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Model-Free Data-Driven Computing

Michael Ortiz
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

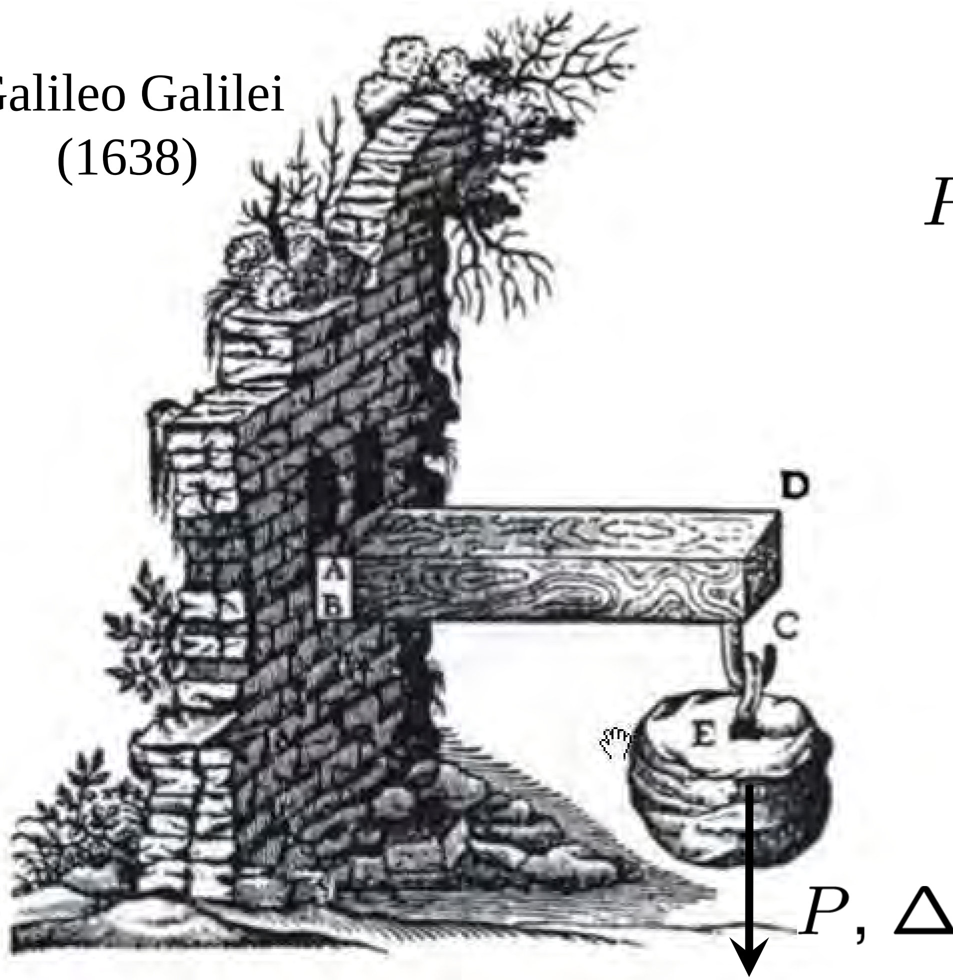
With: K. Karapiperis, J. Andrade (Caltech)
L. Stainier (Central Nantes)
R. Eggersmann, S. Reese (RWTH Aachen)

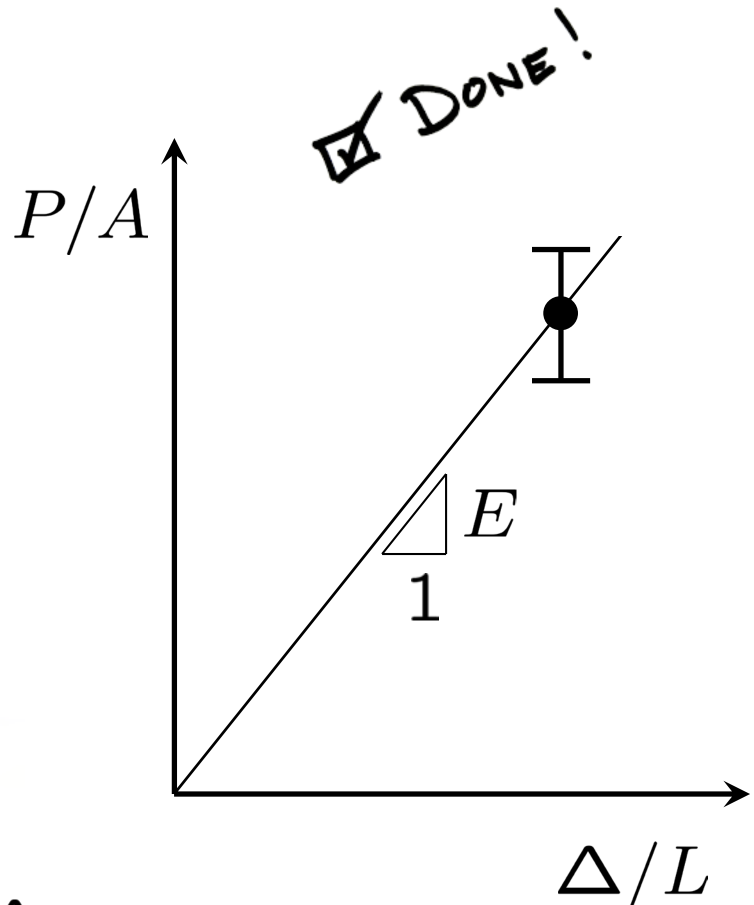
Workshop on Advanced Computing and Big Data
Politecnico di Milano, October 19, 2021

Materials data through the ages…

Traditionally, mechanics of materials has been ***data starved***...

Galileo Galilei
(1638)





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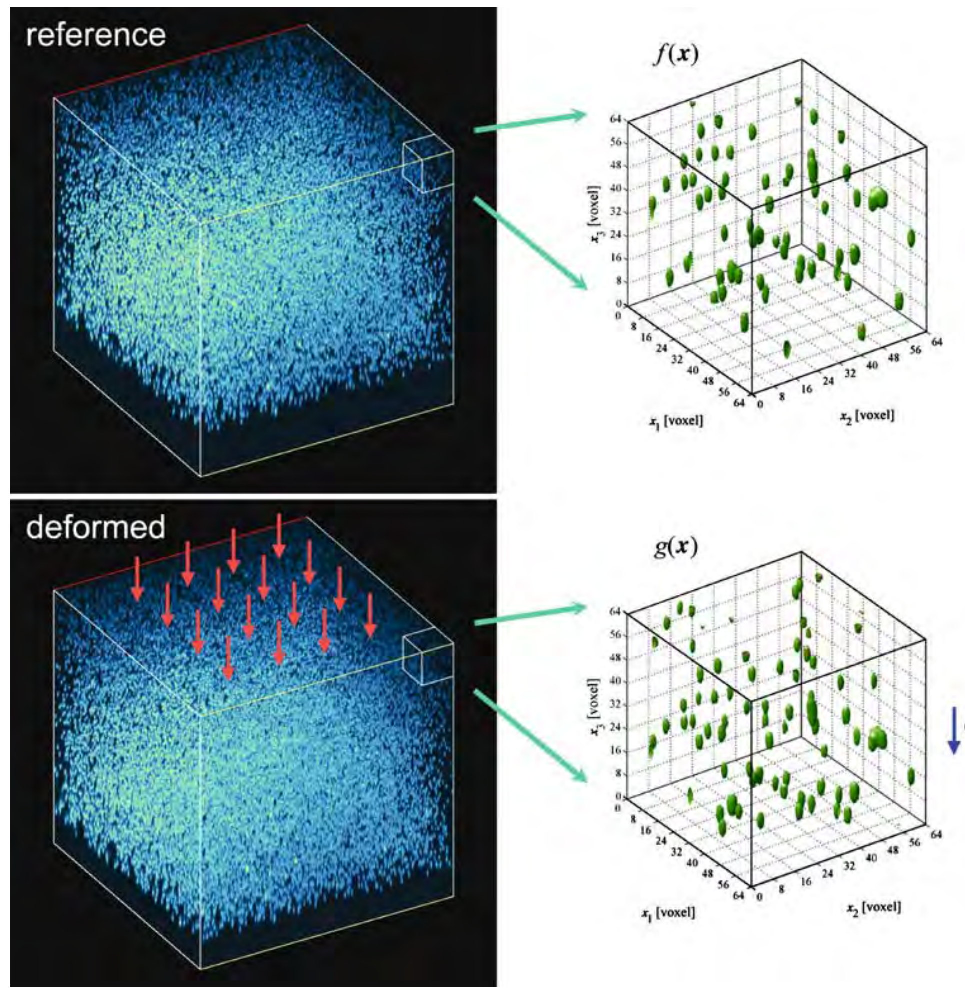
Polimi 10/19/21

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.

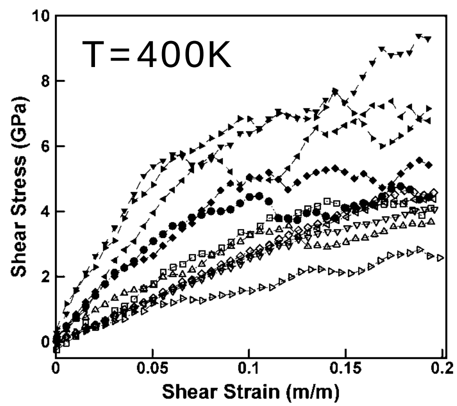
Computational mechanics in a data-rich world

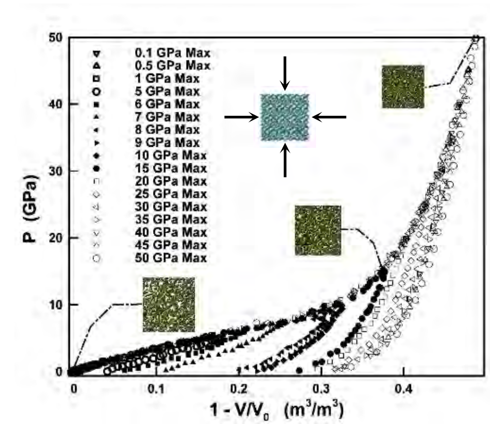
- Material data can also be generated in large volumes from high-fidelity *micromechanical calculations* (DFT, MD, DD...)
- New role for *multiscale analysis*: Data generation

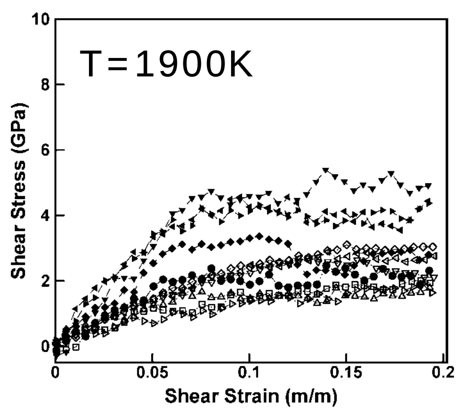
Amorphous SiO_2 glass: LAMMPS MD calculations of amorphous silica glass under *pressure-shear* loading over a range of *temperatures* and *strain rates*. RVEs are quenched from the melt, then analyzed using the BKS potential with Ewald summation.

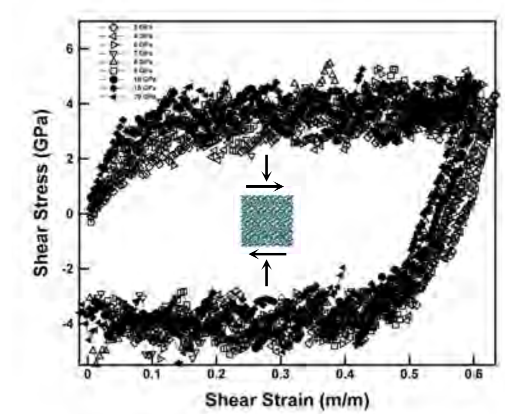
Schill, W., Heyden, S., Conti, S. & MO, *JMPS*, **113** (2018) 105-125.

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









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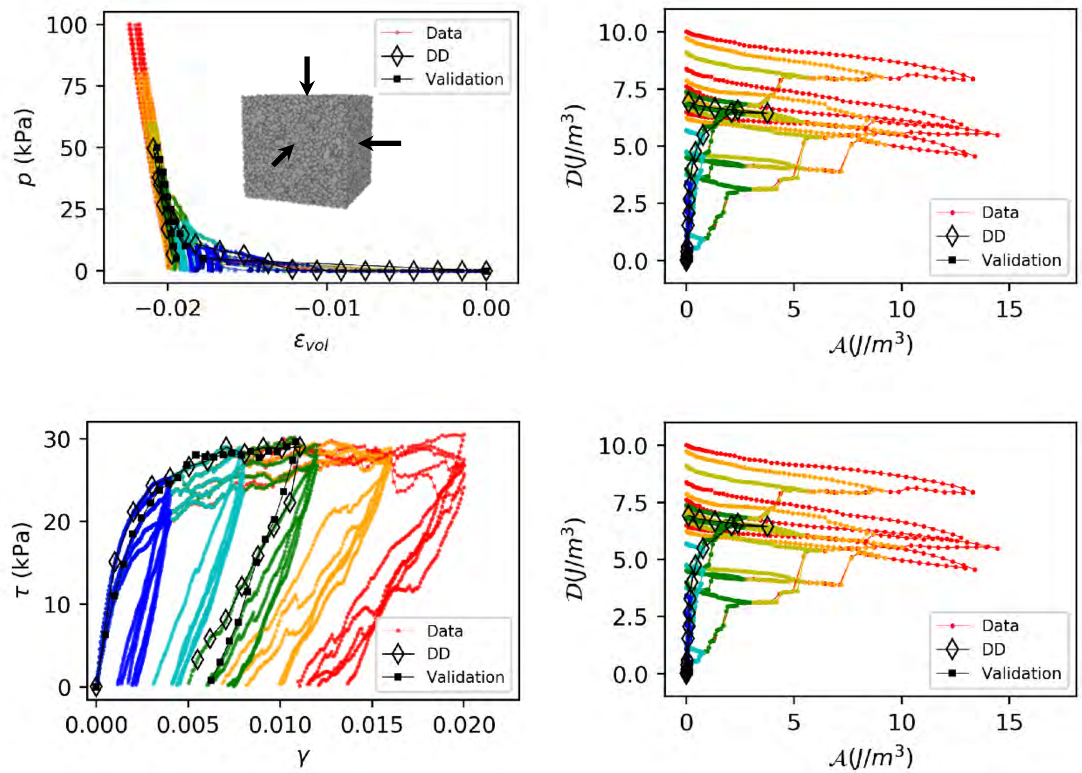
Computational mechanics in a data-rich world

- 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.

Computational mechanics in a data-rich world

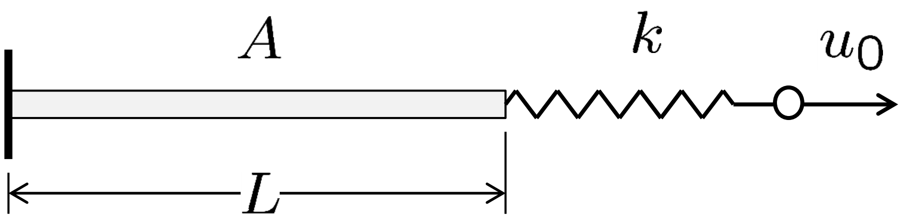
- The unprecedented *abundance of material data* presents new challenges and opportunities
- Two main strategies:
  - *Model the data, use models in BVP calculations*
  - *Embed the data directly into BVP calculations*

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

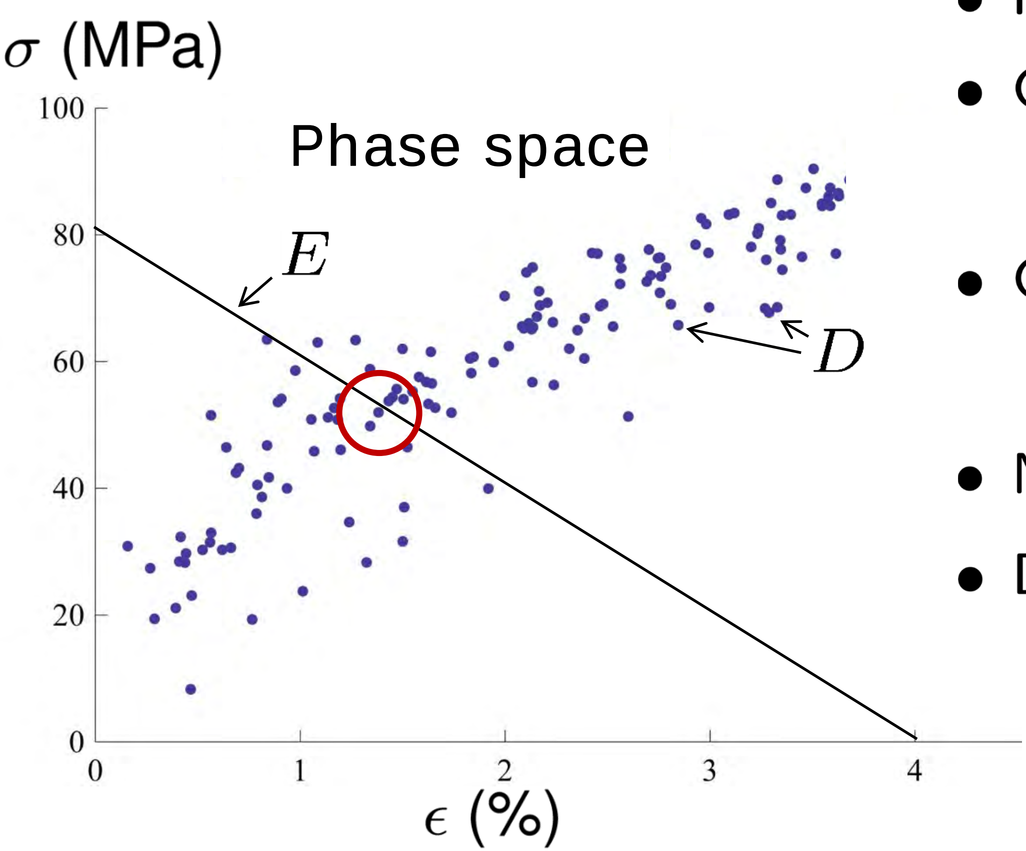
- *Critique of Model-Based computing*: Modeling results in loss of information, introduces biases, modeling error, epistemic uncertainty, is open-ended, *ad hoc*...
- Model-Free computing: *Cut out the middle man!*

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:

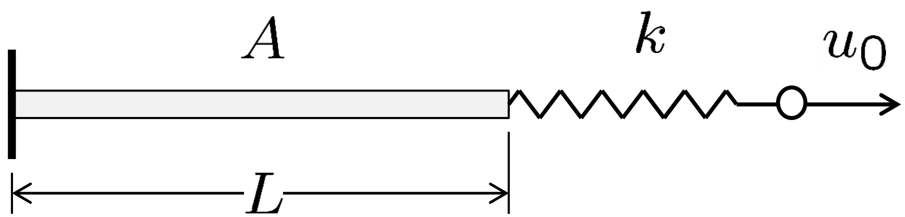
$$E = \{\sigma A = k(u_0 - \epsilon L)\}$$

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

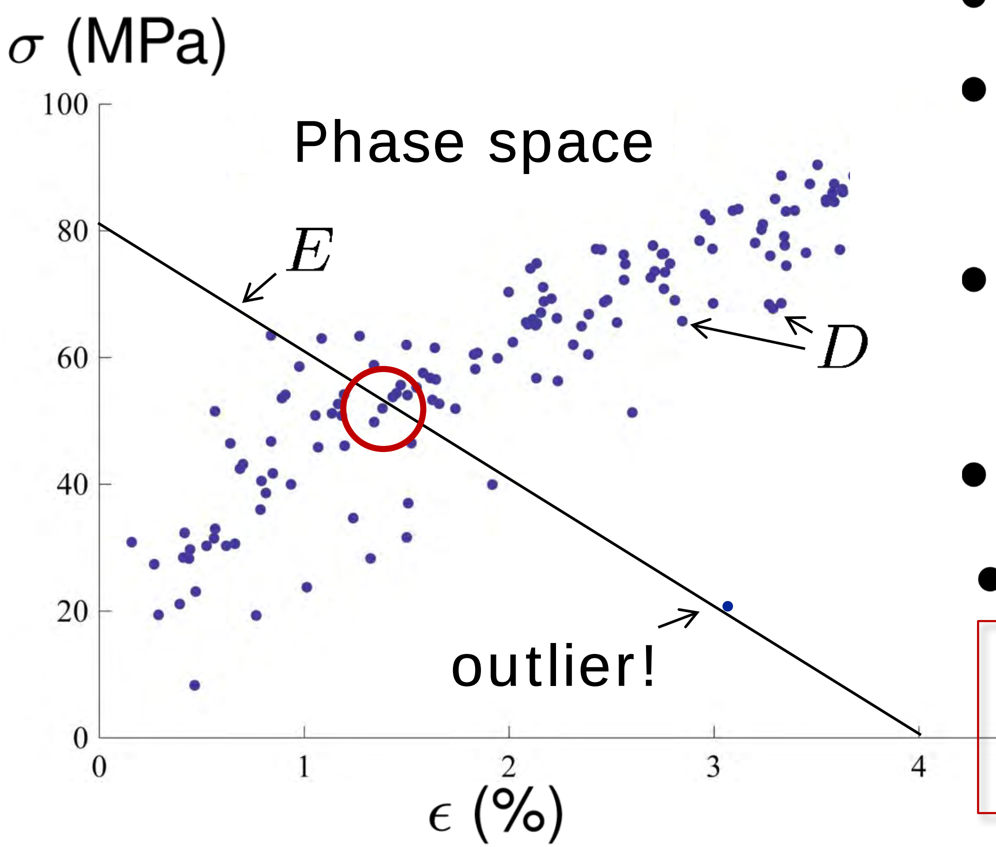
$$\boxed{\min_{z \in E} \text{dist}(z, D)}$$

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

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:

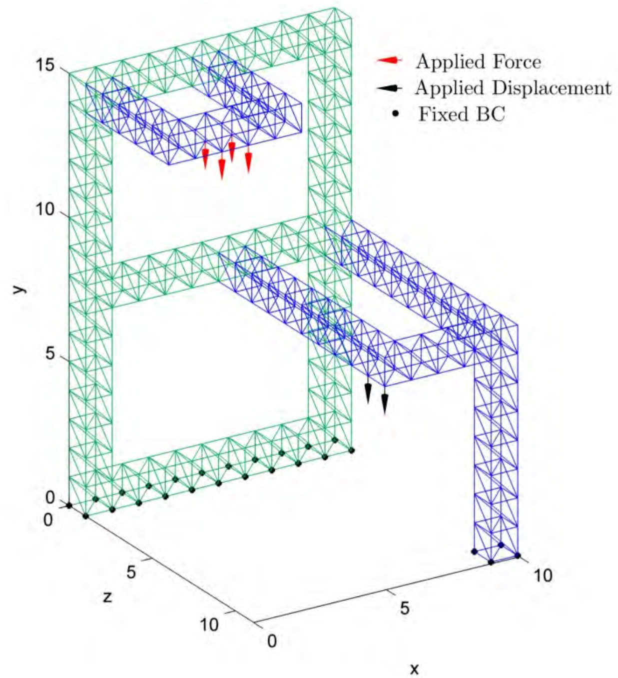
$$E = \{\sigma A = k(u_0 - \epsilon L)\}$$

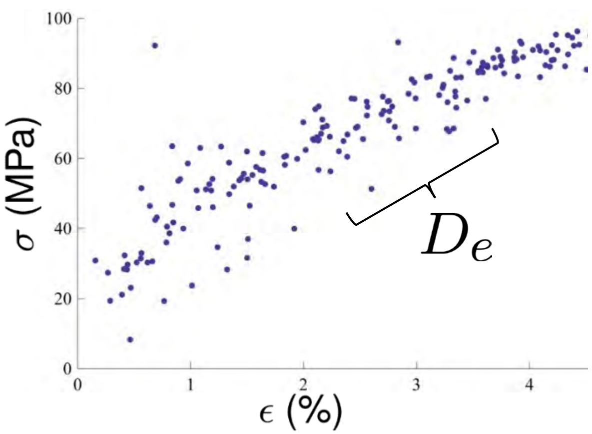
- Material data set: $D \subset Z$
- With outliers (k-means):

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

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:

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

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

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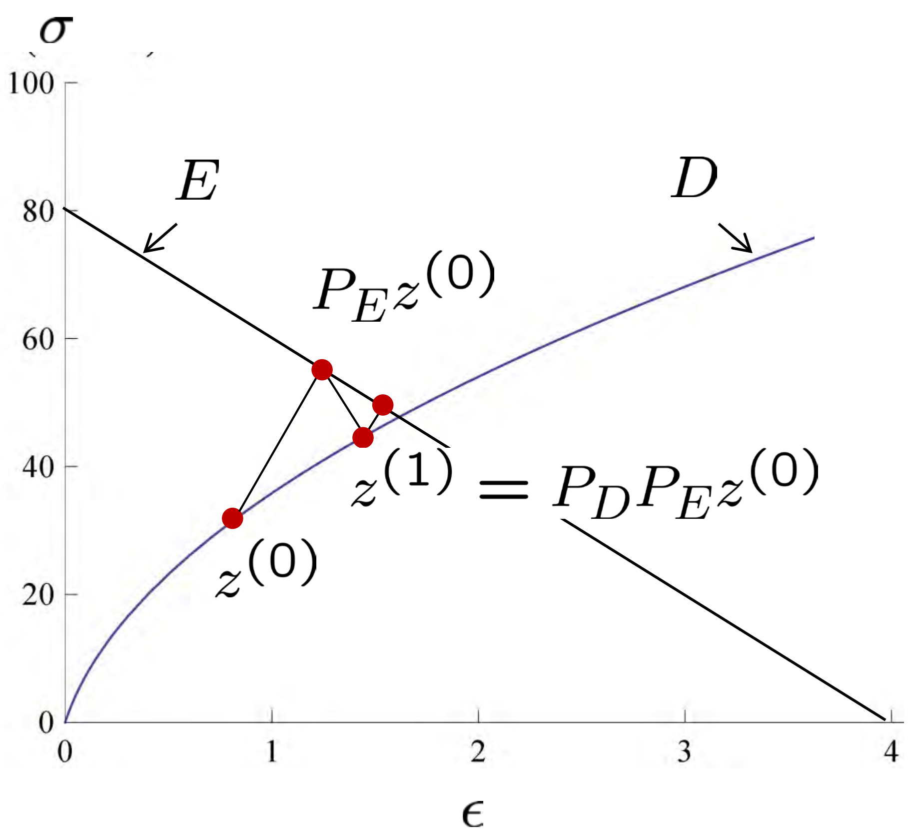
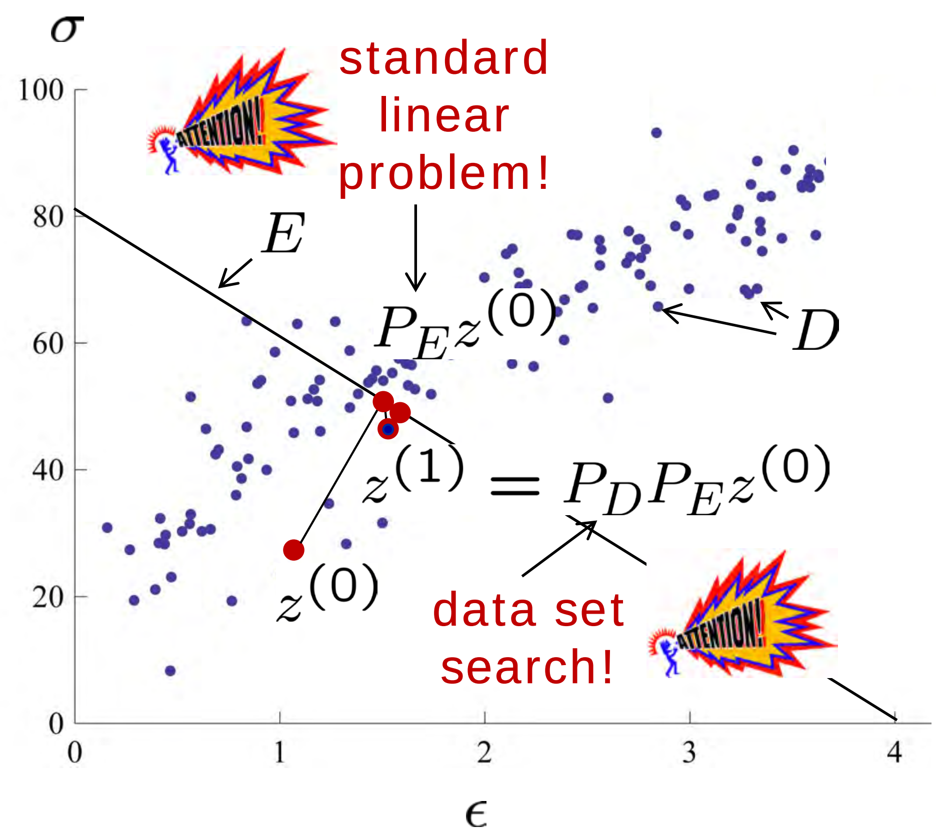
DD solvers: Fixed-point iteration

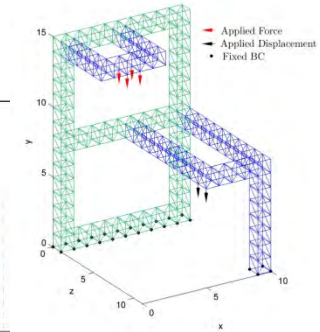
- Find: argmin$\{d(z, D),\ z \in E\}$
- Fixed-point iteration[1]: $z^{(k+1)} = P_D P_E z^{(k)}$

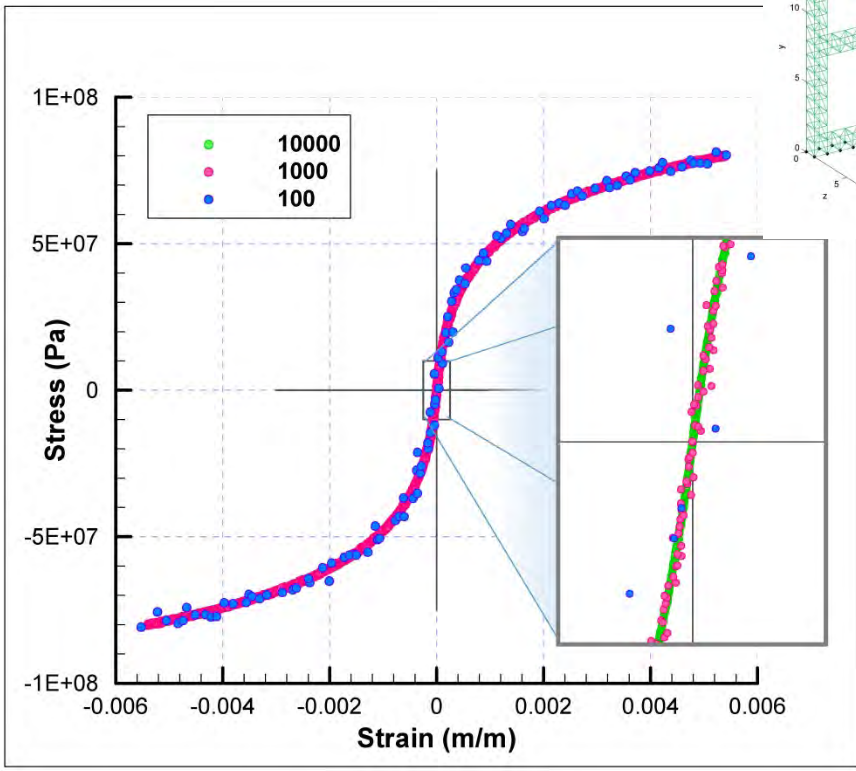


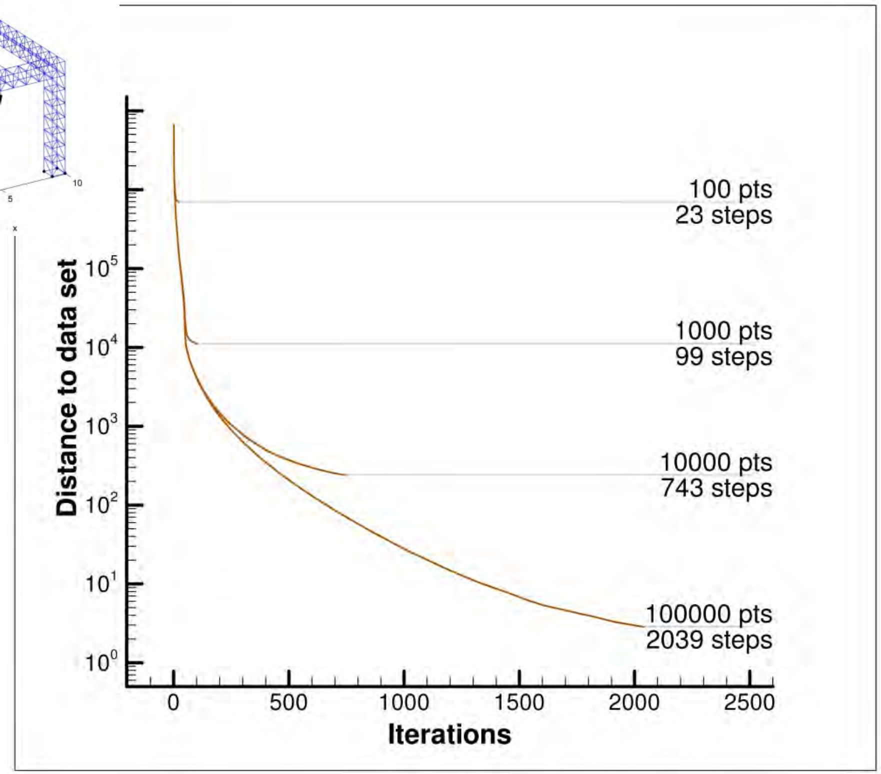


[1]T. Kirchdoerfer and M. Ortiz (2015) arXiv:1510.04232.
[1]T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

Data-Driven solvers – Convergence





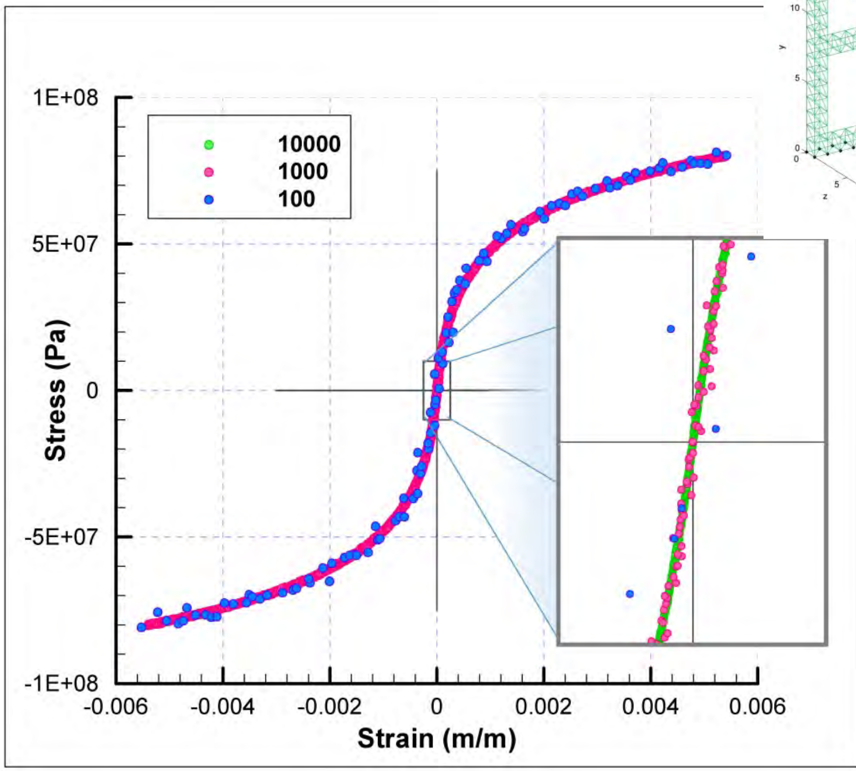


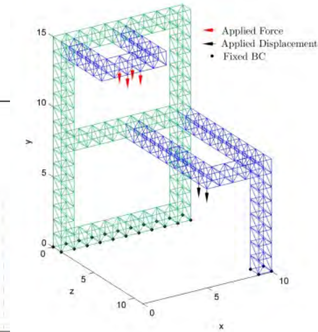
Sequence of uniformly converging data sets (increasing number of points, decreasing scatter)

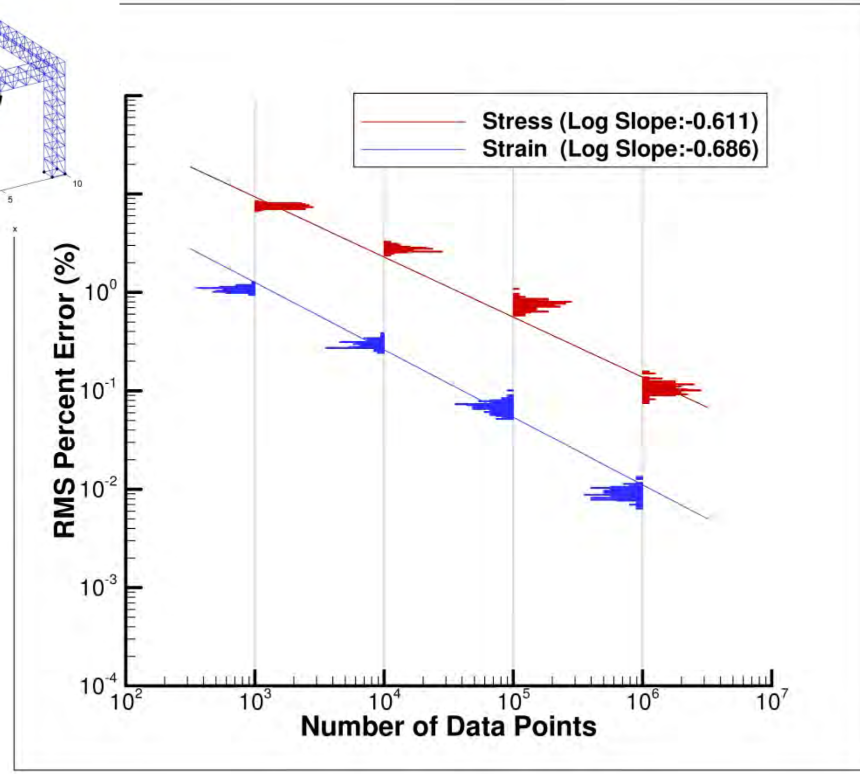
Convergence of fixed-point solver: Each iteration requires two back-substitutions for standard linear systems and one material data search/member

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

Data-Driven solvers – Convergence





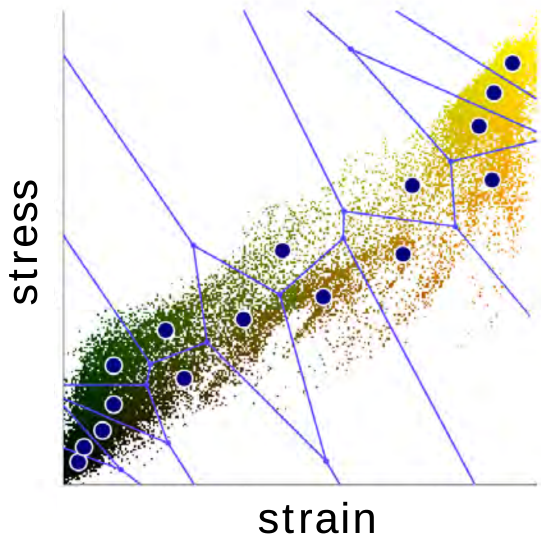


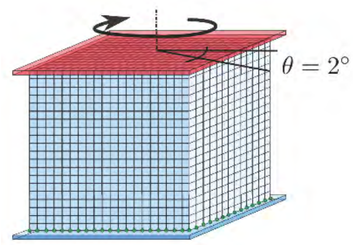
Sequence of
uniformly converging data sets
(increasing number of points,
decreasing scatter)

Convergence with respect to material data set towards
solution of limiting problem
(nonlinear elasticity)

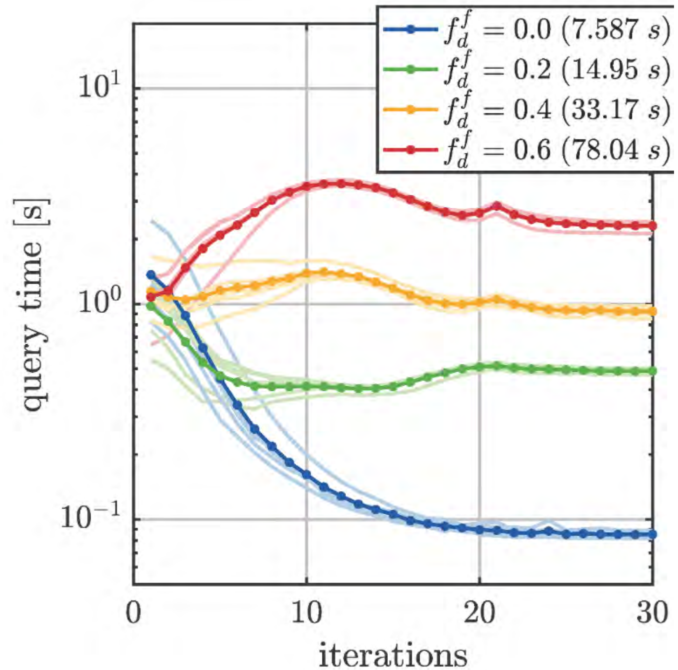
T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

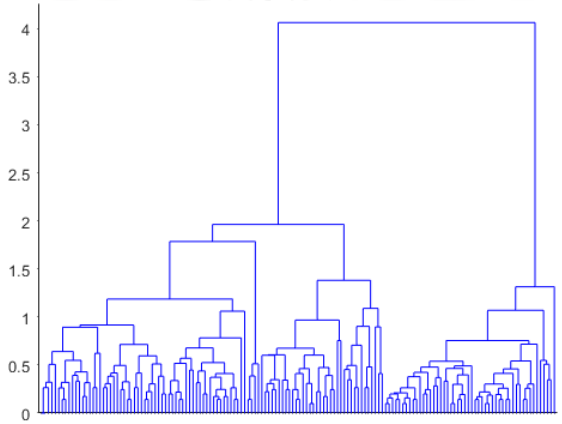
Data-Driven history-independent problems





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!***

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 problems

Plasticity applications - Crashworthiness

Frontal crash test of
Volvo C30


Frontal crash test of
Chevrolet Venture


Offset frontal crash test of
1998 Toyota Sienna


Side-impact test of
1996 Ford Explorer vs.
2000 Ford Focus

Source: http://en.wikipedia.org/wiki/Crash_test

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ROME0611

History-dependent problems

Plasticity applications - Manufacturing

Metal ingot after forging

Lathe cutting metal
from workpiece

Cold rolling
of steel

Deep-drawing of
blank metal sheet
(source: ThomasNet)

Sources: http://en.wikipedia.org/wiki/Forging
http://en.wikipedia.org/wiki/Metal_forming
http://www.kanabco.com/vms/library.html

History-dependent problems

Plasticity applications – Metallic structures

Plastic buckling of storage tank,
1999 Kocaeli earthquake
(PEER 2000/09, Dec. 2000)

Mid-story collapse,
1995 Kobe earthquake
(EQE Summary Rep., 1995)

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History-dependent problems
Plasticity applications –Geotechnical engr.

Some effects of liquefaction after the 1964 Niigata earthquake (Source: Wikipedia)

Foundation Weakening Due to Soil Liquefaction after 1999 Adapazari earthquake, Turkey (Source: USGS)

- Plasticity: history-dependent, irreversible, hysteretic
- *Data-Driven solvers for history-dependent problems?*

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]."

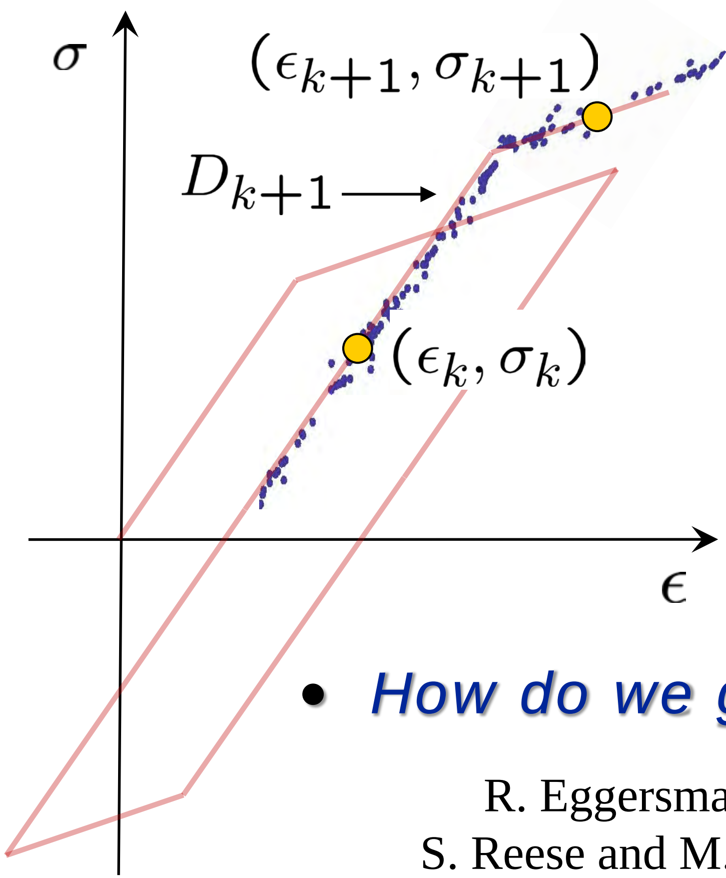
- The theory of *materials with memory* furnishes the most general representation of inelastic materials.
- Alternative: Replace history by the effects of history, the current *microstructure* (internal state)
- *Instead: Develop Data-Driven representations that are internal-variable-free (path-based)! How?*

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

Data-Driven history-dependent problems

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

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



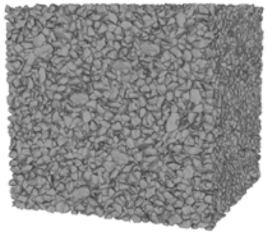
- Data-driven problem:

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

- 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.

Incremental plasticity in phase space



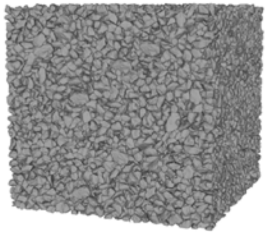
- Summary of governing equations:
  - *Coleman-Noll equilibrium relations,*

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

  - *Incremental kinetic relations,*

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

Incremental plasticity in phase space



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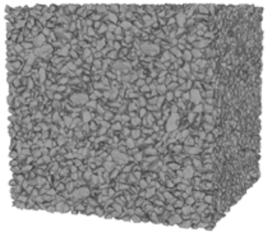
- *Convex analysis* view of plasticity
- Pioneered by *Giulio Maier* at the Politecnico di Milano, and others (Martin, Ponter, Symonds, Moreau…), especially in the area of structural mechanics

Incremental plasticity in phase space



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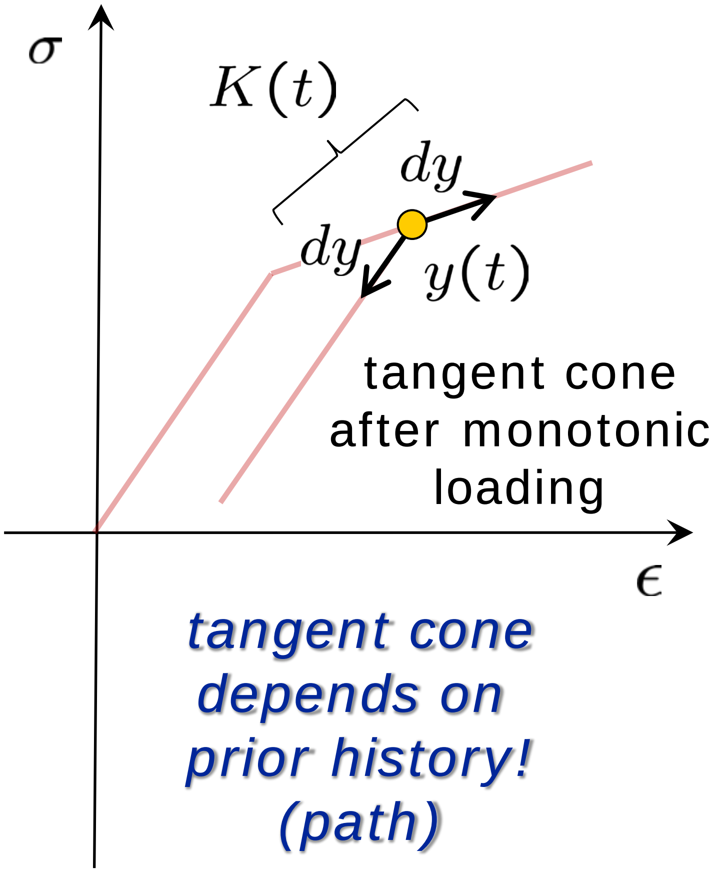
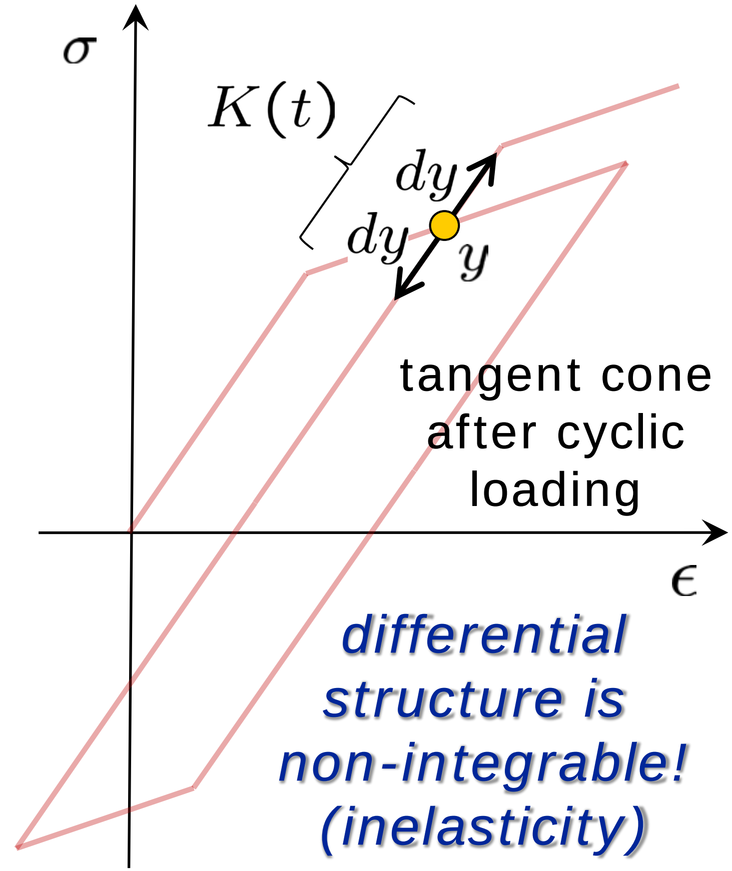
- *Eliminate* $(dq, dp) \Rightarrow$ *tangent cone*

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

- *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...

Carathéodory’s view of plasticity

C. Carathéodory
Berlin, 1873
Munich, 1950

SIAM J. APPL. MATH.
Vol. 25, No. 4, December 1973

CARATHEODORY’S THEOREM ON THE SECOND LAW OF THERMODYNAMICS*

E. C. ZACHMANOGLOU†

1. Introduction and statement of results. We consider the Pfaffian differential equation

$$a^1(x)\,dx_1 + \cdots + a^n(x)\,dx_n = 0, \tag{1}$$

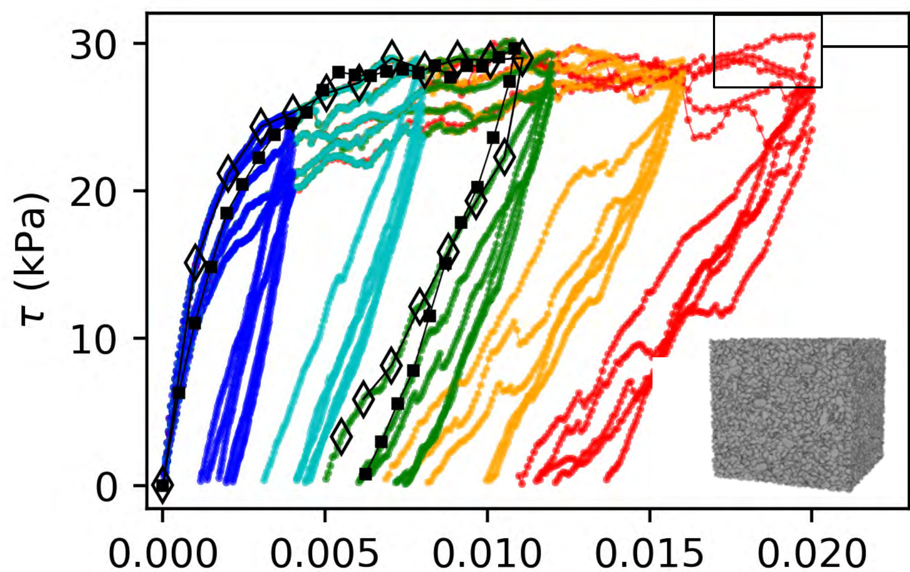
where the coefficients $a^1, \cdots, a^n$ are real-valued C^∞ functions in some open set Ω in R^n and do not vanish simultaneously at any point $x = (x_1, \cdots, x_n)$ of Ω. An integral curve of (1) is any solution $x = x(t)$ of the differential equation

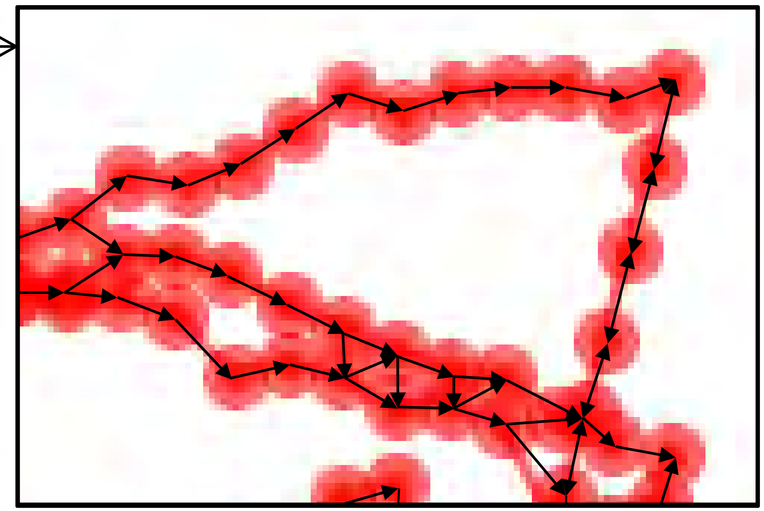
$$a^1(x)\frac{dx_1}{dt} + \cdots + a^n(x)\frac{dx_n}{dt} = 0, \tag{2}$$

and a trajectory of (1) is a piecewise C^∞ curve, each $C^\propto$ piece of which is an integral curve of (1).

An integral surface of (1) is any $(n-1)$-dimensional surface which envelopes the field of surface elements defined by $a = (a^1, \cdots, a^n)$. When $n = 2$ the concepts

Building path data from micromechanics





Data points and connections

i) Evaluate RVE for selected loading paths

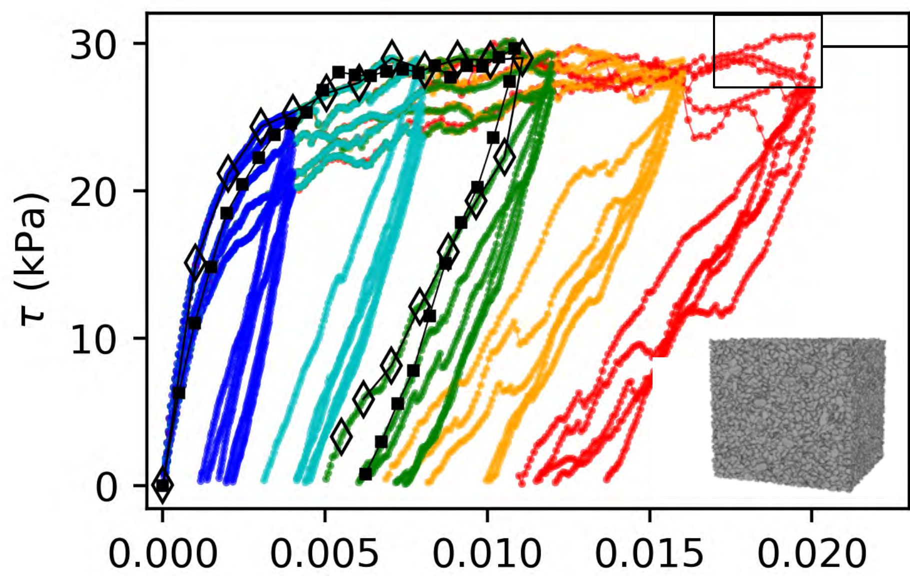
ii) Record $(\epsilon_i, \theta_i; \sigma_i, \eta_i)$, connect points i and j if

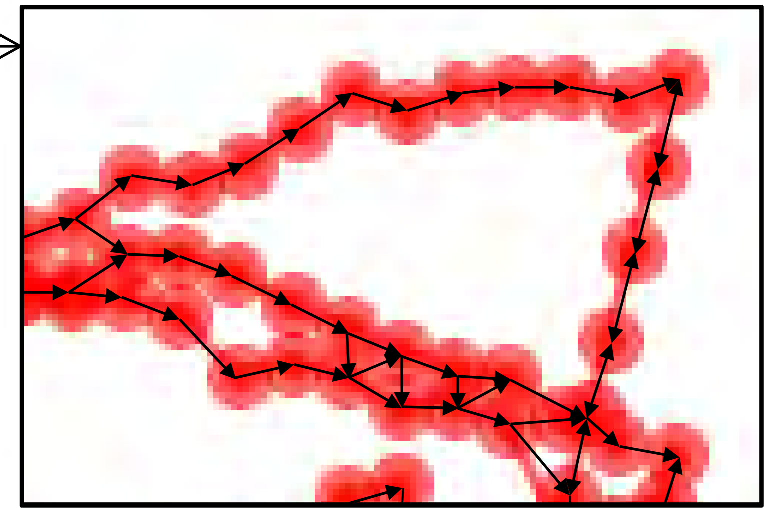
$$\psi(q_j - q_i) - \langle \frac{p_i + p_j}{2}, q_j - q_i \rangle \leq \text{TOL}$$

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

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

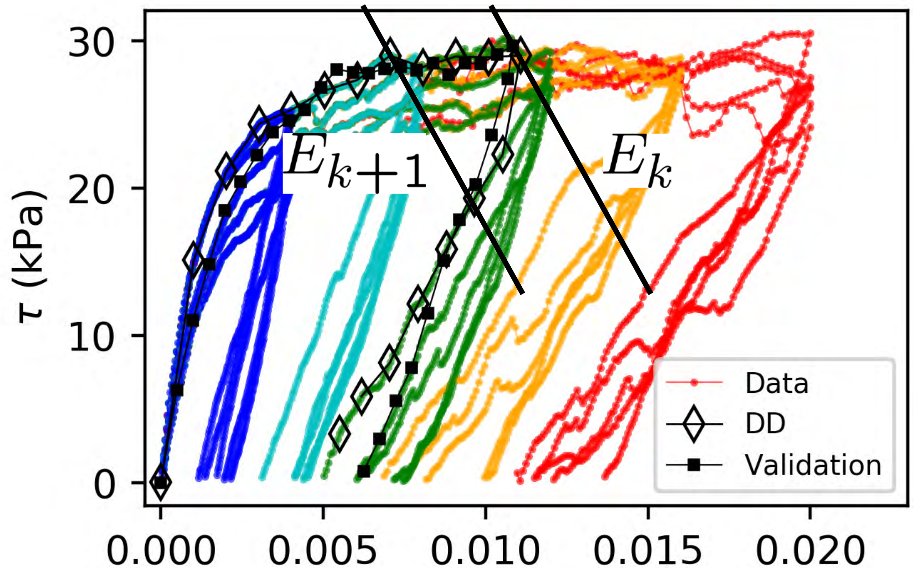
ii) Record $(\epsilon_i, \theta_i; \sigma_i, \eta_i)$, connect points i and j if

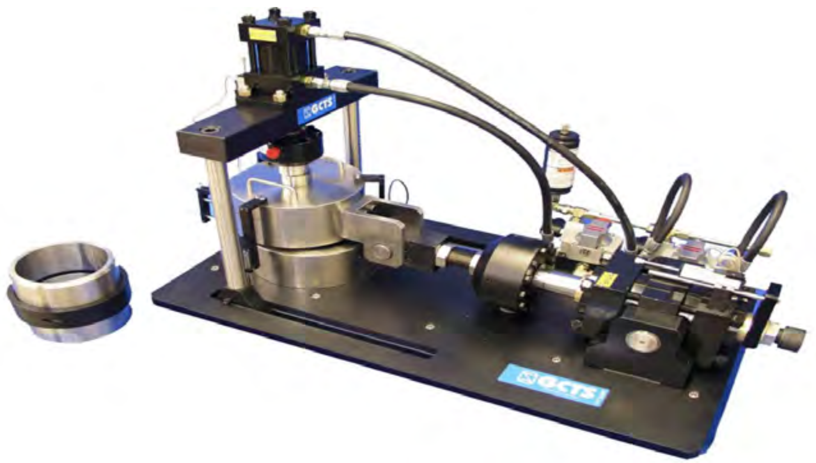
$$Diss_{i \to j} + A_j - A_i - \langle \frac{\sigma_i + \sigma_j}{2}, \epsilon_j - \epsilon_i \rangle \leq \text{TOL}$$

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

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

Incremental Data-Driven plasticity problem





Direct shear test device

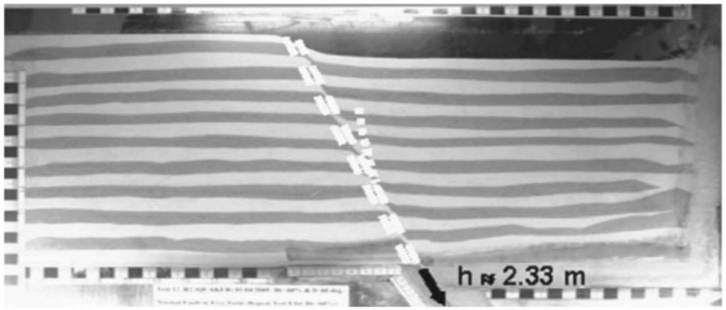
- *Material data set: Directed graphs in phase space!*
- Incremental material data set:

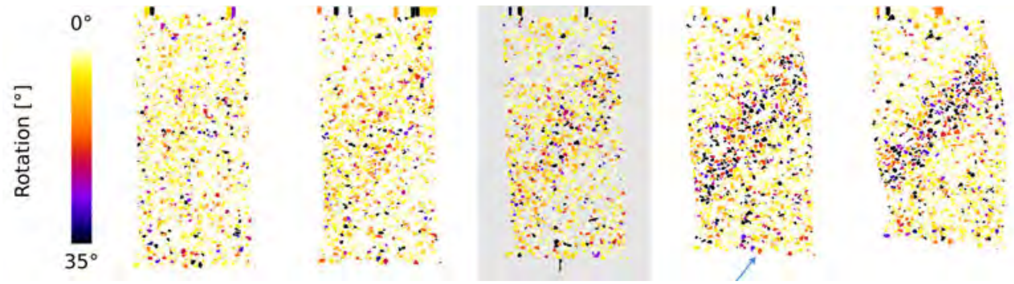
$$D_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \ : \text{ accessible from } (\epsilon_k, \sigma_k)\}$$

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

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

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

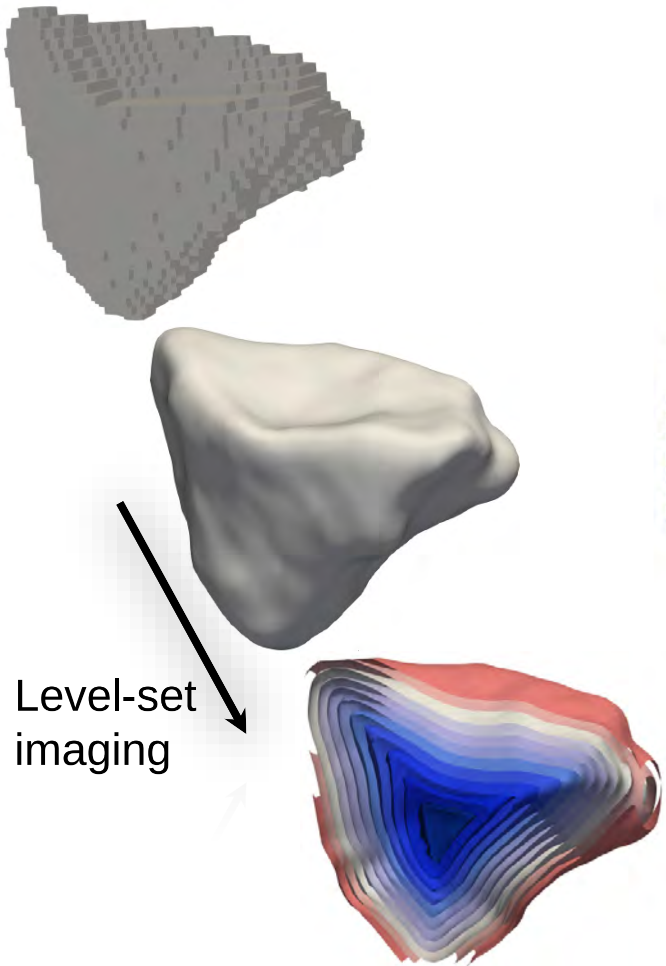
[1]Anastasopoulos, I., *et al.*, *J. Geotech. Geoenviron. Eng.*, **133** (2007) 943–958.

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

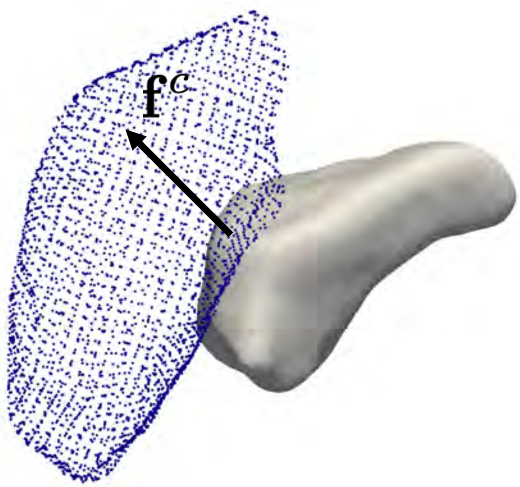
[2]Andò, E., *et al.*, *Acta Geotech.*, **7** (2012) 1-13.

Virtual experiments with LS-DEM

Morphology



Grain-grain interaction

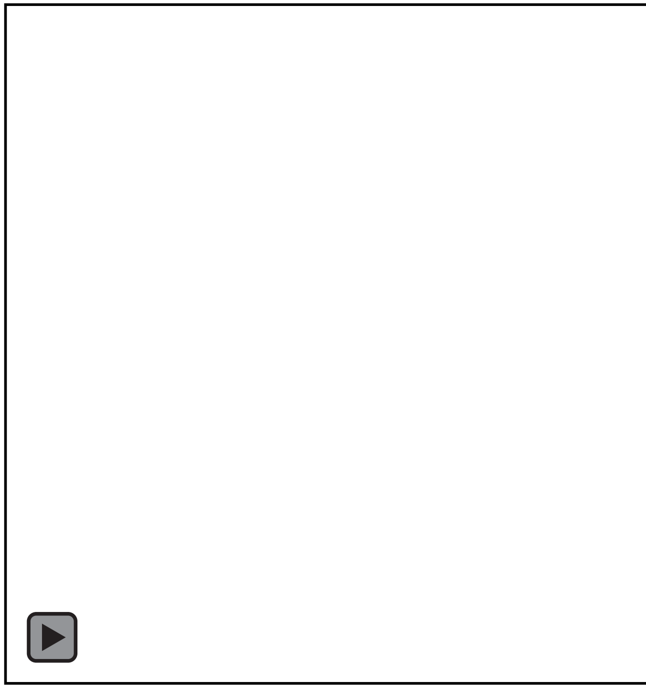


$$f^c = f_n^c + f_t^c$$

f_n^c : Hertzian

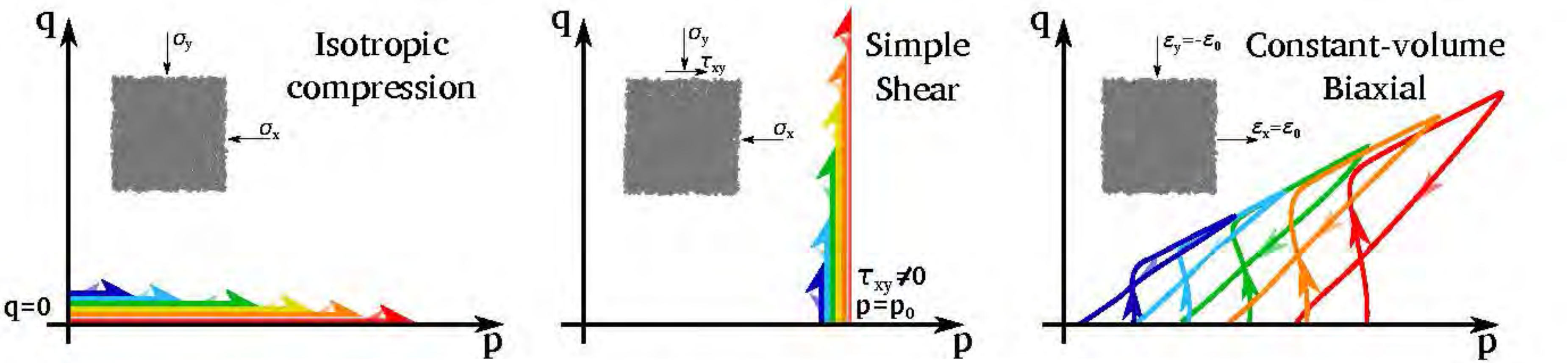
f_t^c : Coulomb

RVE generation

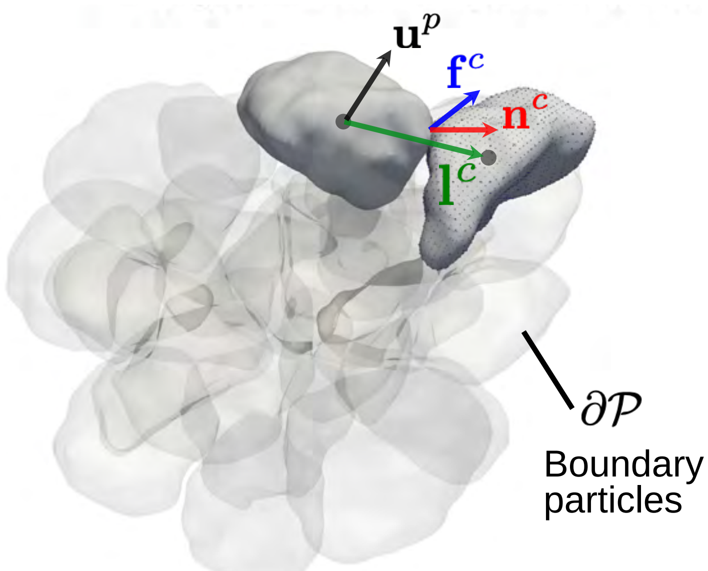


Kawamoto, R., Andò, E., Viggiani, G., Andrade, J.E., *JMPS*, **91** (2016) 1-13.

Hastun angular sand – Path sampling



Selected paths for building the material data repository



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

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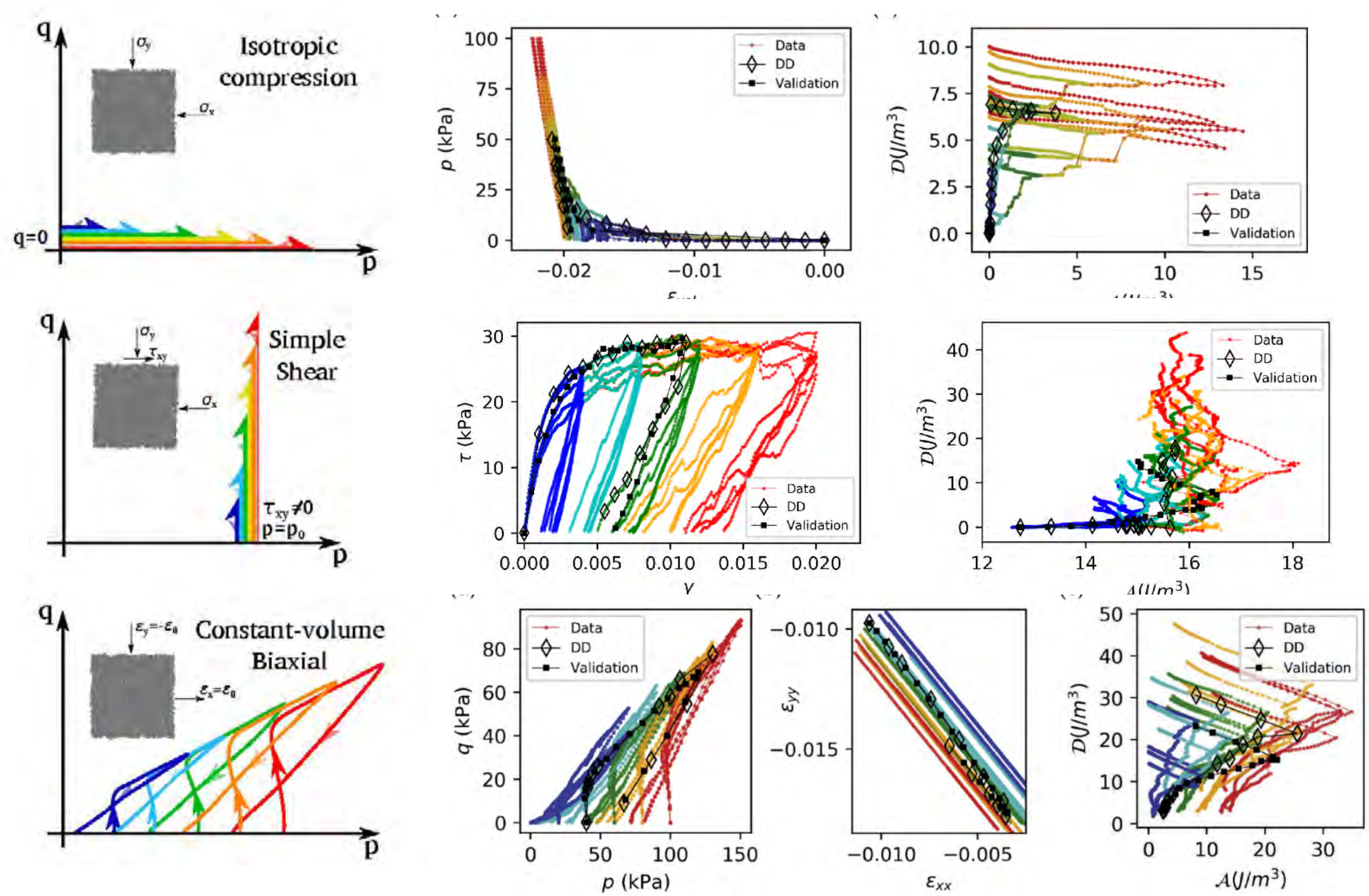
Hastun angular sand – Path sampling

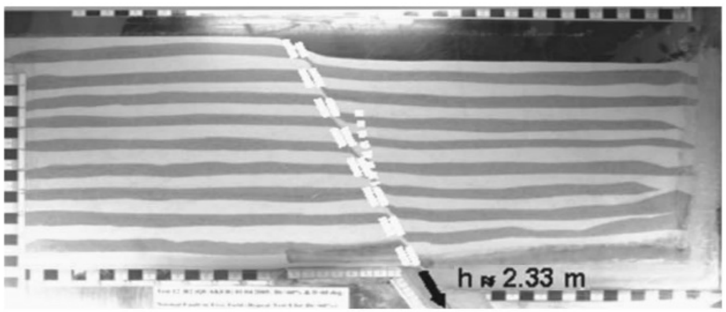


path | stress-strain | energy-dissipation

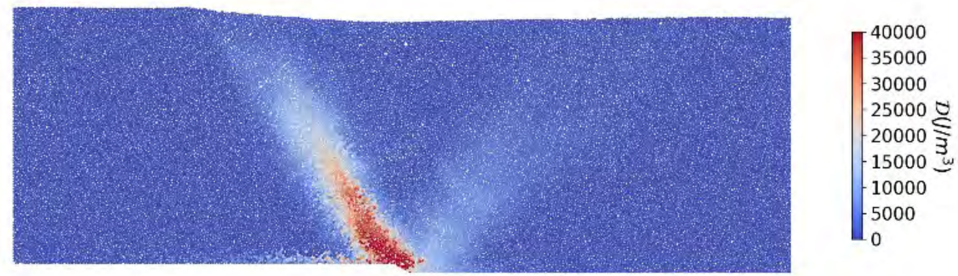
Compilation of path data for Hatsun angular sand computed from RVEs using LS-DEM

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

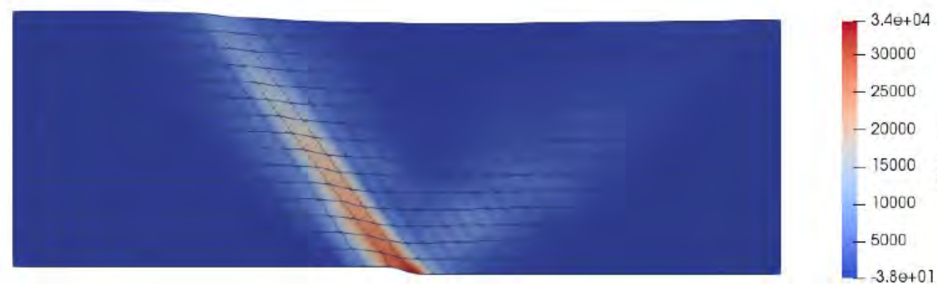
Sand mechanics – Fault rupture experiment



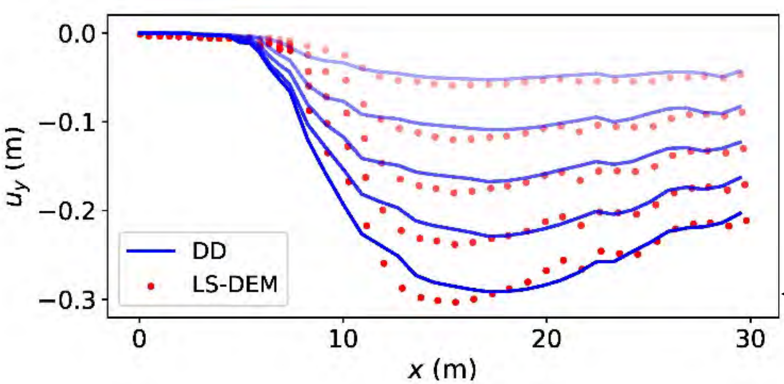
Experimental fault rupture experiment



LS-DEM simulation



Data-Driven simulation

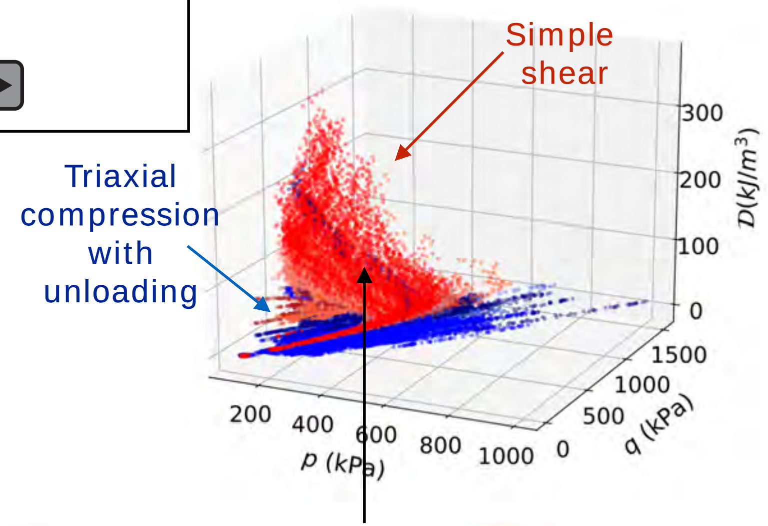


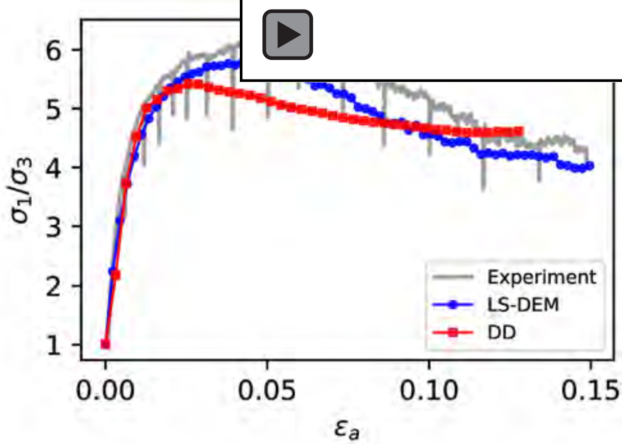
Evolution of surface settlement LS-DEM *vs*. DD simulations

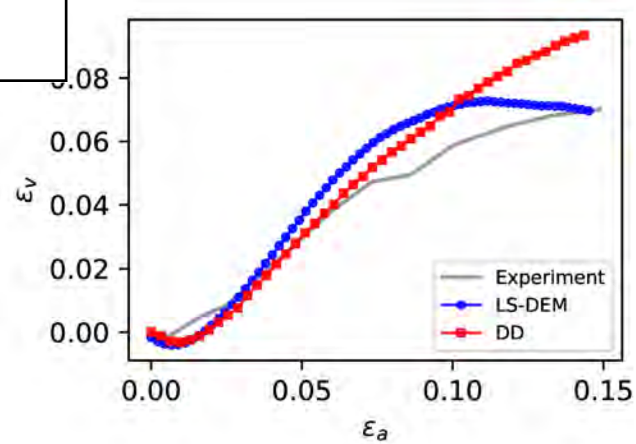
Anastasopoulos, I., *et al*., *J. Geotech. Geoenviron. Eng*., **133** (2007) 943–958.
K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

Data-Driven – Fault rupture experiment

LS-DEM





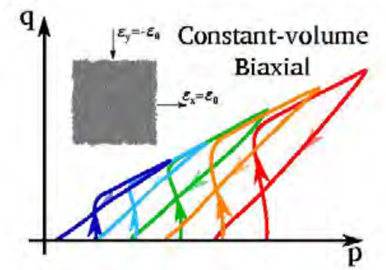


K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

Michael Ortiz
Polimi 10/19/21

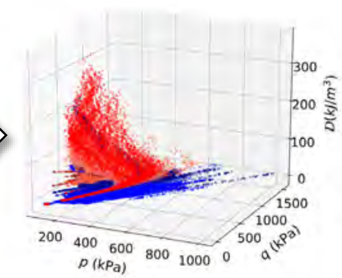
Path selection, coverage, convergence

- Path coverage must be ***goal oriented*** (tailored to specific problems, cannot sample entire path-space)
- ***Main path types*** are often known beforehand for specific problems (initial path-data repository)
- DD is ***self-correcting*** (reinforcement learning):

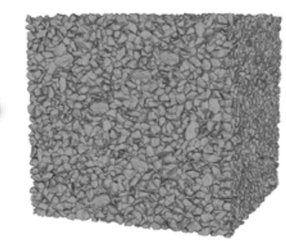


Initial path-data repository

Application, DD analysis



Monitor actual local paths at material points

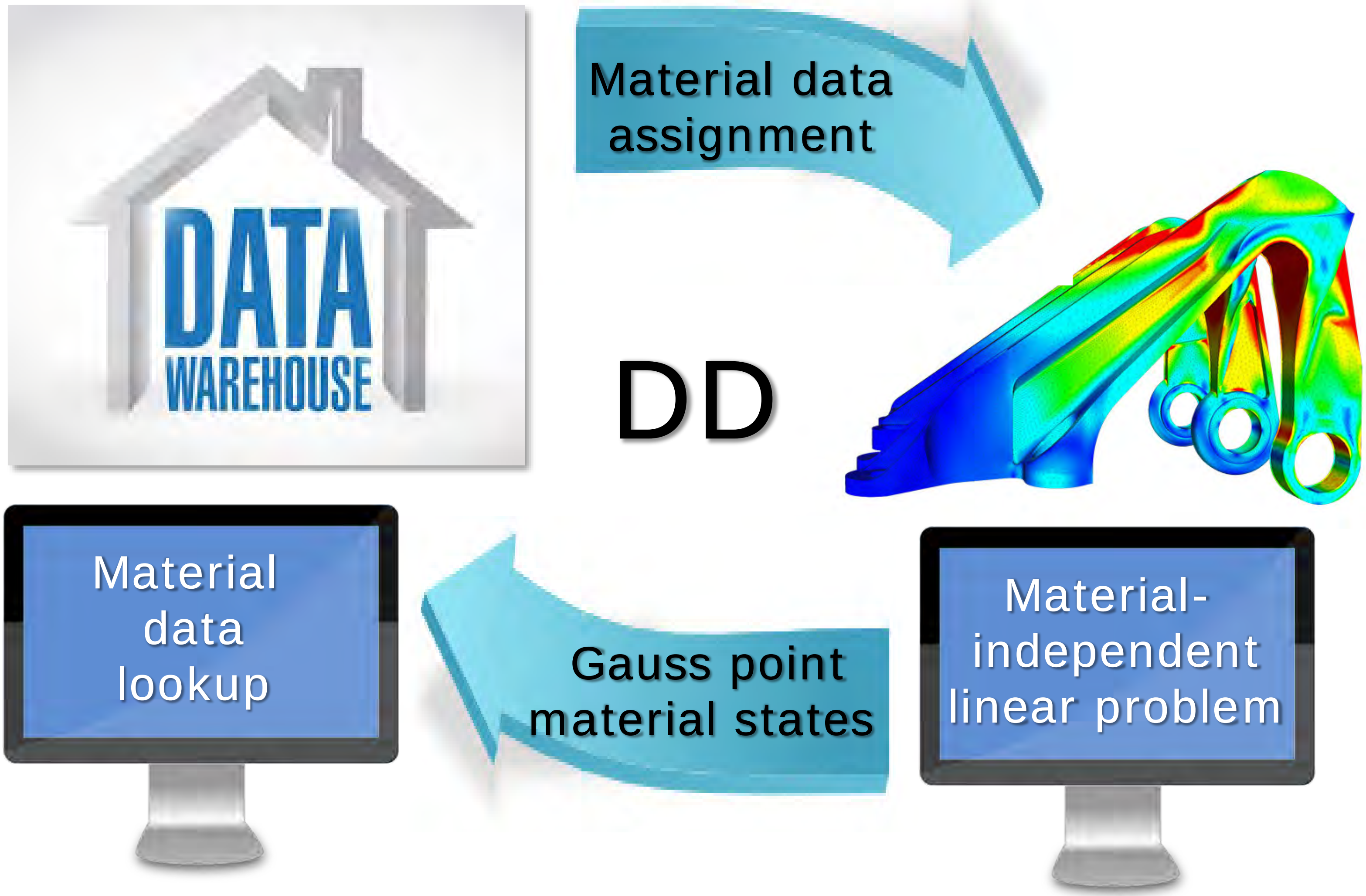


Generate RVE data if distance to repository > TOL

Iterate to convergence

K. Karapiperis, PhD dissertation, Caltech (2021)
A. Platzer, PhD dissertation, École Central Nantes (2020)

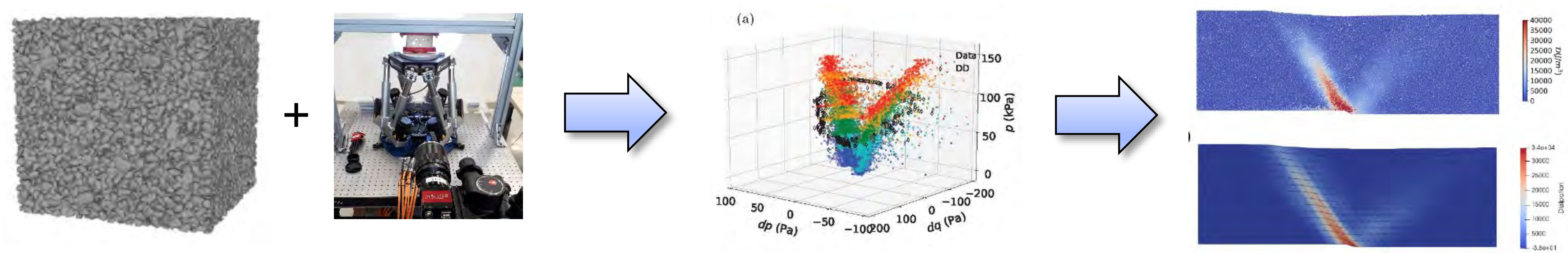
Concluding remarks



The Data-Driven information flow

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!