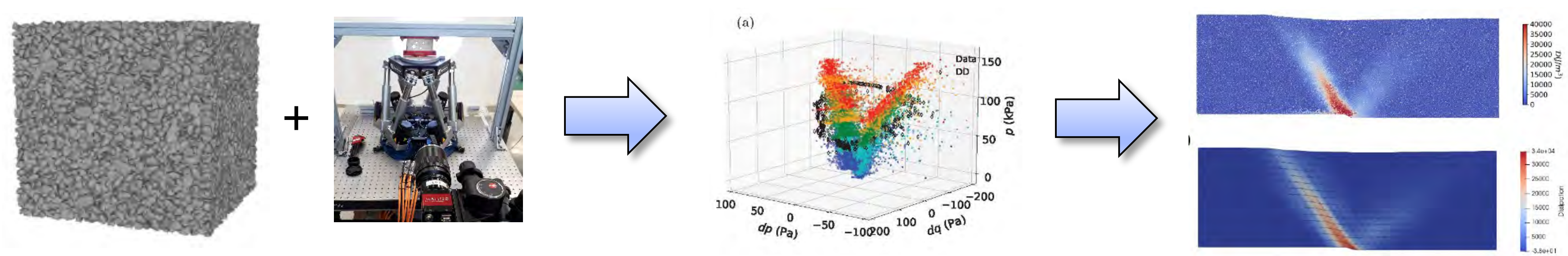
Path selection, coverage, convergence

- Path coverage must be *goal oriented* (tailored to specific problems)
- *Main path types* are often known beforehand for specific problems (initial path-data repository)
- Monitor local *path-distance error* at individual material points
- *Evaluate RVEs for local paths* that are *farther* from the existing path repository *than a given tolerance*
- *Add new RVE path data to repository*
- *Iterate till convergence*

Karapiperis, Konstantinos (2021) *Multiscale, Data-Driven and Nonlocal Modeling of Granular Materials.* Dissertation (Ph.D.) California Institute of Technology. doi:10.7907/7rtg-x780. https://resolver.caltech.edu/CaltechTHESIS:12182020-181342301

Concluding remarks

- *It is possible to formulate DD approximation schemes for history-dependent materials that are model-free and internal-variable free*
- *Path data for rate-independent plasticity has the structure of directed graphs in phase space*
- *DD sets forth new opportunities for synergism between experimental science and scientific computing, new multiscale analysis paradigm*



- *Model-free DD mechanics represents a paradigm shift in material data management and exchange in the mechanics of materials community*

Concluding remarks

Thank you!