universitätbonn

Model-Free Data-Driven Science: Cutting out the Middleman

$$\inf_{y \in D} \inf_{z \in E} \|y - z\| = \inf_{z \in E} \inf_{y \in D} \|y - z\|$$

Michael Ortiz
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn
With: Sergio Conti and Stefan Müller (uni-Bonn)

Oberseminar "Mathematische Modelle“
Fakultät für Mathematik (M6)
Technische Universität München
Garching bei München, 21. April, 2021

Outline

- Background and motivation:
  - *New emerging paradigm: Data-Driven Science*
  - *How does Data Science intersect with the physical sciences? With experimental science?*
  - *Why Data-Driven science now? What has changed?*
  - *What are* Model-Free Data-Driven problems*?*
  - *Theory vs. practice: Solvers, fast search algorithms, set-oriented machine learning, data mining, data repositories, data management…*
- Analysis: *Data-Driven problems in elasticity*:
  - Existence and uniqueness of solutions
  - The topology of data convergence
  - Data-Driven relaxation
  - Extension to finite kinematics

The anatomy of field theories

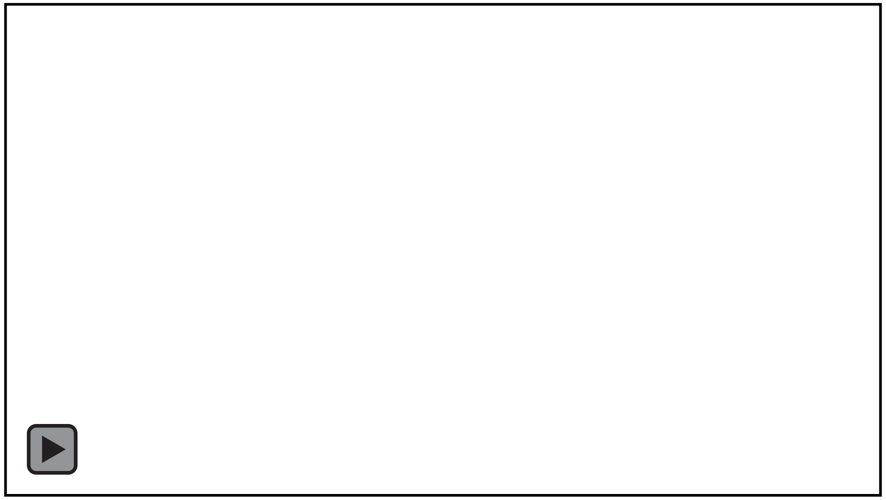
- Focus on problems in the *physical sciences* (as opposed to finance, marketing, social sciences…)
- Problems in the physical sciences deal with *field theories*
- All field theories have a *common structure*:

Field	Potential	Conservation	Material law
Gravitation	$g = -\nabla\phi$	$\nabla \cdot f + 4\pi\rho = 0$	$f = g/G$ (Newton)
Electrostatics	$E = -\nabla V$	$\nabla \cdot D = 4\pi\rho$	$D = \epsilon\, E$
Electromagnetics	$B = \nabla \times A$	$\nabla \times H = J$	$H = B/\mu$
Diffusion	$g = -\nabla c$	$\nabla \cdot J + s = 0$	$J = D\, g$ (Fick)
Heat transfer	$g = -\nabla T$	$\nabla \cdot J + s = 0$	$J = \kappa\, g$ (Fourier)
Elasticity	$\epsilon = \mathrm{sym}\nabla u$	$\nabla \cdot \sigma + f = 0$	$\sigma = \mathbb{C}\,\epsilon$ (Hooke)
General	$\epsilon = \delta u$	$\partial\sigma + f = 0$	??

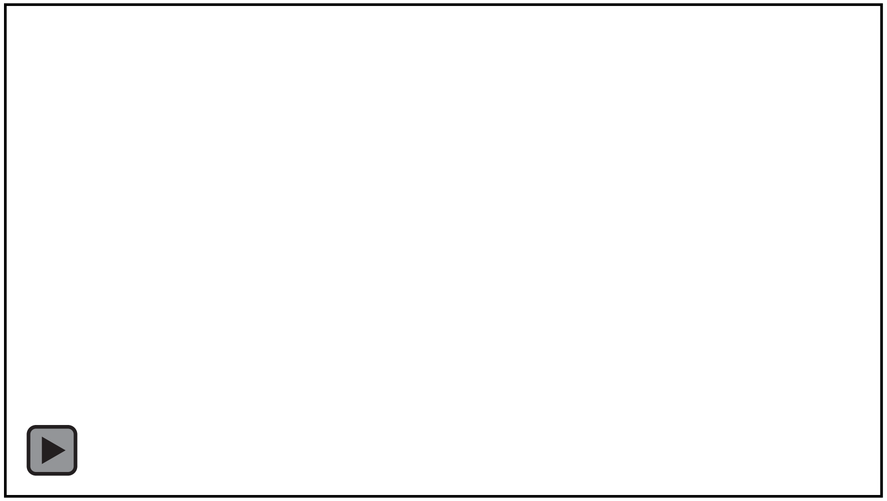
- Potential relations and conservation laws are *universal*!
- *Material laws need to be defined empirically!*

The new data-rich world…

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



3D tomographic reconstruction of particles in battery electrode

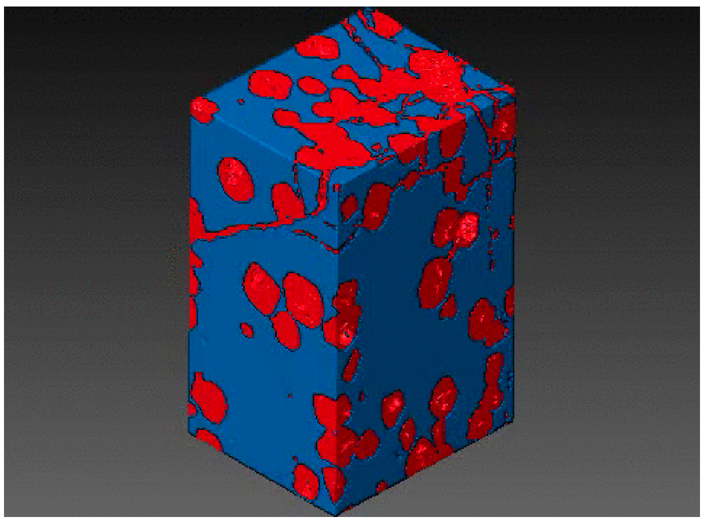


3D DIC-measured internal-strain full-field compressed PDMS sample

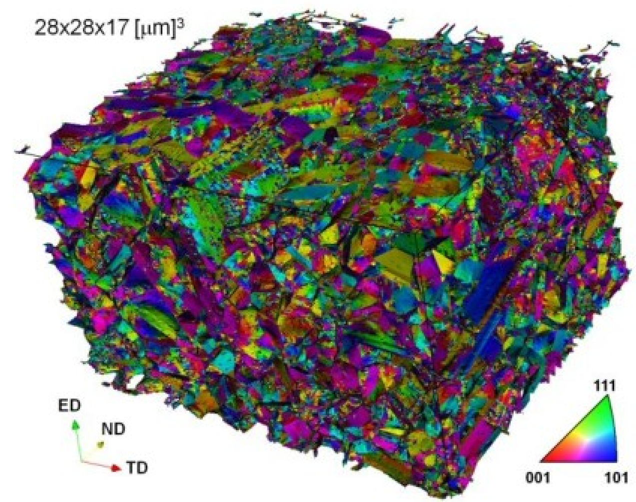
John Lambros, UIUC, https://lambros.ae.illinois.edu/moviesimages/

The new 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)



Two-phase μCT analysis of Ti2AlC/Al composite[1]



3D EBSD microstructure in Cu-0.17wt%Zr after ECAP[2]

[1]Hanaor *etal*, *Mater Sci Eng A*, **672** (2019) 247.
[2]Khorashadizadeh, *Adv Eng Mater*, **13** (2011) 237.

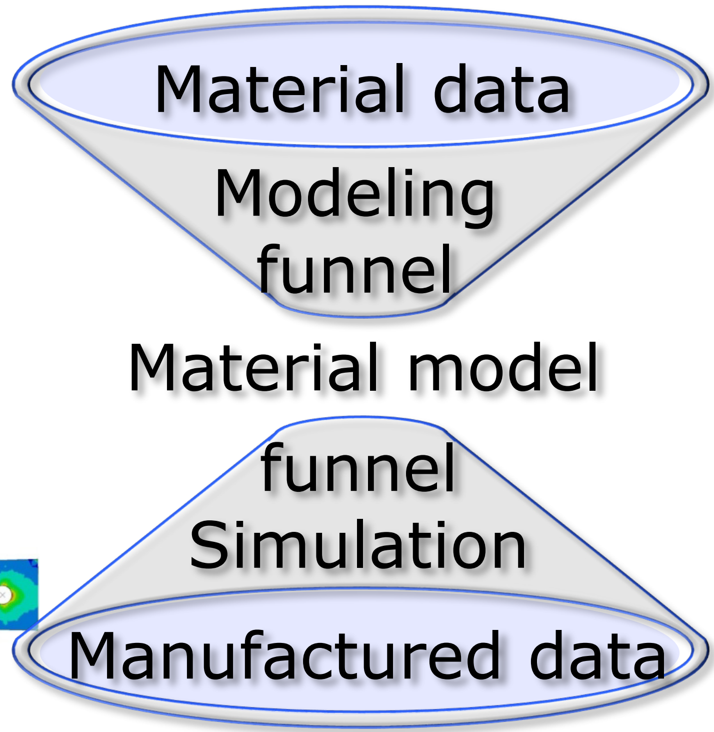
Michael Ortiz
TUM 2021

Adapting to a new data-rich world...

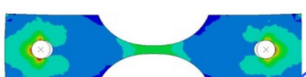
Classical Model-Based Computational Science...

Modern microscopy generates massive data sets

$$\sigma = \mathbb{C}\epsilon$$



Modelling entails massive loss of information!



Adapting to a new data-rich world...

- *Modeling* = Any operation that changes the data set
- Modeling usually entails *massive loss of information* from material data sets, *epistemic uncertainty…*
- Material modeling is *ad hoc, open ended, ill-posed*
- There is *no theory* that determines material models from first principles to a desired level of accuracy
- Modeling requires *heuristics and intuition*: Models are *only as good as the modeler*'s physical intuition
- Example of modeling: *Deep Learning = piecewise-linear regression* (cf., e.g., Gilbert Strang, 2019), requires *ad hoc guessing* of effective variables (a.k.a. 'features')
- *Direct connection between data and prediction*? Goal:

$$\begin{array}{rl} \text{Classical inference:} & \text{Data} \;\rightarrow\; \text{Model} \;\rightarrow\; \text{Prediction} \\ \text{Model-Free Data-Driven inference:} & \text{Data} \;\longrightarrow\; \text{Prediction} \end{array}$$

(cut out the middleman!)

Adapting to a new data-rich world...

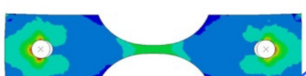
Classical Model-Based Computational Science...

Alternative: Model-Free Data-Driven Computing!

Modern microscopy generates massive data sets

$\sigma = \mathbb{C}\epsilon$

Modelling entails massive loss of information!



Material data

Modeling funnel

Material model

funnel

Simulation

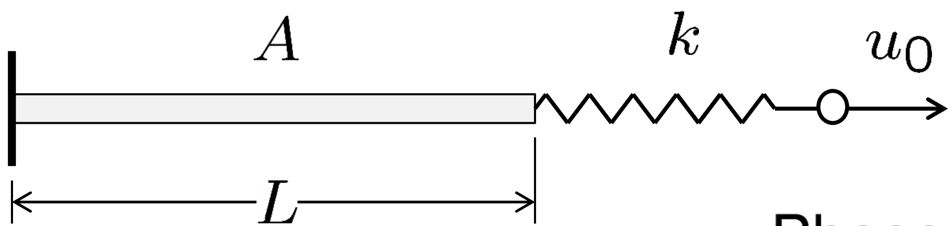
Manufactured data

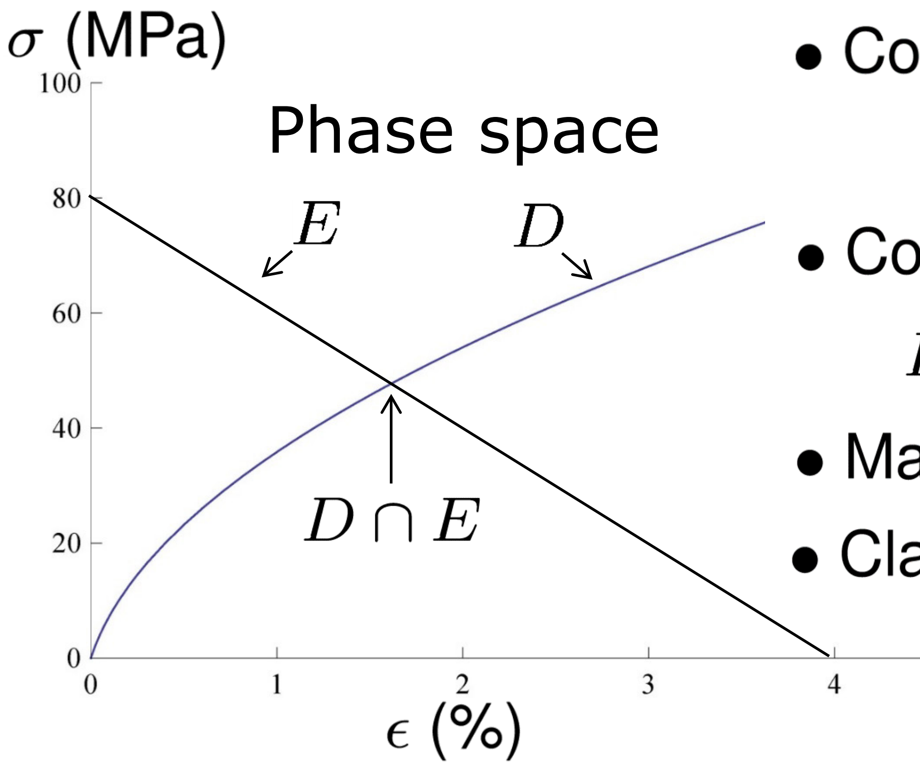
Set/solve problems directly from data!

Eliminate modeling bottleneck!

How?

Elementary example: Bar and spring





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

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

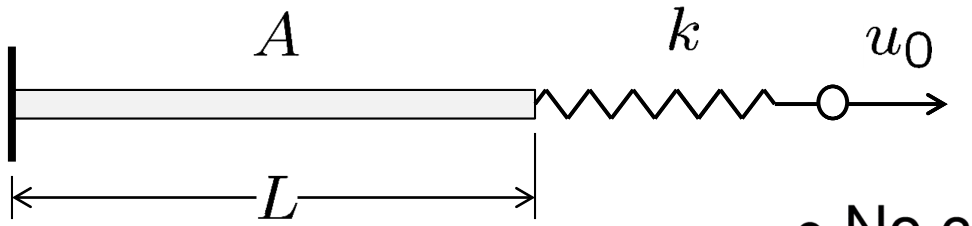
- Constraint set:

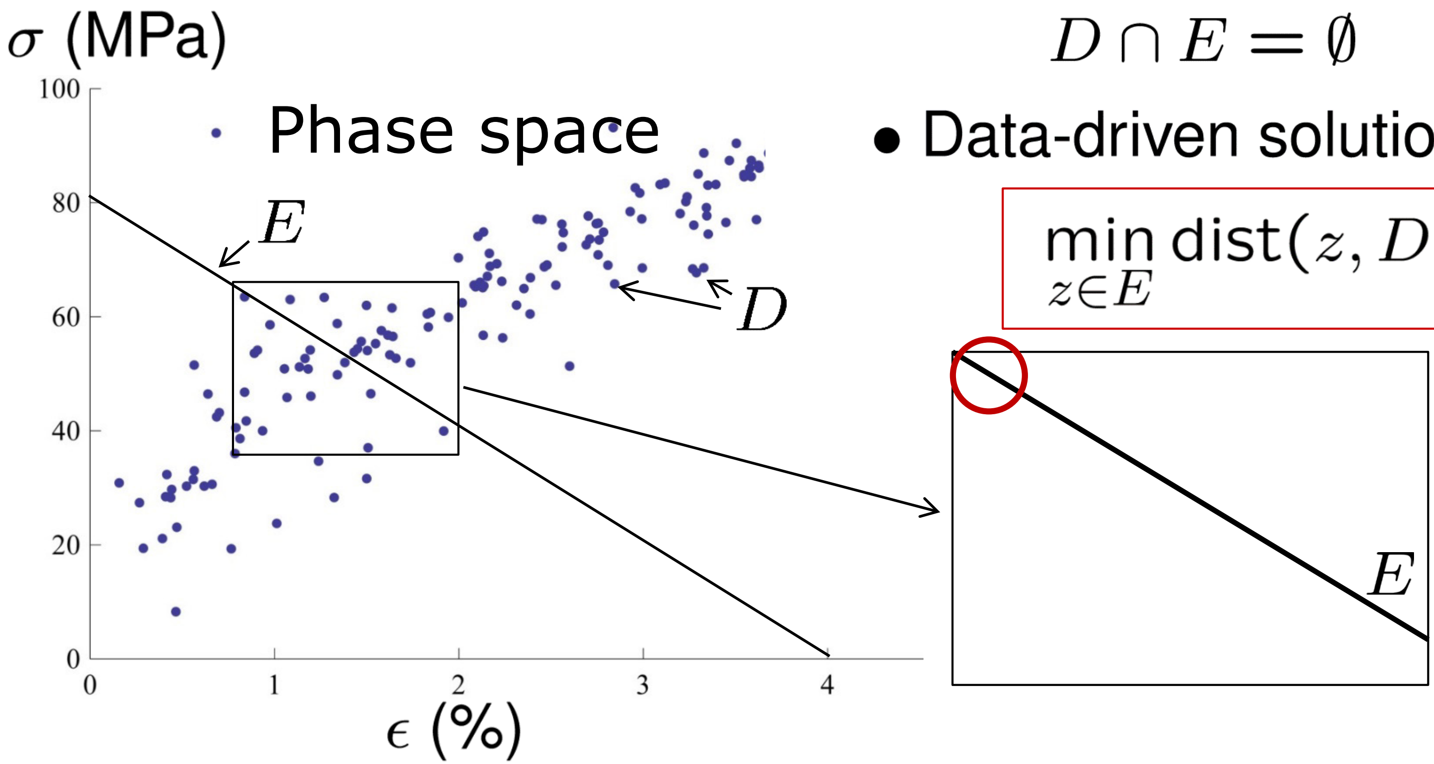
$$E = \{\sigma A = k(u_0 - \epsilon L)\}$$

- Material data set: $D \subset Z$
- Classical solution set: $D \cap E$

Michael Ortiz
TUM 2021

Elementary example: Bar and spring





- No classical solutions!

$$D \cap E = \emptyset$$

- Data-driven solution:

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

Michael Ortiz
TUM 2021

Model-Free Data-Driven paradigm

- The *Model-Free Data-Driven paradigm*[1]: Given,
  - *D = {fundamental material data},*
  - *E = {compatibility + equilibrium},*

$$\inf_{y\in D}\inf_{z\in E}\|y-z\| = \inf_{z\in E}\inf_{y\in D}\|y-z\|$$

- *Aim of Model-Free Data-Driven problems is to find the admissible state (compatibility and equilibrium) in phase space (stress, strain) closest to the material data set*
- Raw *fundamental material data* (stress *and* strain) is used (unprocessed) in the formulation of the problems
- *No material modeling, no biasing, no loss of information:*

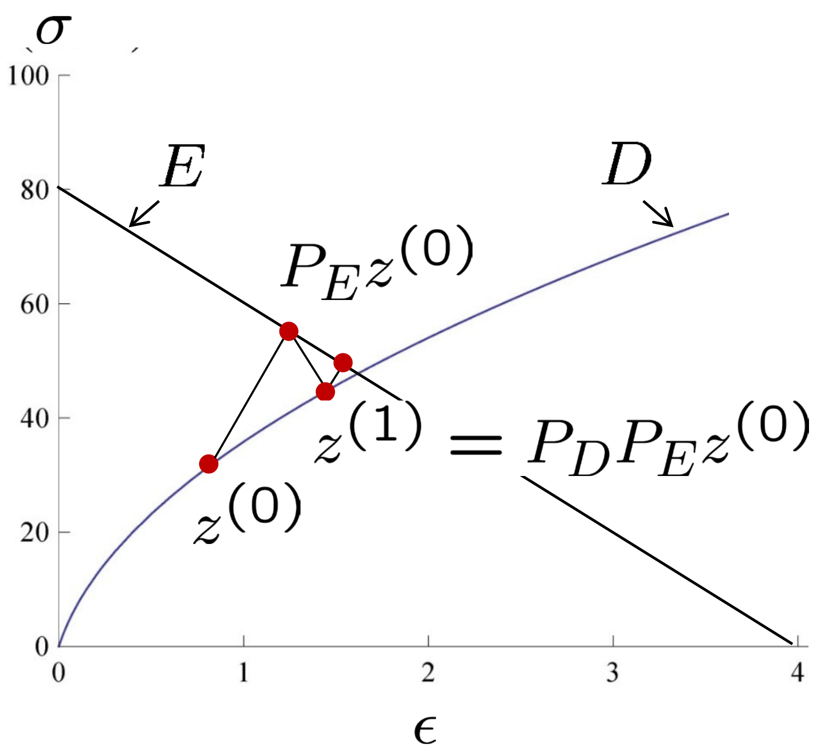
  The data, all the data, nothing but the data!

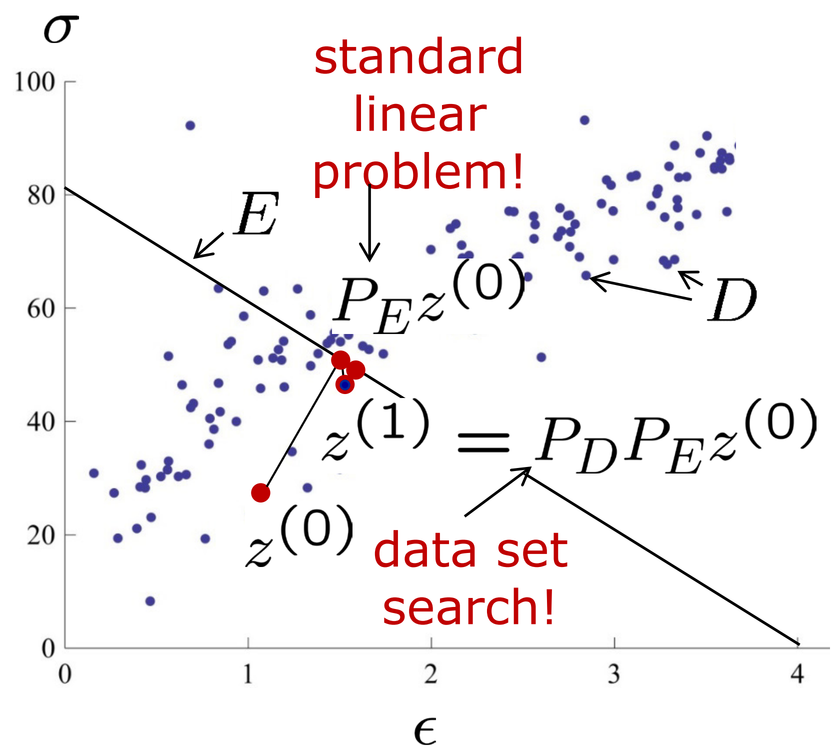
[1]T. Kirchdoerfer and M. Ortiz (2015) arXiv:1510.04232.
[1]T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

Michael Ortiz
TUM 2021

DD solvers: Fixed-point iteration

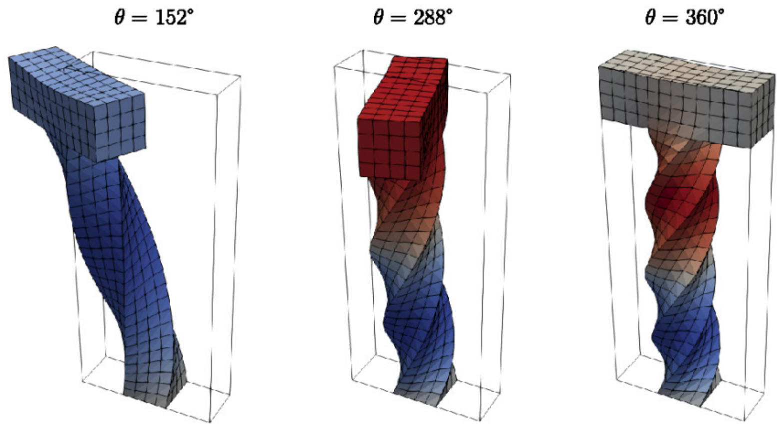
- Closest-point projections to E and D: $P_E,\ P_D$
- *Fixed-point iteration*: $z^{(k+1)} = P_E P_D\, z^{(k)}$



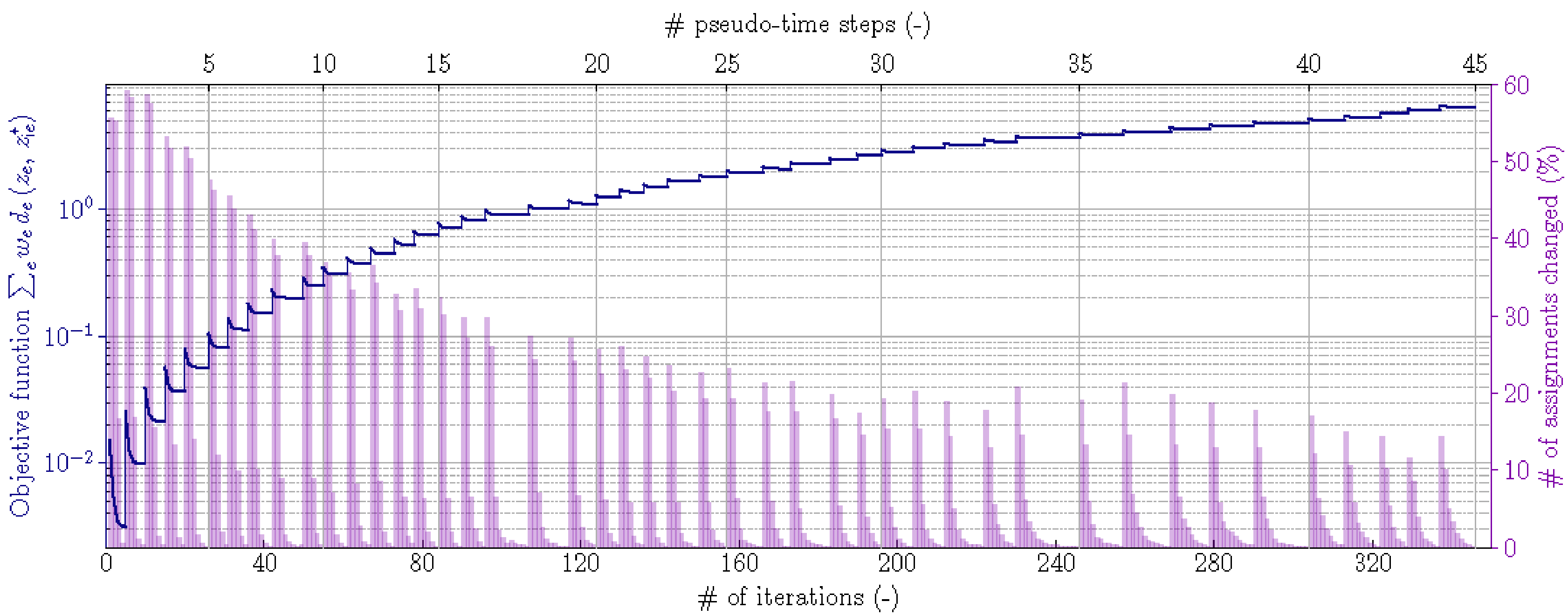


[1]T. Kirchdoerfer and M. Ortiz (2015) arXiv:1510.04232.
[1]T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

DD solvers: Fixed-point iteration



- Twisting of isotropic-elastic rod
- Randomized Green-Saint Venant
- 10,000,000 data points
- Linear convergence of fixed-point iteration wrt number of iterations
- Convergence with respect to data set size (uniform approximation)

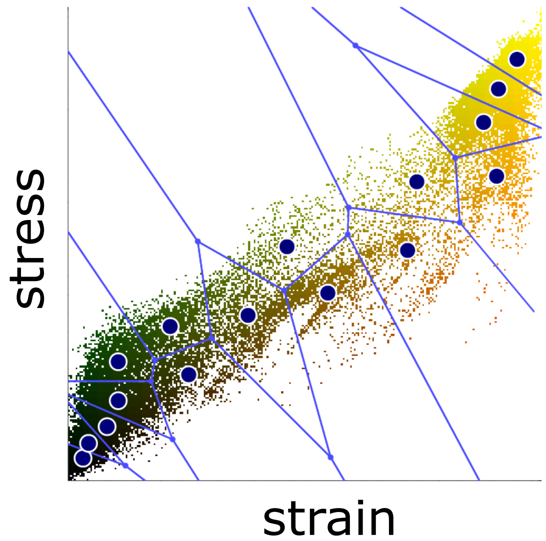


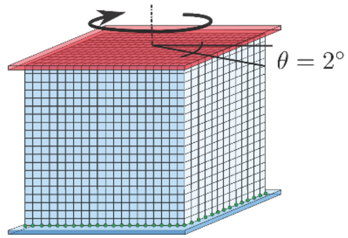
A. Platzer, Doctoral Thesis, Ecole Centrale de Nantes, 2020.

z

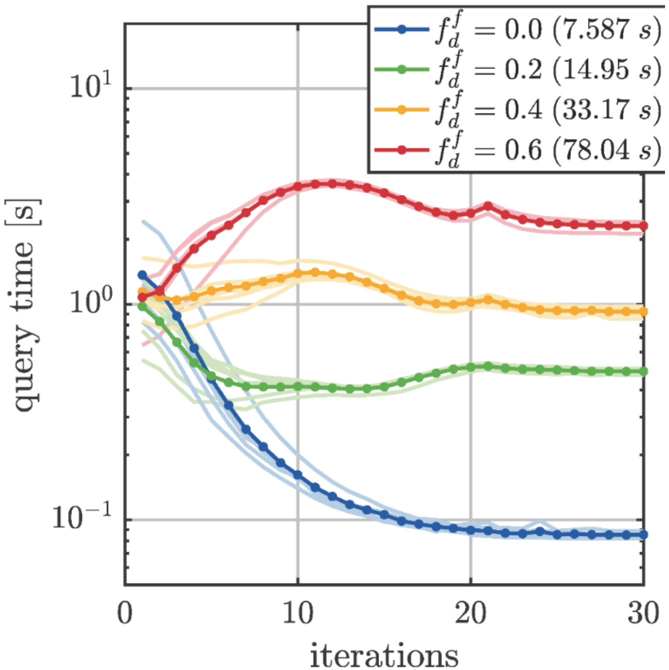
TUM 2021

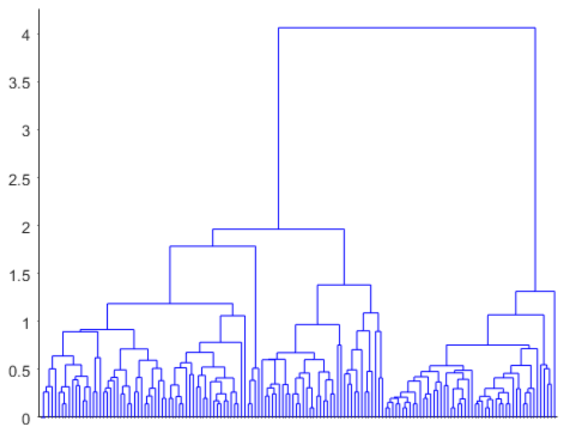
Connection with Machine Learning





Test problem:
Torsion of
20x20x20 cube
64000 mat pts





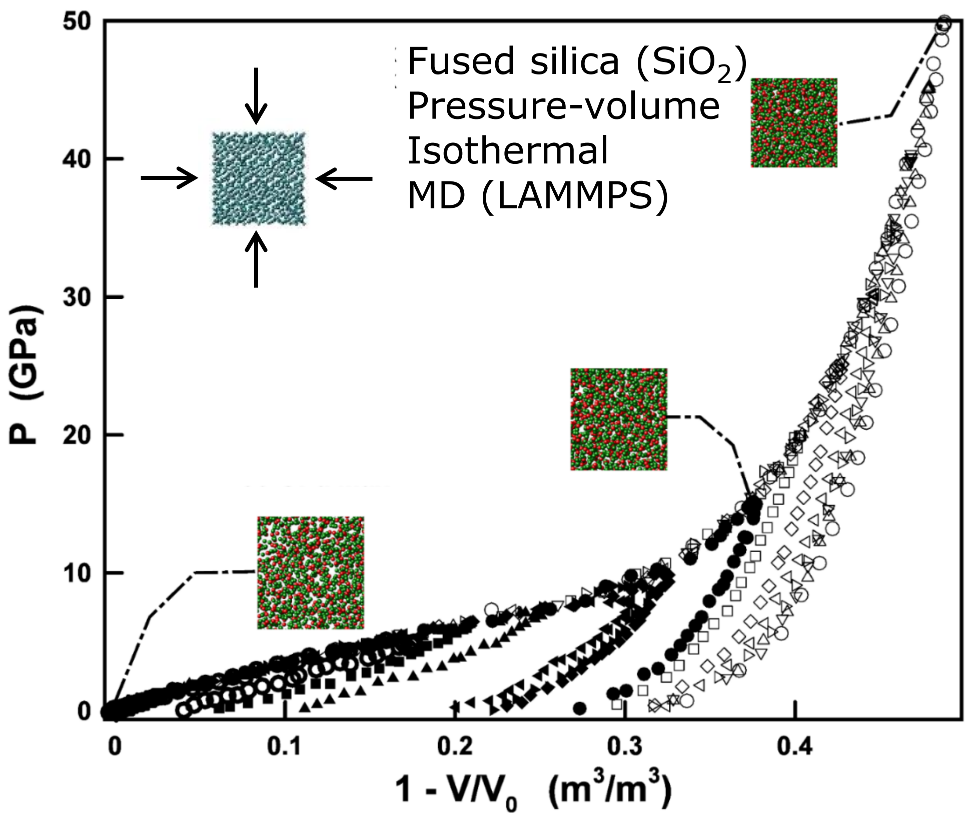
K-means hierarchical structure

- 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!*
- *The data, all the data, nothing but the data!*

Michael Ortiz
TUM 2021

Connection with multiscale analysis

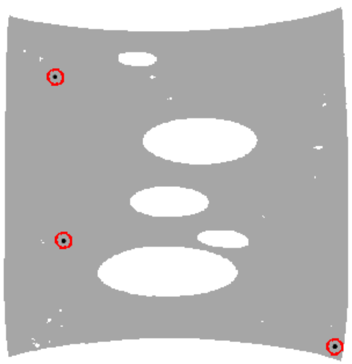
- Generate *material data* from microscale *RVE calculations*
- *Upscale data directly to macroscale* (*no effective model!*)

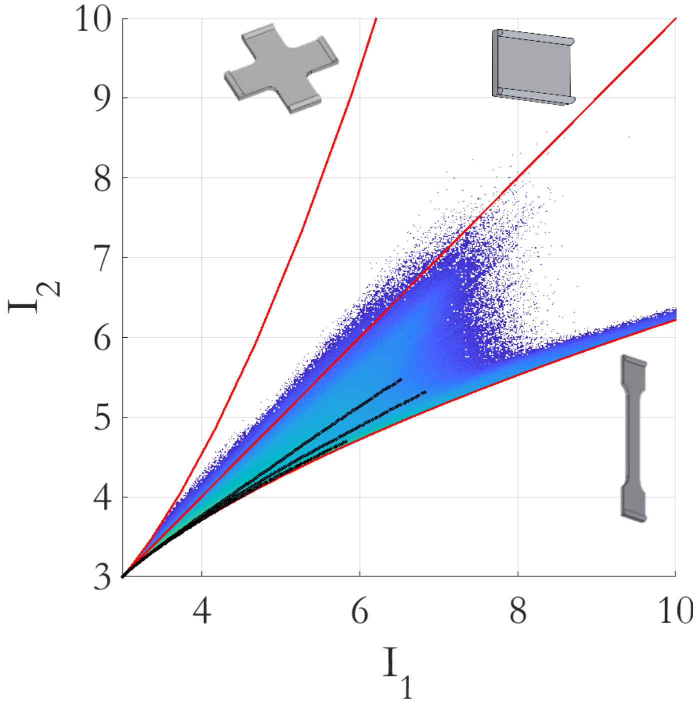


Schill, W., Heyden, S., Conti, S. and Ortiz, M., JMPS (2017) 113.

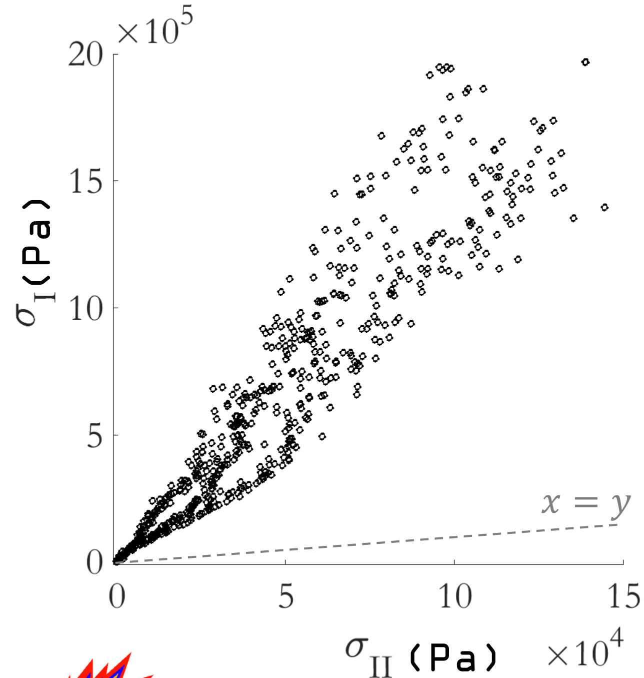
Connection with experimental science

- Generate full-field microscopy data using DIC
- *Infer stresses from inverse Data-Driven problem!*





Strain data



Stress data

M. Dalémat, M. Coret, A. Leygue and E. Verron, *Mechanics of Materials*, **136** (2019) 103087.

Michael Ortiz
TUM 2021

Data-Driven problems – Analysis

Problem (General Data-Driven problem)

Given:

- *Phase space* $\mathcal{Z}$ *(determined by field equations)*
- *Material-data set* $\mathcal{D} = \{y \in \mathcal{Z} : \text{observed}\}$ *(measured, ab initio)*
- *Constraint set* $\mathcal{E} = \{z \in \mathcal{Z} : \text{field equations}\}$ *(from field theory)*

Minimize: $d(z, \mathcal{D}) + I_{\mathcal{E}}(z)$, *or* $d^2(y, z) + I_{\mathcal{D}}(y) + I_{\mathcal{E}}(z)$

- Well-posedness? (existence, uniqueness)
- Convergence with respect to data?
- Relaxation, weak convergence?
- Extension to finite kinematics?

Conti, S., Müller, S. & MO. Data-Driven Problems in Elasticity. *ARMA* **229,** 79–123 (2018).
Conti, S., Müller, S. & MO. Data-Driven Finite Elasticity. *ARMA* **237,** 1–33 (2020).

Data-Driven (small-strain) elasticity

$\Omega \subset \mathbb{R}^n$ open, bounded, Lipschitz boundary
$\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, Γ_D, Γ_N sufficiently regular, $\mathcal{H}^{n-1}(\Gamma_D) \neq 0$

Phase space: $\mathcal{Z} = \{(\epsilon, \sigma) \, : \, \epsilon \in L^2(\Omega, \mathbb{R}^{n\times n}_{\rm sym}), \; \sigma \in L^2(\Omega, \mathbb{R}^{n\times n}_{\rm sym})\}$

Constraint set $\mathcal{E} \subset \mathcal{Z}$ consists of pairs (ϵ, σ) which satisfy:

i) Compatibility: $\epsilon = 1/2(Du + Du^T)$, $\quad u = g$ on Γ_D.
ii) Equilibrium: $\operatorname{div} \sigma + f = 0$, $\quad \sigma\nu = h$ on Γ_N.

Material data set $\mathcal{D} = \{(\epsilon, \sigma) \in \mathcal{Z} \, : \, (\epsilon(x), \sigma(x)) \in \mathcal{D}_{\rm loc}$ a. e.$\}$
Hooke's law: $\mathcal{D}_{\rm loc} = \{(\epsilon, \sigma) \in \mathcal{Z}_{\rm loc} = \mathbb{R}^{n\times n}_{\rm sym} \times \mathbb{R}^{n\times n}_{\rm sym} \, : \, \sigma = \mathbb{C}\epsilon\}$

Distance on $\mathcal{Z}$, $d(y, z) = \|y - z\|$,

$$\|z\|^2 = \int_\Omega \frac{1}{2}\Big(\mathbb{C}\epsilon \cdot \epsilon + \mathbb{C}^{-1}\sigma \cdot \sigma\Big)\, dx, \quad z = (\epsilon, \sigma), \quad \mathbb{C} > 0$$

NB: *Universal field equations* and *material-specific data* (field-theories of physics, rational mechanics, Truesdell, Noll, . . . , Tartar'70s)

Classical solutions are subsumed within DD solutions

Theorem

Assume: $f \in L^2(\Omega; \mathbb{R}^n)$, $g \in H^{1/2}(\partial\Omega; \mathbb{R}^n)$, $g \in H^{-1/2}(\partial\Omega; \mathbb{R}^n)$. *Let* $\mathcal{E}$ *be the constraint set and let*

$$\mathcal{D} = \{(\epsilon, \sigma) \in \mathcal{Z} \, : \, \sigma(x) = \mathbb{C}\epsilon(x), \text{ a. e.}\}, \quad \mathbb{C} > 0,$$

be the material data set for Hooke's law. Then, the Data-Driven problem

$$\min\{d(z, \mathcal{D}), \; z \in \mathcal{E}\},$$

has a unique solution in $\mathcal{Z}$*. Furthermore, the Data-Driven solution satisfies*

$$\sigma = \mathbb{C}\epsilon.$$

NB: Similarly for $\mathcal{D}_{\rm loc} = \{(\epsilon, \sigma) \in \mathcal{Z}_{\rm loc} \, : \, \sigma = \hat{\sigma}(\epsilon)\}$ with $\hat{\sigma}$ uniformly monotone (using div-curl Lemma of Murat-Tartar)

Classical solutions are subsumed within DD solutions

Distance identity: $d^2(z,\mathcal{D}) = \int_\Omega \frac{1}{4}\mathbb{C}^{-1}(\sigma - \mathbb{C}\epsilon)\cdot(\sigma - \mathbb{C}\epsilon)\,dx.$

Lemma (Power identity)

$$(\epsilon,\sigma)\in\mathcal{E} \Rightarrow \int_\Omega \sigma(x)\cdot\epsilon(x)\,dx = \int_\Omega f(x)\cdot u(x)\,dx +$$
$$\int_{\Gamma_D} \sigma(x)\nu(x)\cdot g(x)\,d\mathcal{H}^{n-1}(x) + \int_{\Gamma_N} h(x)\cdot u(x)\,d\mathcal{H}^{n-1}(x).$$

Lemma (Tensor Helmholtz decomposition)

$$M = \{e(u),\ u\in H^1(\Omega;\mathbb{R}^n),\ u=0 \textit{ on } \Gamma_D\}\ ,$$
$$N = \{\sigma\in L^2(\Omega;\mathbb{R}^{n\times n}_{\rm sym}),\ \operatorname{div}\sigma = 0,\ \sigma\nu = 0 \textit{ on } \Gamma_N\}\ ,$$

are strongly (and weakly) closed in $L^2(\Omega,\mathbb{R}^{n\times n}_{\rm sym})$, $L^2(\Omega;\mathbb{R}^{n\times n}_{\rm sym}) = M\oplus N$ *and the decomposition is orthogonal.*

Classical solutions are subsumed within DD solutions

Proof.

Apply direct method of the CoV to $F(z) = d^2(z, \mathcal{D}) + I_{\mathcal{E}}(z)$.

i) *Lower-semicontinuity:* By the tensor Helmholtz decomposition lemma and Hahn-Banach, $\mathcal{E}$ is weakly closed in $\mathcal{Z}$ and $I_{\mathcal{E}}(z)$ is weakly lower-semicontinuous. By the convexity of $\mathcal{D}$, $d^2(z, \mathcal{D})$ is also weakly lower-semicontinuous in $\mathcal{Z}$.

ii) *Compactness:* With $z = (\epsilon, \sigma)$, we have the identity

$$\|z\|^2 = 2d^2(z, \mathcal{D}) - \int_\Omega \sigma \cdot \epsilon \, dx$$

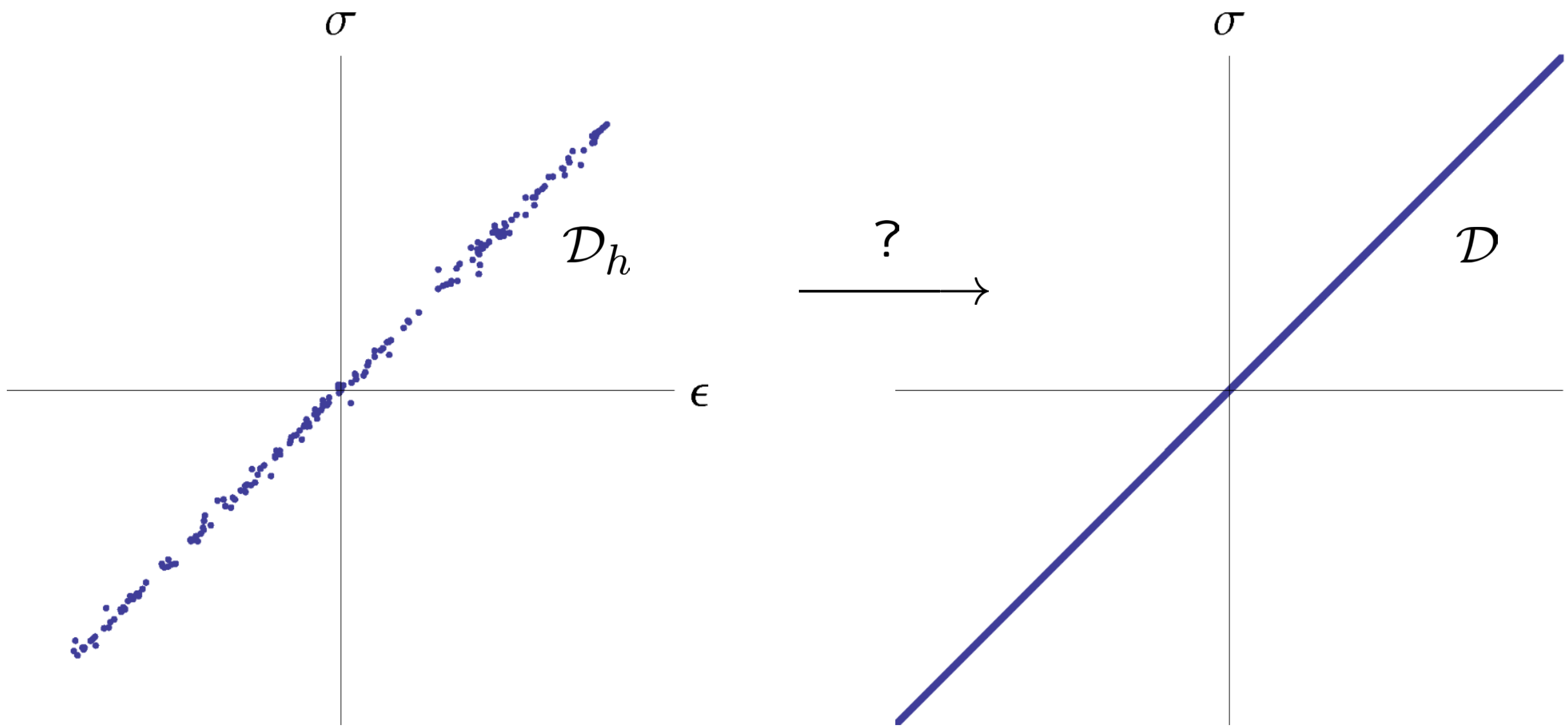
By the power identity, Korn, Poincaré and trace theorems, with $z \in \mathcal{E}$,

$$\|z\|^2 \leq 2d^2(z, \mathcal{D}) + C\|z\| \Rightarrow \text{coercivity}$$

iii) *Uniqueness* follows from convexity and $\sigma = \mathbb{C}\epsilon$ from the Euler-Lagrange equations.

$\square$

The topology of data convergence



- We are given a *sequence* of material data sets (sampling)
- The sequence *approximates* a *limiting material data set*
- What *topology of convergence* of material data sets ensures convergence of the corresponding Data-Driven solutions?
- *Two cases*: Limiting material data set is: i) weakly closed; ii) not weakly closed.

Michael Ortiz
TUM 2021

The topology of data convergence

Definition (Mosco convergence of functions and sets)

A sequence (F_h) of functions from a Banach space X to $\overline{\mathbb{R}}$ converges to $F : X \to \overline{\mathbb{R}}$ in the sense of Mosco, or $F = M\!-\lim_{h\to\infty} F_h$, if

i) For every sequence (x_h) converging weakly to x in X, $\liminf_{h\to\infty} F_h(x_h) \geq F(x)$.

ii) For every $x \in X$, there is a sequence (x_h) converging strongly to x in X such that $\lim_{h\to\infty} F_h(x_h) = F(x)$.

A sequence $(\mathcal{E}_h)$ of subsets of X converges to $\mathcal{E} \subset X$ in the sense of Mosco, or $\mathcal{E} = M\!-\lim_{h\to\infty} \mathcal{E}_h$, if $I_{\mathcal{E}} = M\!-\lim_{h\to\infty} I_{\mathcal{E}_h}$.

Lemma

Every Mosco limit functional F is weakly sequentially lower semicontinuous. In particular, every Mosco limit set $\mathcal{E}$ is weakly sequentially closed and $\mathcal{E} = M\!-\lim_{h\to\infty} \mathcal{E}$ if and only if $\mathcal{E}$ is weakly sequentially closed.

The topology of data convergence

Theorem

Let Z be a reflexive, separable Banach space, $\mathcal{D}$ and $(\mathcal{D}_h)$ subsets of Z, $\mathcal{E}$ a weakly sequentially closed subset of Z. Suppose:

i) *(Mosco convergence)* $\mathcal{D} = M-\lim_{h\to\infty} \mathcal{D}_h$ *in* Z.

ii) *(Equi-transversality) There are constants* $c > 0$ *and* $b \geq 0$ *such that, for all* $y \in \mathcal{D}_h$ *and* $z \in \mathcal{E}$,

$$\|y - z\| \geq c(\|y\| + \|z\|) - b.$$

Then, $I_{\mathcal{E}}(\cdot) + d^2(\cdot, \mathcal{D}) = \Gamma-\lim_{h\to\infty} \Big(I_{\mathcal{E}}(\cdot) + d^2(\cdot, \mathcal{D}_h) \Big)$, *with respect to the weak topology of* Z.

NB Mosco convergence supplies the right topology for sequences of material data sets when the limiting set is weakly continuous.

The topology of data convergence

Proof.

i) *Equi-coercivity*. With $F_h(z) = I_{\mathcal{E}}(z) + d^2(z, \mathcal{D}_h)$, by transversality,

$$\sqrt{F_h(z)} \geq I_{\mathcal{E}}(z) + \inf_{y \in \mathcal{D}_h} \|z - y\| \geq \inf_{y \in \mathcal{D}_h} c(\|y\| + \|z\|) - b \geq c\|z\| - b.$$

ii) *Limsup inequality*. Let $z \in \mathcal{E}$. By lemma, $\mathcal{D}$ is weakly closed and $d(z, \mathcal{D}) = \|y - z\|$. By Mosco, there is $y_h \to y$, $y_h \in \mathcal{D}_h$. Hence,

$$\limsup_{h \to \infty} d(z, \mathcal{D}_h) \leq \limsup_{h \to \infty} \|z - y_h\| \leq \|z - y\| = d(z, \mathcal{D}).$$

iii) *Liminf inequality*. Let $z_h \rightharpoonup z$, can take $z_h \in \mathcal{E}$. Let $y_h \in \mathcal{D}_h$ s. t. $\lim_{h \to \infty} d^2(z_h, \mathcal{D}_h) = \lim_{h \to \infty} \|y_h - z_h\|^2$. By equi-transversality and Mosco, there is $y \in \mathcal{D}$ s. t. $y_h \rightharpoonup y$. Hence,

$$\liminf_{h \to \infty} F_h(z_h) = \liminf_{h \to \infty} \|z_h - y_h\|^2 \geq \|z - y\|^2 \geq d^2(z, \mathcal{D}) = F(z).$$

$\square$

The topology of data convergence

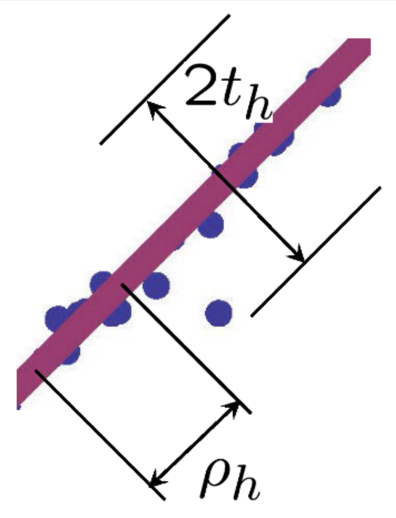
Theorem (Uniform approximation)

Suppose that $\mathcal{D}_h = \{z \in Z \,:\, z(x) \in \mathcal{D}_{\text{loc},h}$ *a. e. in* $\Omega\}$, *for some sequence of local material data sets* $\mathcal{D}_{\text{loc},h} \subset \mathbb{R}^{n\times n}_{\text{sym}} \times \mathbb{R}^{n\times n}_{\text{sym}}$. *Let* $\mathcal{D} = \{z \in Z \,:\, z(x) \in \mathcal{D}_{\text{loc}}$ *a. e. in* $\Omega\}$, *where* $\mathcal{D}_{\text{loc}} = \{\sigma = \mathbb{C}\epsilon\}$. *Assume:*

i) *(Fine approximation) There is a sequence* $\rho_h \downarrow 0$ *such that* $d(\xi, \mathcal{D}_{\text{loc},h}) \leq \rho_h$, $\forall \xi \in \mathcal{D}_{\text{loc}}$.

ii) *(Uniform approximation) There is a sequence* $t_h \downarrow 0$ *such that* $d(\xi, \mathcal{D}_{\text{loc}}) \leq t_h$, $\forall \xi \in \mathcal{D}_{\text{loc},h}$.

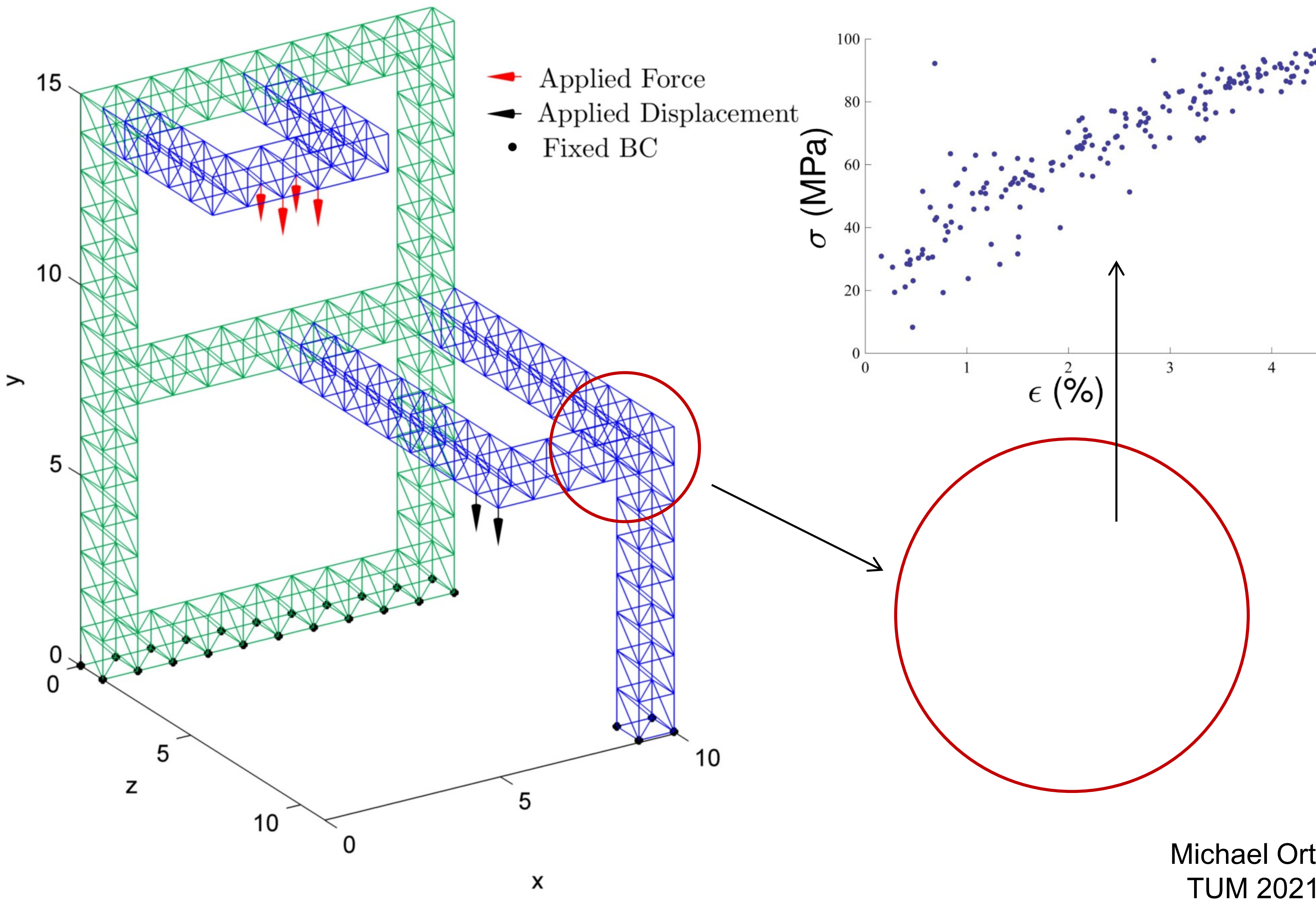
Then, $\mathcal{D} = M\!-\!\lim_{h\to\infty} \mathcal{D}_h$ *in* Z.



Proof.

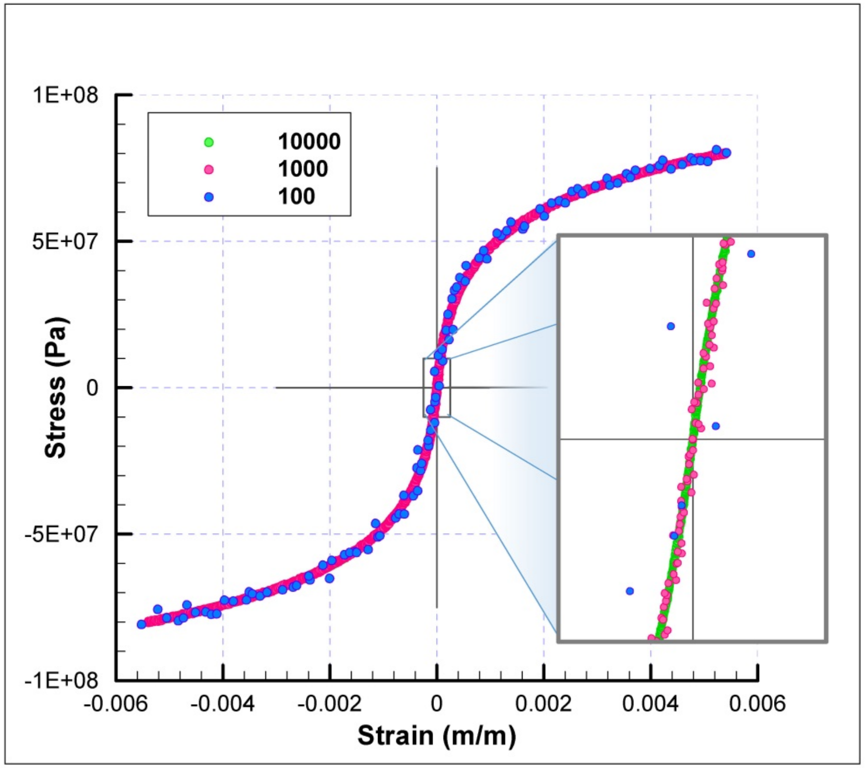
Equi-coercivity from (ii) and coercivity of the limit.
Lower bound from weak closedness of $\mathcal{D}$ and (ii).
Recovery sequence from (i). □

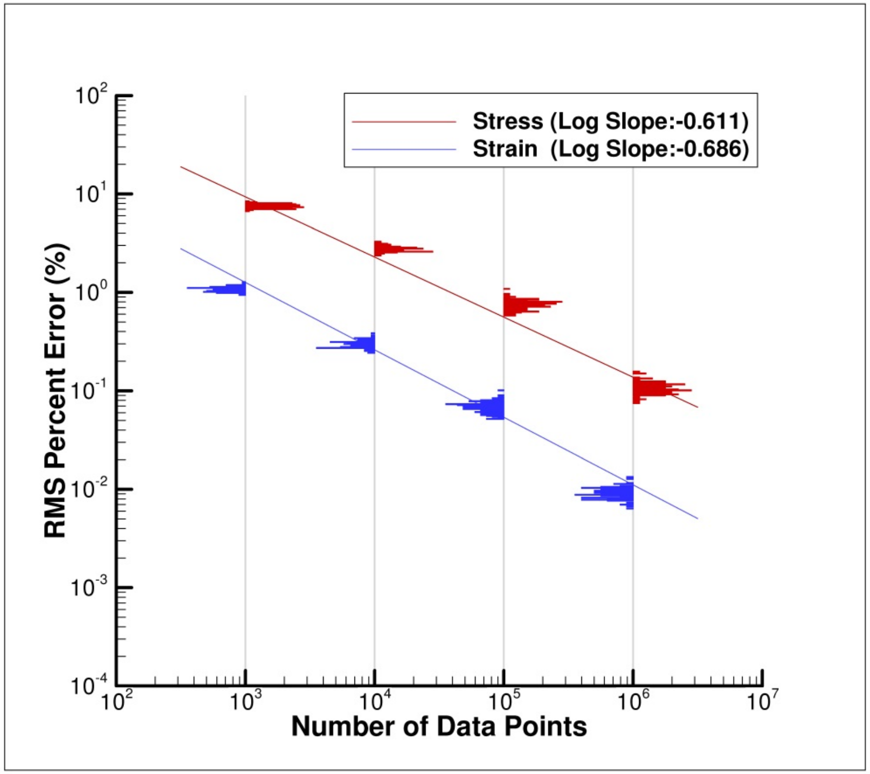
Numerical example: 3D Truss structure



Michael Ortiz
TUM 2021

Numerical example: 3D Truss structure





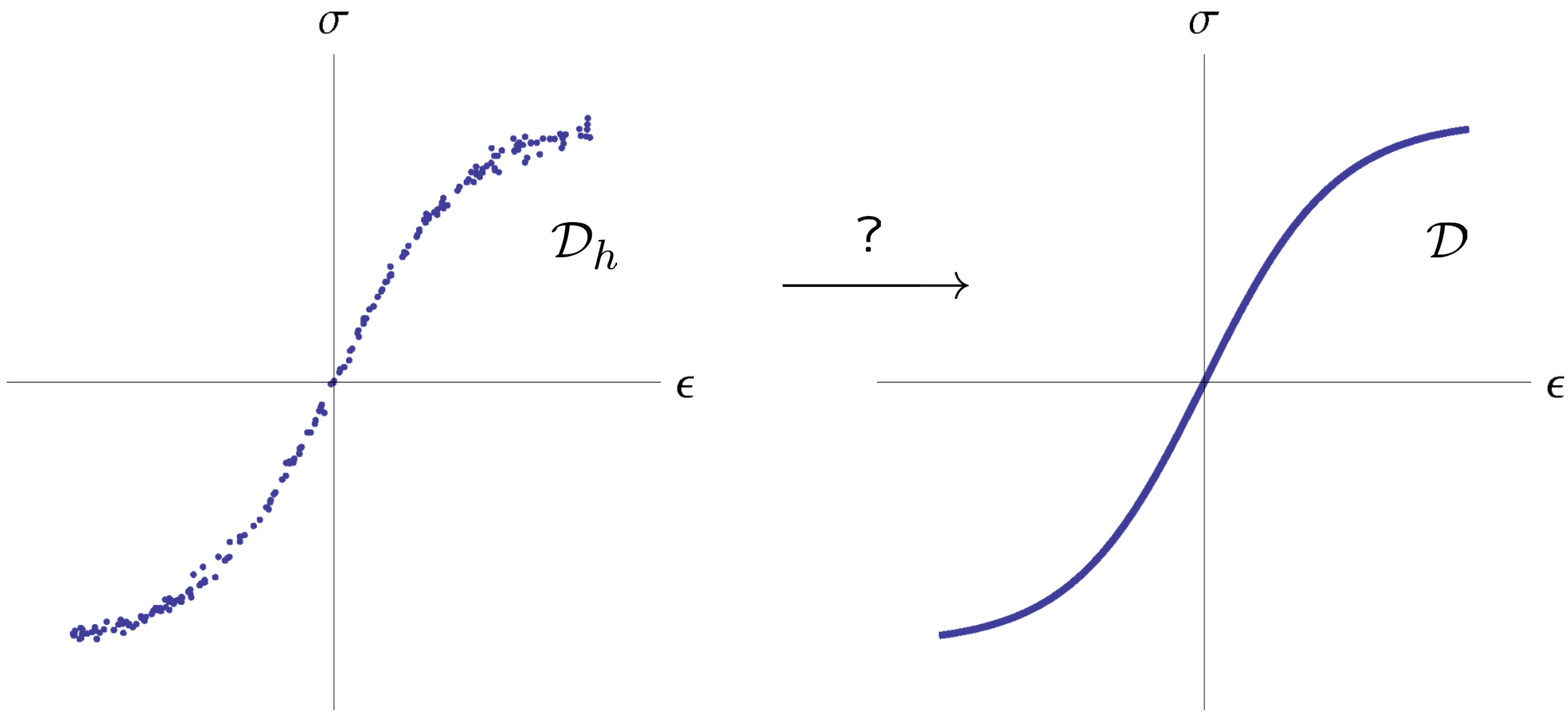
Randomized material-data sets of increasing size and decreasing scatter

Convergence with respect to data set size

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

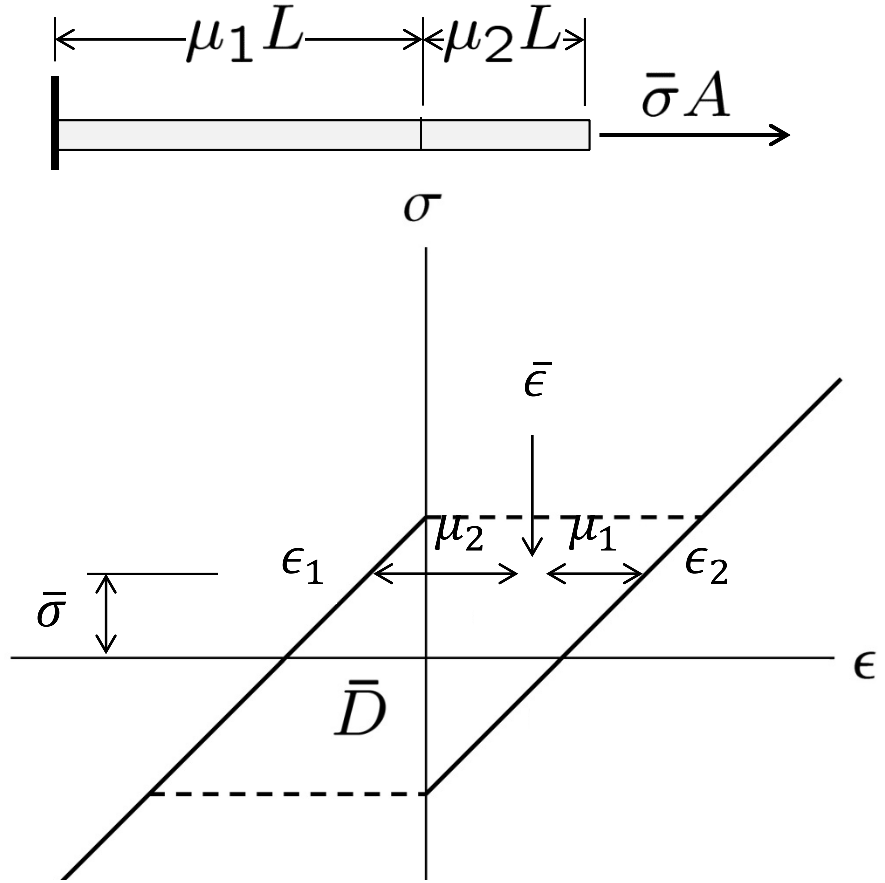
Michael Ortiz
TUM 2021

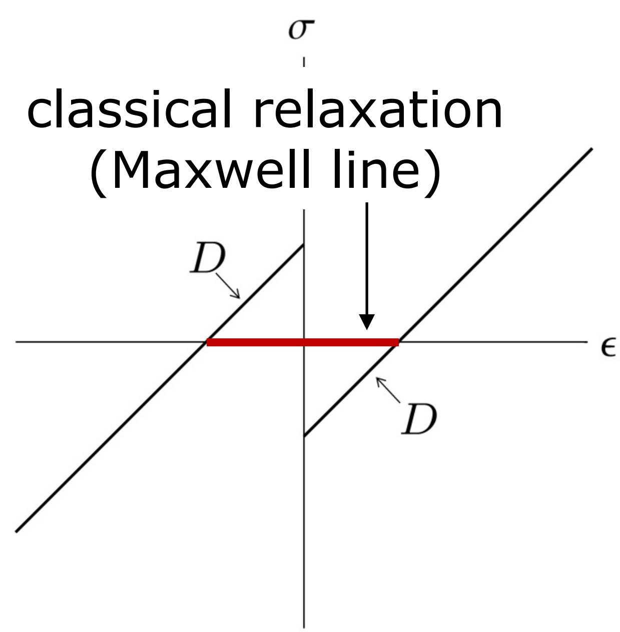
The topology of Δ-convergence



- Suppose now that the limiting set is *not weakly closed*
- Infimum of the distance may not be attained: *Relaxation*
- What *topology* describes material data set relaxation?
- What are the *relaxed material data sets?*

Data-Driven elasticity - Relaxation





Conjecture (DD relaxation)

$$D \equiv \{double\ well\} \Rightarrow \{(\bar{\epsilon}, \bar{\sigma})\} = \overline{D}.$$

Conti, S., Müller, S. & Ortiz, M., *ARMA,* **229** (2018) 79-123.

The topology of Δ-convergence

Henceforth: $\mathcal{Z}$ reflexive separable Banach space; $\mathcal{E}$ weakly-closed subset.

Definition (Δ convergence)

A sequence (y_h, z_h) in $\mathcal{Z} \times \mathcal{Z}$ is said to converge to $(y, z) \in \mathcal{Z} \times \mathcal{Z}$ in the Δ topology, denoted $(y, z) = \Delta\!-\lim_{h\to\infty}(y_h, z_h)$, if $y_h \rightharpoonup y$, $z_h \rightharpoonup z$ and $y_h - z_h \to y - z$.

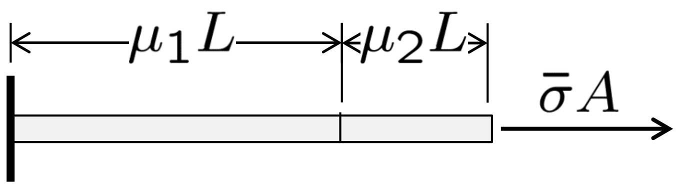
NB: We denote by $\Gamma(\Delta) - \lim_{h\to\infty} F_h$ the Γ-limit of sequences (F_h) of functions over $\mathcal{Z} \times \mathcal{Z}$ in the Δ-topology, and by $K(\Delta) - \lim_{h\to\infty} \mathcal{A}_h$ the Kuratowski-limit of sequences $(\mathcal{A}_h)$ of subsets of $\mathcal{Z} \times \mathcal{Z}$.

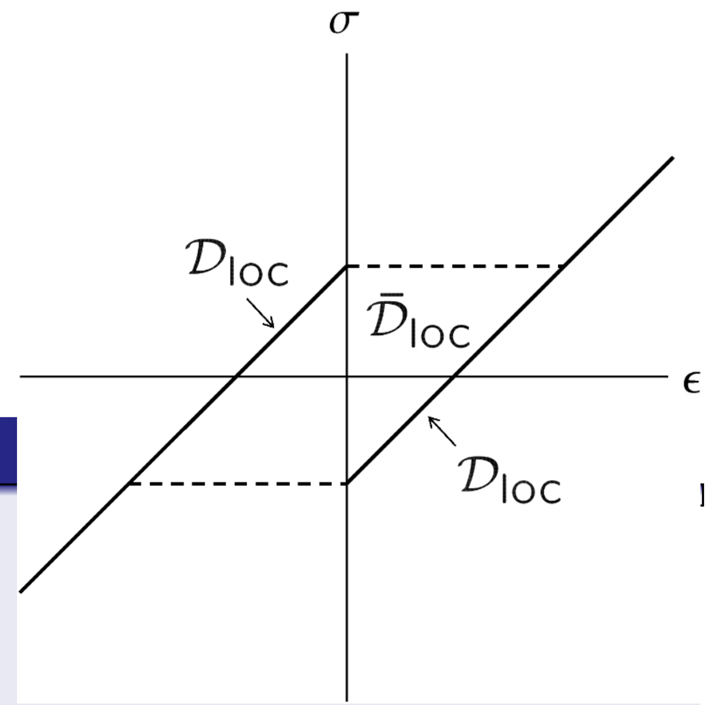
Theorem (One-dimensional bistable material)

Let $\mathcal{Z} = L^2(0,1) \times L^2(0,1)$, $\mathcal{E} \subset \mathcal{Z}$ as before, $\mathcal{D}_{\rm loc}$ bistable and $\overline{\mathcal{D}}_{\rm loc}$ the corresponding flag. Then, $\overline{\mathcal{D}} \times \mathcal{E} = K(\Delta)\!-\lim_{h\to\infty} \mathcal{D} \times \mathcal{E}$.

NB: Can be extended to 3D bistable materials (CMO'2018)

The topology of Δ-convergence





Proof.

Need to show that $\bar{F} = \Gamma(\Delta)-\lim_{h\to\infty} F_h$, $F_h(y,z) = d^2(y,z) + I_{\mathcal{D}}(z) + I_{\mathcal{E}}(z)$ and $\bar{F}(y,z) = d^2(y,z) + I_{\bar{\mathcal{D}}}(z) + I_{\mathcal{E}}(z)$.

Main idea: σ_h does not oscillate. Can add arbitrary oscillations in ϵ_h.

Lower bound: Let $(y_h, z_h) \stackrel{\Delta}{\to} (y,z)$. By strong convergence, have $y_h \sim z_h \sim (\epsilon_h, \sigma_h) \in \mathcal{E} \cap \mathcal{D}$. Then, $\sigma_h \sim \bar{\sigma}$ and $\epsilon_h \rightharpoonup \bar{\epsilon}$, $(\bar{\epsilon}, \bar{\sigma}) \in \bar{\mathcal{D}}$.

Upper bound: By strong convergence, enough to consider $y \sim z \sim (\epsilon, \sigma) \in \bar{\mathcal{D}}$. Then $\sigma = \bar{\sigma}$. Add piecewise-constant oscillations to ϵ to obtain $\epsilon_h \rightharpoonup \epsilon$, with $(\epsilon_h, \bar{\sigma}) \in \mathcal{E} \cap \mathcal{D}$.

Equi-transversality: Follows from $\sigma \sim \bar{\sigma}$, $|\sigma(x) - \mathbb{C}\epsilon(x)| \leq \sigma_0$. □

The topology of Δ-convergence

Connection between convergence of data sets and DD solutions?

Let: $F_h(y,z) = I_{\mathcal{D}_h}(y) + I_{\mathcal{E}}(z) + \|y-z\|^2 = I_{\mathcal{D}_h \times \mathcal{E}}(y,z) + \|y-z\|^2.$

Theorem

Let $\mathcal{D}$ and $(\mathcal{D}_h)$ be subsets of a reflexive separable Banach space $\mathcal{Z}$, $\mathcal{E}$ a weakly sequentially closed subset of $\mathcal{Z}$. For $(y,z) \in \mathcal{Z} \times \mathcal{Z}$. Suppose:

i) *(Data convergence) $\mathcal{D} \times \mathcal{E} = K(\Delta)\!-\lim_{h\to\infty}(\mathcal{D}_h \times \mathcal{E})$.*

ii) *(Equi-transversality) There are constants $c > 0$ and $b \geq 0$ such that, for all $y \in \mathcal{D}_h$ and $z \in \mathcal{E}$, $\|y-z\| \geq c(\|y\| + \|z\|) - b$.*

Then:

a) *If $F_h(y_h, z_h) \to 0$, there exists $z \in \mathcal{D} \cap \mathcal{E}$ such that, up to subsequences, $(z,z) = \Delta\!-\lim_{h\to\infty}(y_h, z_h)$.*

b) *If $z \in \mathcal{D} \cap \mathcal{E}$, there exist a sequence (y_h, z_h) in $\mathcal{Z} \times \mathcal{Z}$ such that $(z,z) = \Delta\!-\lim_{h\to\infty}(y_h, z_h)$ and $F_h(y_h, z_h) \to 0$.*

The topology of Δ-convergence

Proof.

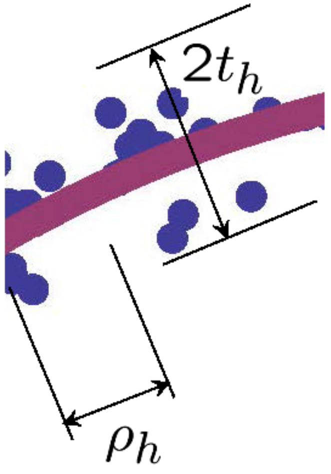
a) Since $F_h(y_h, z_h) \to 0$, it follows that $y_h \in \mathcal{D}_h$, $z_h \in \mathcal{E}$, $\|y_h - z_h\| \to 0$. By (ii), (y_h) and (z_h) are bounded. Therefore, there are $y \in \mathcal{Z}$ and $z \in \mathcal{Z}$ such that $y_h \rightharpoonup y$ and $z_h \rightharpoonup z$ up to subsequences. By the weak closedness of $\mathcal{E}$, $z \in \mathcal{E}$. By weak lower-semicontinuity, $y = z$ and $(y, z) = \Delta\!-\lim_{h\to\infty}(y_h, z_h)$. By (i), $y \in \mathcal{D}$.
b) Let $z \in \mathcal{D} \cap \mathcal{E}$. Then, by (i) there exists a sequence $(y_h, z_h) \in \mathcal{D}_h \times \mathcal{E}$ with limit $(z, z) = \Delta\!-\lim_{h\to\infty}(y_h, z_h)$. In particular, we have $y_h - z_h \to z - z = 0$. Hence, by continuity of the norm,

$$\lim_{h\to\infty} F_h(y_h, z_h) = \lim_{h\to\infty} \left(I_{\mathcal{D}_h}(y_h) + I_{\mathcal{E}}(z_h) + \|y_h - z_h\|^2 \right) = 0,$$

as required. □

The topology of Δ-convergence

Example of Delta-convergence of sets



Theorem (Uniform set convergence)

Let $\mathcal{E} \subset \mathcal{Z}$ *be weakly sequentially closed,* $\mathcal{D}$, $\overline{\mathcal{D}} \subset \mathcal{Z}$. *Suppose:*

i) *(Data convergence)* $\overline{\mathcal{D}} \times \mathcal{E} = K(\Delta) - \lim_{h\to\infty} (\mathcal{D} \times \mathcal{E})$.

ii) *(Fine approximation) There is a sequence* $\rho_h \downarrow 0$ *such that* $d(\xi, \mathcal{D}_{\mathrm{loc},h}) < \rho_h$, $\forall \xi \in \mathcal{D}_{\mathrm{loc}}$.

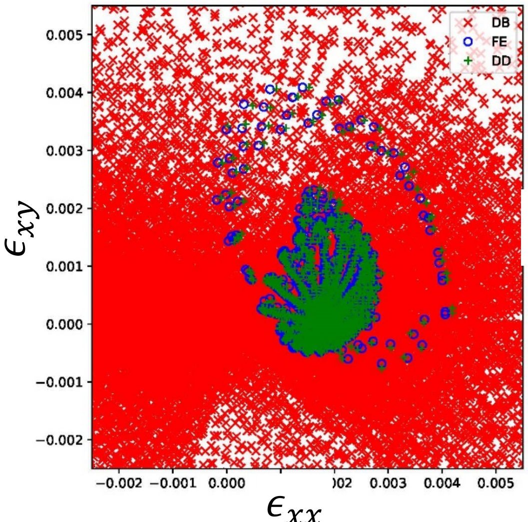
iii) *(Uniform approximation) There is a sequence* $t_h \downarrow 0$ *such that* $d(\xi, \mathcal{D}_{\mathrm{loc}}) < t_h$, $\forall \xi \in \mathcal{D}_{\mathrm{loc},h}$.

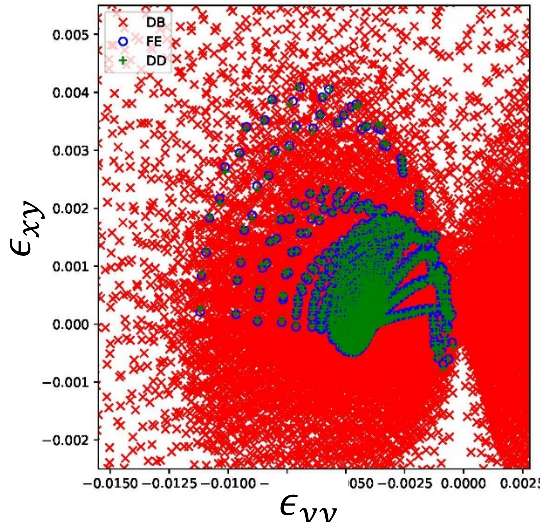
iv) *(Transversality) There are constants* $c > 0$ *and* $b \geq 0$ *such that, for all* $y \in \mathcal{D}$ *and* $z \in \mathcal{E}$, $\|y - z\| \geq c(\|y\| + \|z\|) - b$.

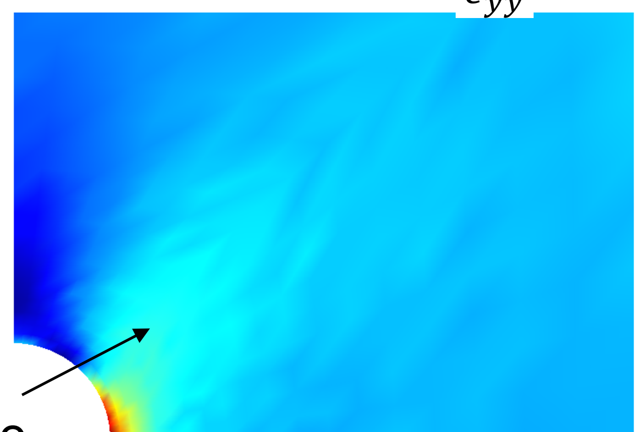
Then, $\overline{\mathcal{D}} \times \mathcal{E} = K(\Delta) - \lim_{h\to\infty} (\mathcal{D}_h \times \mathcal{E})$.

DD relaxation – Finite elements

strain coverage



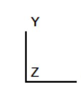




Gauss-point to Gauus-point oscillations!

Stress (DD)

Stress (FE)



Nonlinear elasticity – set-up

Phase space: For $p \in (1, \infty)$, $\frac{1}{p} + \frac{1}{q} = 1$
$Z = X_{p,q} := \{(F, P) \in L^p(\Omega; \mathbb{R}^{n \times n}) \times L^q(\Omega; \mathbb{R}^{n \times n})\}$,
Constraint set: $\mathcal{E}_0$ consists of $(F, P) \in X_{p,q}$ s.t. $\exists u \in W^{1,p}$

$$F = Du \quad \text{in } \Omega, \quad u = g_D \quad \text{on } \Gamma_D,$$
$$\operatorname{div} P + f = 0 \ \text{ in } \Omega, \quad P\nu = h_N \quad \text{on } \Gamma_N.$$

$\mathcal{E} := \{(F, P) \in \mathcal{E}_0 : FP^T \text{symmetric a.e.}\}$ (angular momentum)
Local data sets:
$\mathcal{D} = \{(F, P) \in X_{p,q} : (F(x), P(x)) \in \mathcal{D}_{\text{loc}} \text{ a.e.}\}$.

Deviation function measures distance from the data set
$\psi_{\mathcal{D}_{\text{loc}}}(F, P) := \inf\{\frac{1}{p}|F - F'|^p + \frac{1}{q}|P - P'|^q : (F', P') \in \mathcal{D}_{\text{loc}}\}$
$J(F, P) = \int_\Omega \psi_{\mathcal{D}_{\text{loc}}}(F, P)\, dx$
Goal: minimize J in $\mathcal{E}$

$$\psi_{\mathcal{D}_{\rm loc}}(F,P) := \inf\{\tfrac{1}{p}|F-F'|^p + \tfrac{1}{q}|P-P'|^q : (F',P') \in \mathcal{D}_{\rm loc}\}$$

$J(F,P) = \int_\Omega \psi_{\mathcal{D}_{\rm loc}}(F,P)\,dx$, $\mathcal{E}$ equilibrium set

Theorem

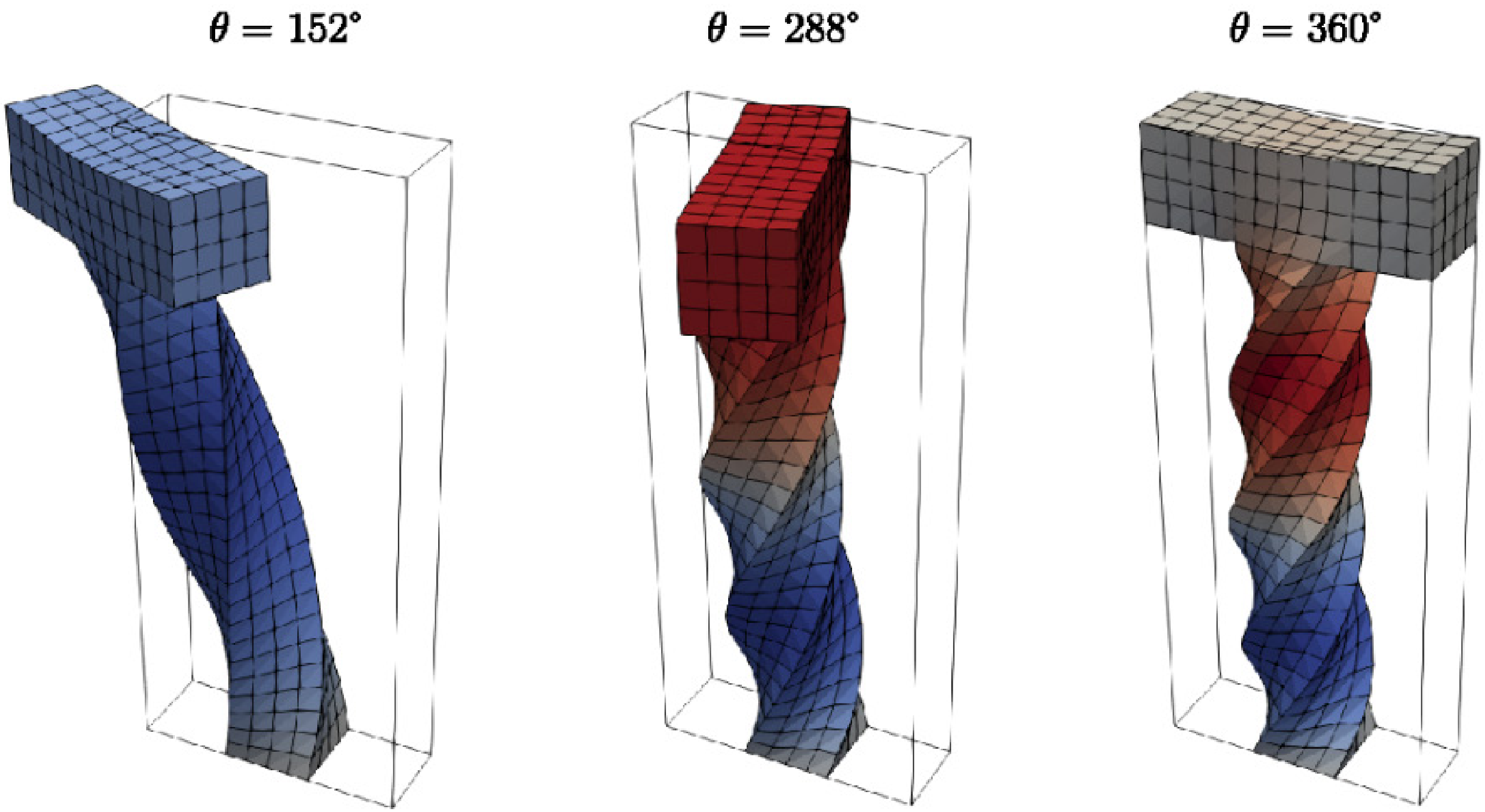
Assume $\inf_{\mathcal{E}} J = 0$. *If* $\mathcal{D}_{loc}$ *is* (p,q) *coercive and div-curl closed then the infimum is attained by* $(F,P) \in \mathcal{E} \cap \mathcal{D}$.

(p,q)-coercive:
$\exists c > 0\ \forall (F,P) \in \mathcal{D}_{\rm loc} \quad F \cdot P \geq \frac{1}{c}|F|^p + \frac{1}{c}|P|^q - C$

(p,q) div-curl closed: $(F_k,P_k) \rightharpoonup (F_*,P_*)$, $\quad (F_k,P_k) \in \mathcal{D}_{\rm loc}$ a.e.,
$\operatorname{curl} F_k$ compact in $W^{-1,p}$, $\quad \operatorname{div} P_k$ compact in $W^{-1,q}$
$\Longrightarrow (F_*,P_*) \in \mathcal{D}_{\rm loc}$ a.e.

There are interesting examples for $D_{\rm loc}$ of the form
$\{(F, DW(F)) : F \in \mathbb{R}^{n\times n}\}$
with $W : \mathbb{R}^{n\times n} \to \mathbb{R}$ which satisfies $\min W = W(\mathrm{Id})$
and $W(QF) = W(F)$ for all $Q \in SO(n)$.

DD finite elasticity - Numerics



A. Platzer, Doctoral Thesis, Ecole Centrale de Nantes, 2020.

Concluding remarks

- *Model-Free Data-Driven computing: The data, all the data, nothing but the data!*
- New class of variational problems in phase space
- New natural notion of convergence of data sets and relaxation (different from relaxation of the energy)
- Connections with compensated compactness, A-quasiconvexity, G-closure in homogenization
- Natural connections with div-curl quasiconvexity, quasimonotonicity (K. Zhang), polymonotonicity
- *Data-driven computing is likely to be a growth area in an increasingly data-rich world and to change the way in which data is mined, stored, exchanged, disseminated and utilized in science and in industry!*

Concluding remarks

Thank you!

Michael Ortiz
TUM 2021