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

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

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Mathematics Colloquium
University of Warwick
June 18, 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
  - Extension to stochastic materials…

Motivation, background, hype...

The anatomy of field theories

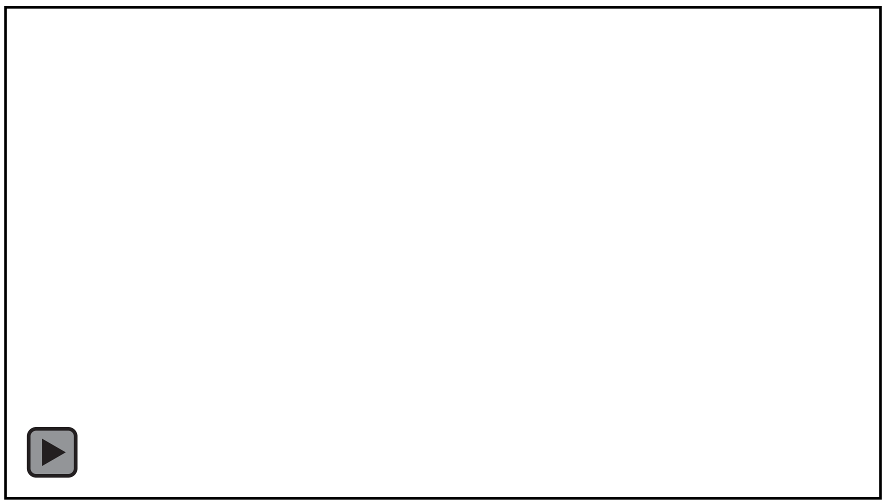
- Focus on problems in the *physical sciences* (as opposed to finance, marketing, social sciences…)
- Problems in the physical sciences deal with *field theories*
- All field theories have a *common structure*:

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	$\epsilon = \delta u$	$\partial\sigma + f = 0$	??

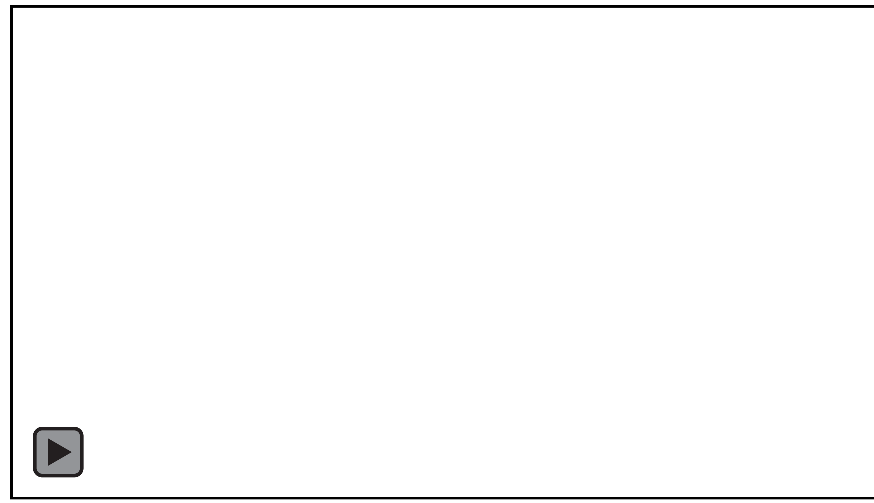
- Potential relations and conservation laws are *universal*!
- *Material laws need to be defined empirically!*

The new data-rich world…

- Material *data is currently plentiful* due to dramatic advances in experimental science
- How do we *rise to the challenge* of rich data sets?



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
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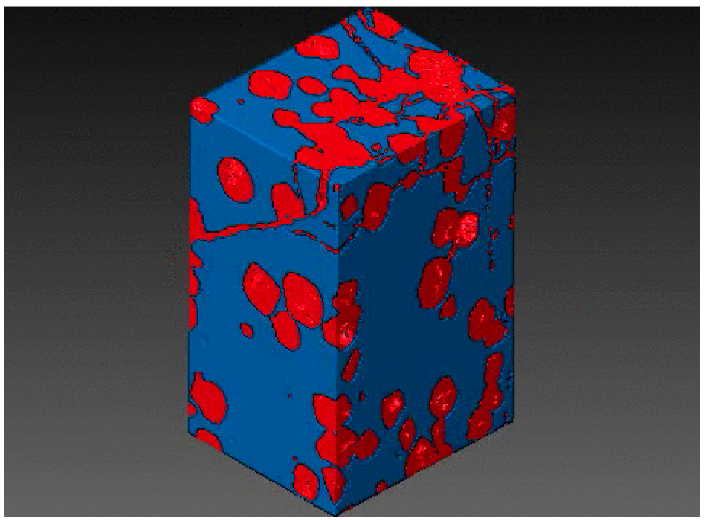
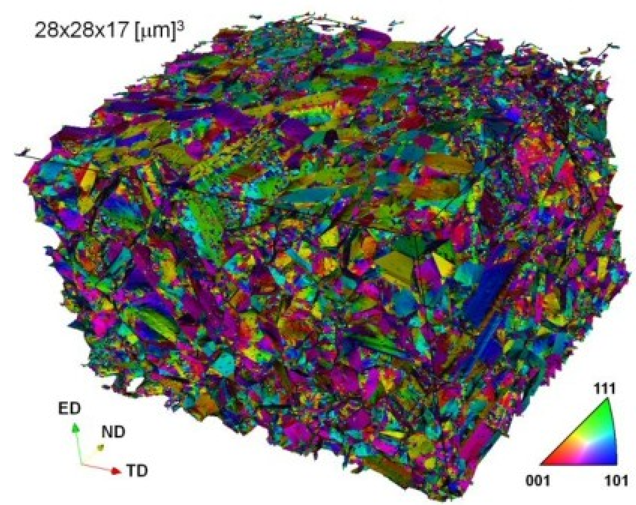


Two-phase μCT analysis of Ti2AlC/Al composite[1]



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.

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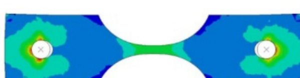
Adapting to a new data-rich world...

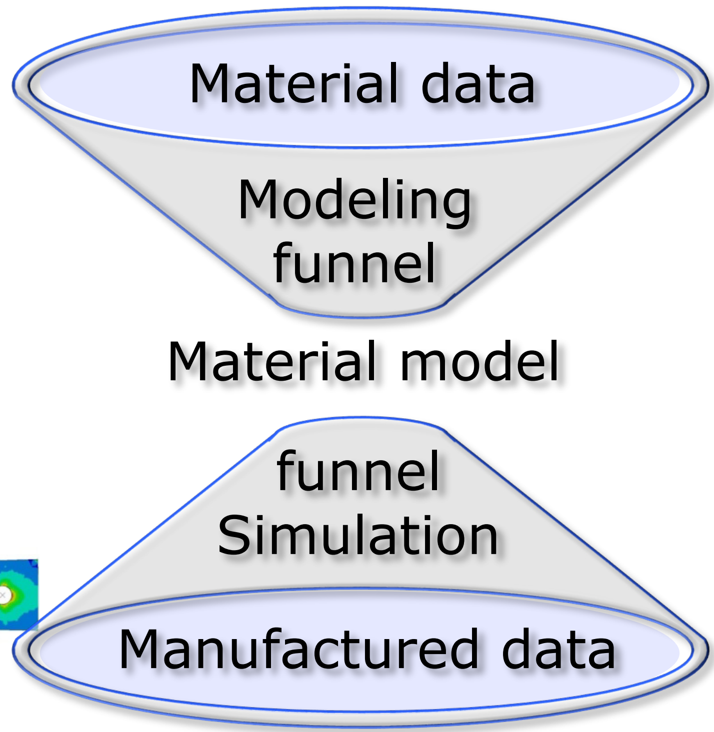
Classical Model-Based
Computational Science...

Modern
microscopy
generates
massive
data sets

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

*Modelling
entails
massive
loss of
information!*





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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:

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

(cut out the middleman!)

Adapting to a new data-rich world...

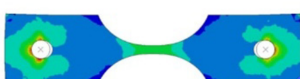
Classical Model-Based Computational Science...

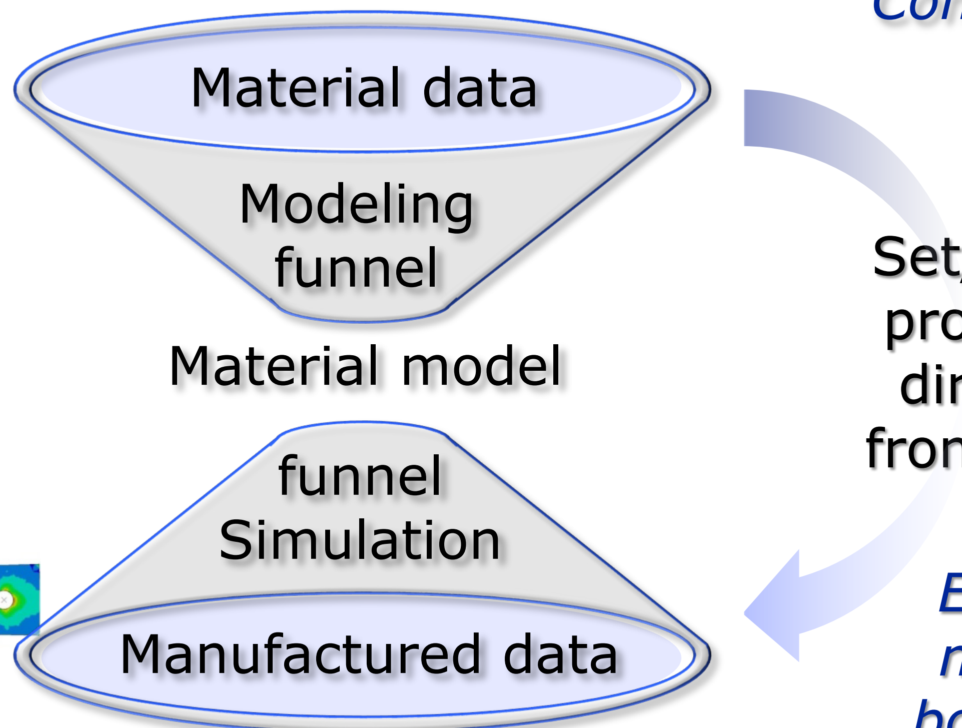
Alternative: Model-Free Data-Driven Computing!

Modern microscopy generates massive data sets

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

Modelling entails massive loss of information!



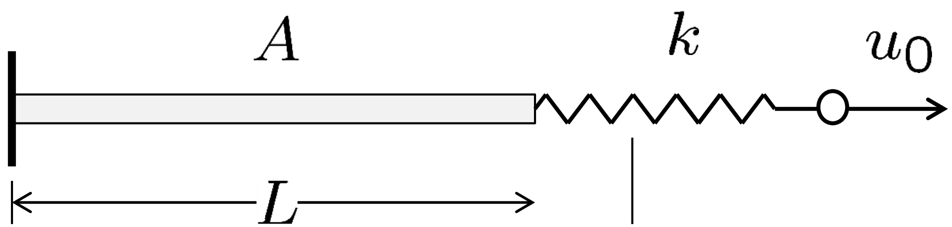


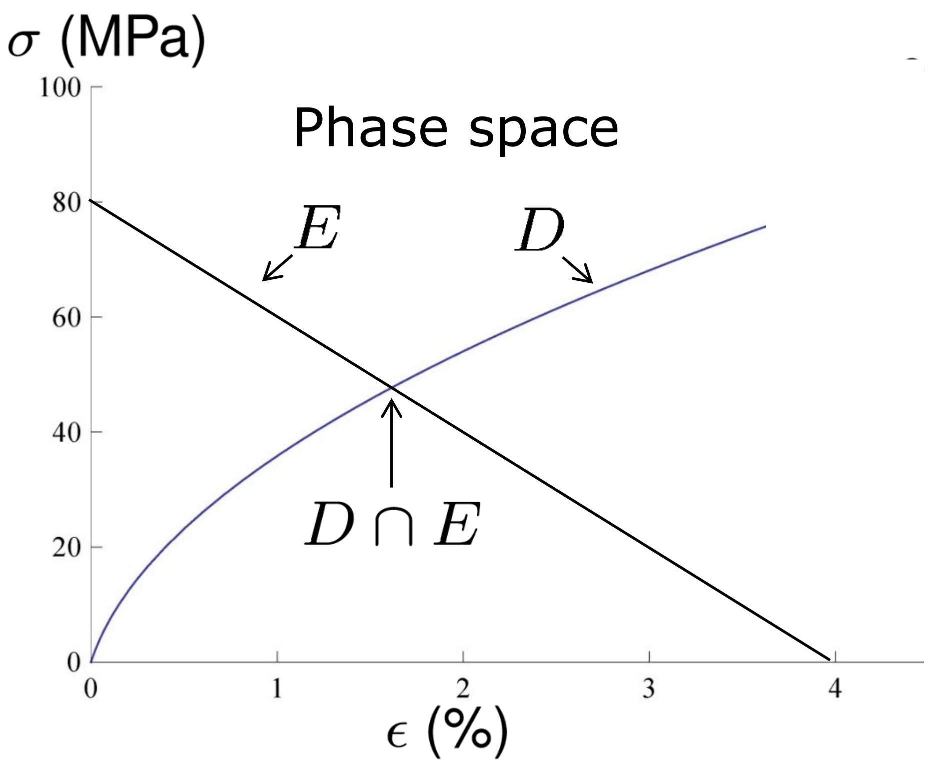
Set/solve problems directly from data!

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: $D \cap E$

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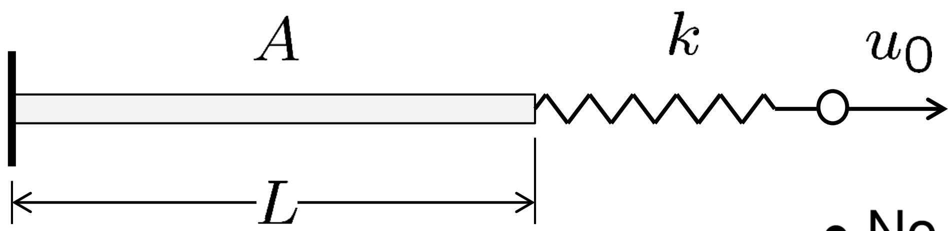
Elementary example: Bar and spring

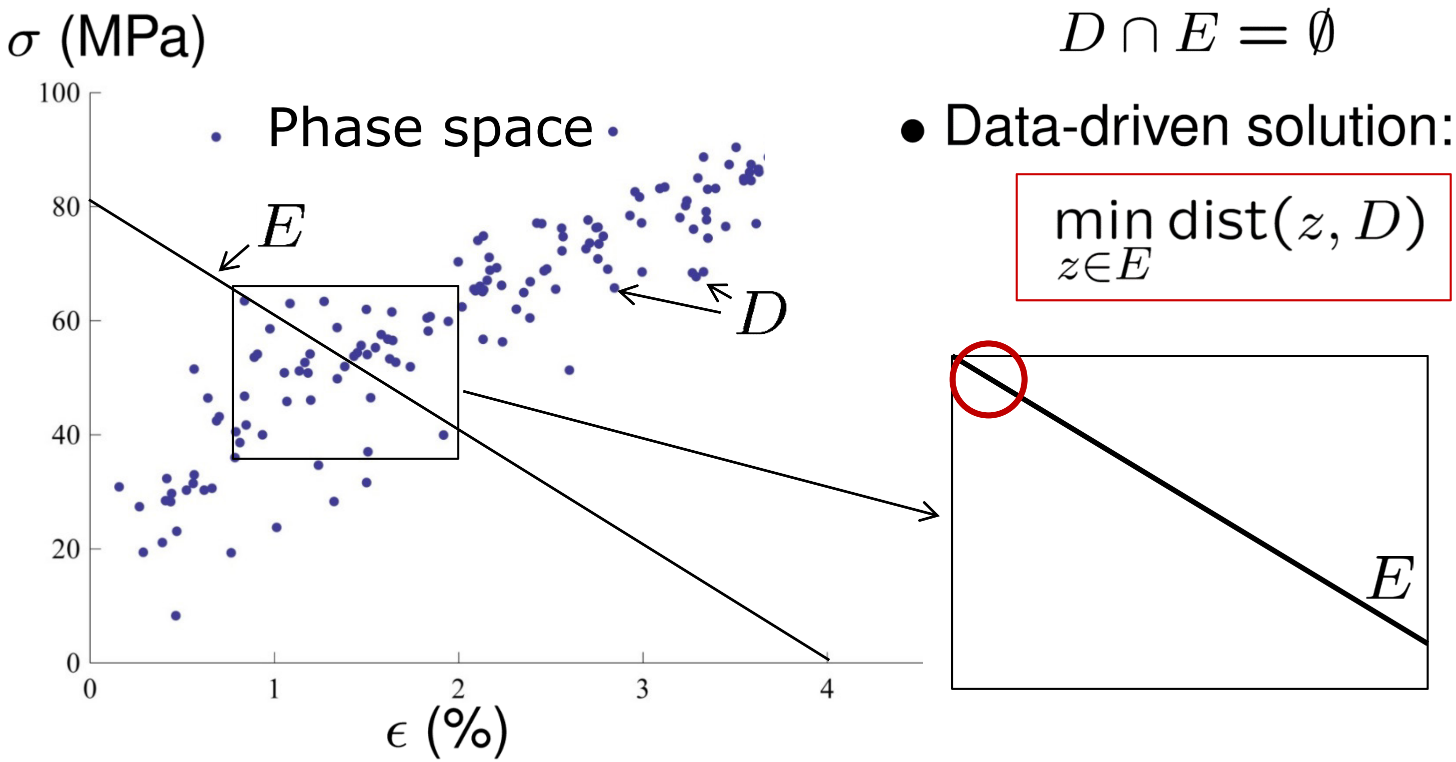


- No classical solutions!

$$D \cap E = \emptyset$$

- Data-driven solution:

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



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Model-Free Data-Driven paradigm

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

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

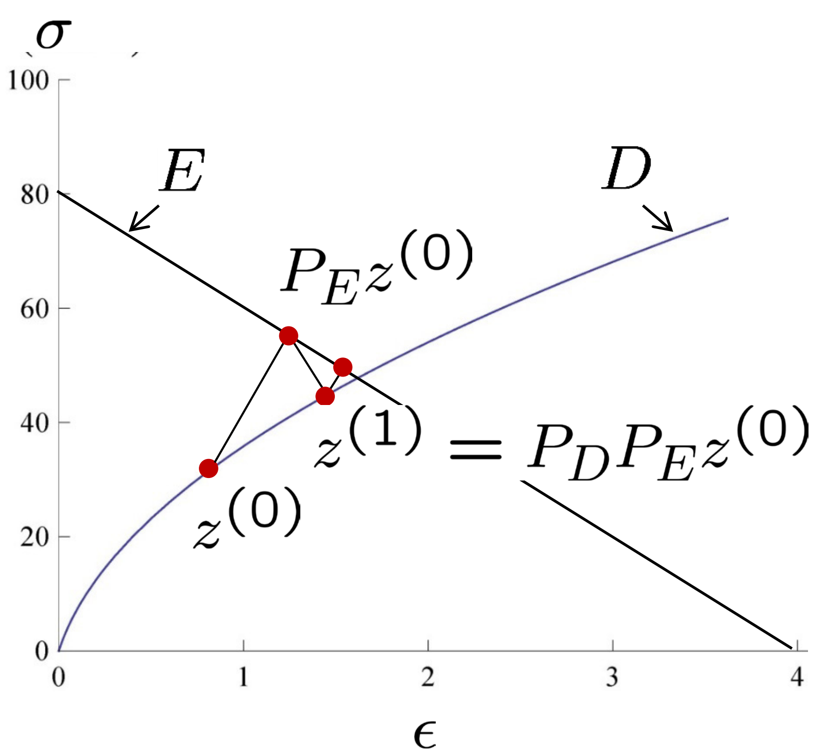
- *Aim of Model-Free Data-Driven problems is to find the admissible state (compatibility and equilibrium) in phase space (stress, strain) closest to the material data set*
- Raw *fundamental material data* (stress *and* strain) is used (unprocessed) in the formulation of the problems
- *No material modeling,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

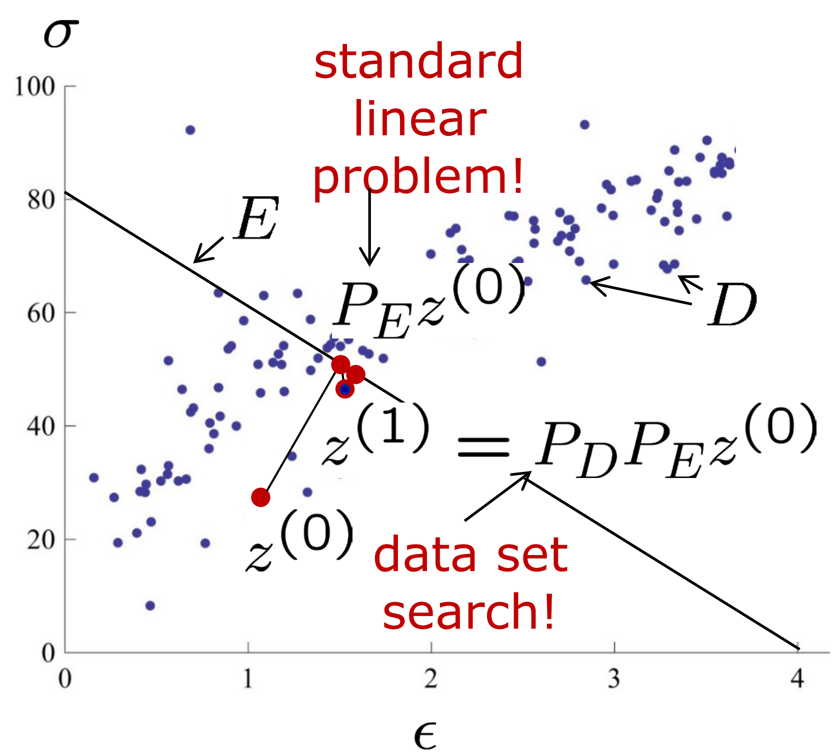
  The data, all the data, nothing but the data!

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

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.
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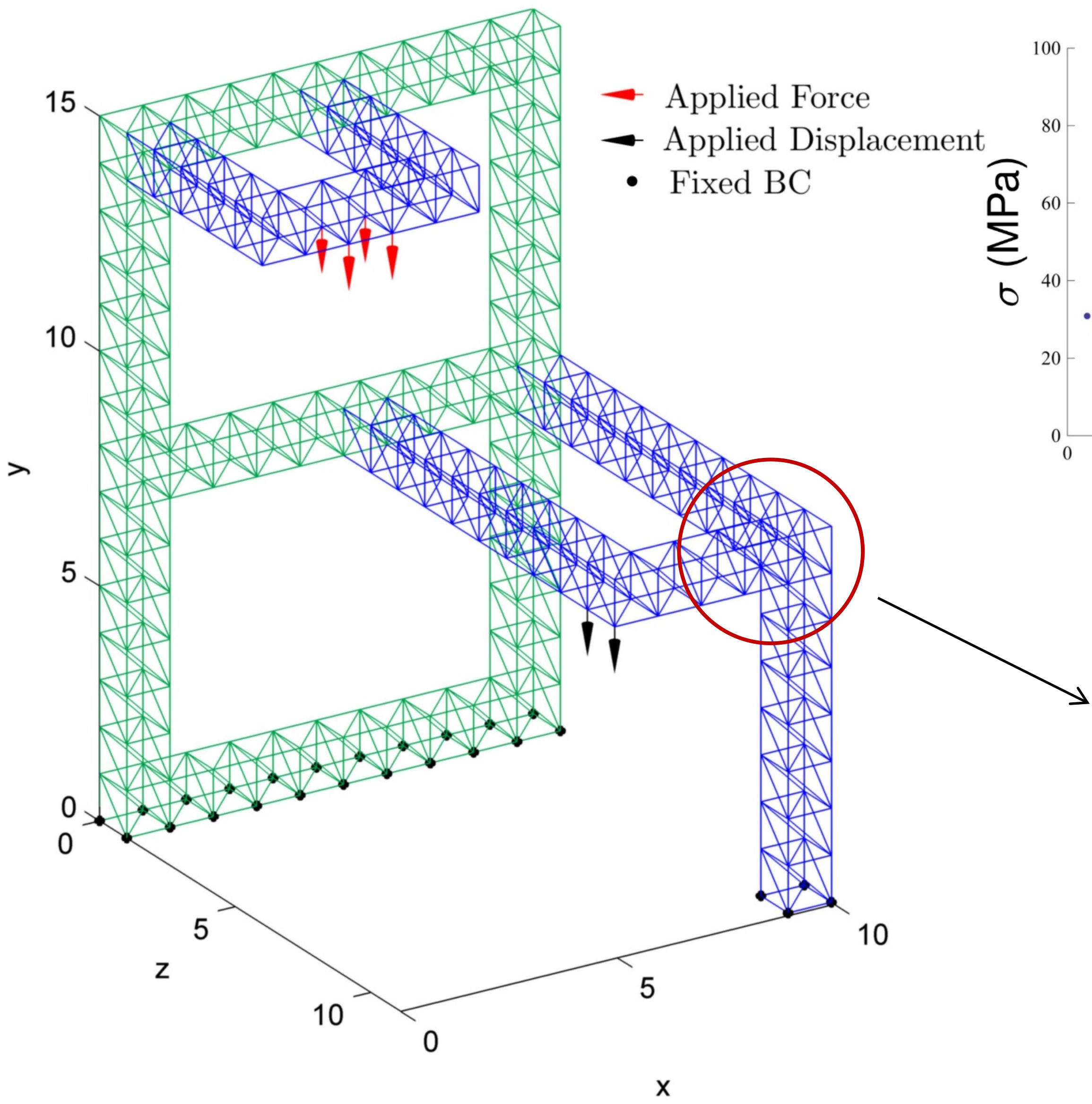
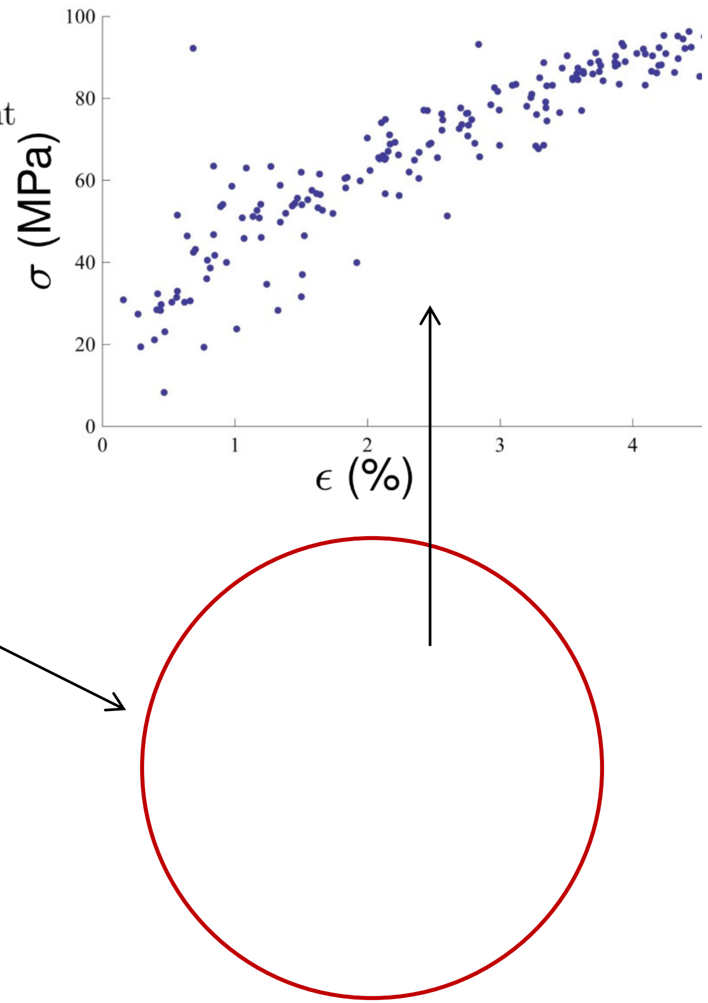
Numerical example: 3D Truss structure





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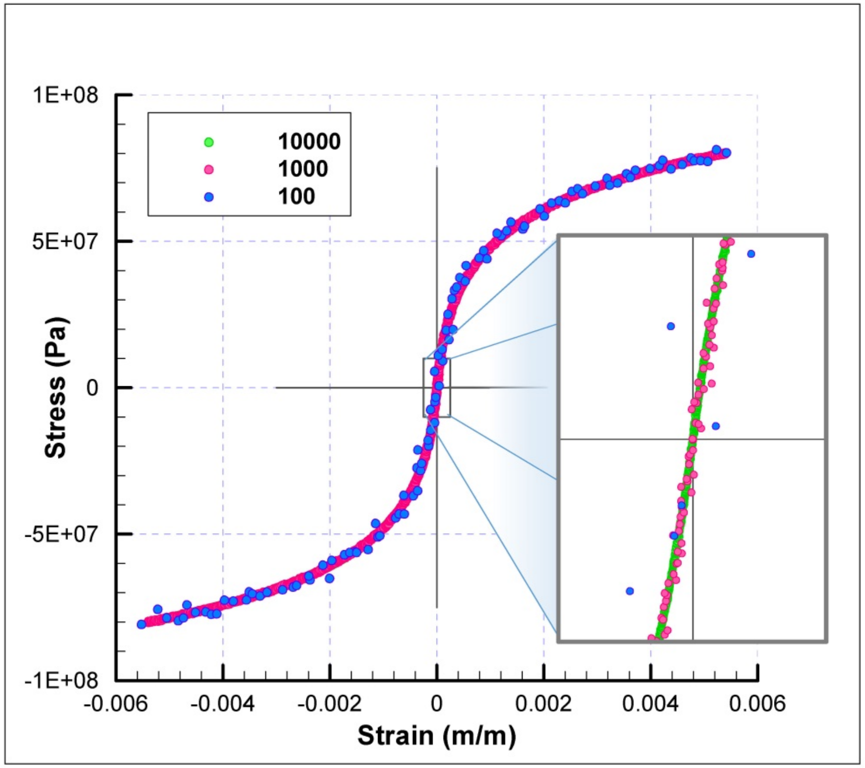
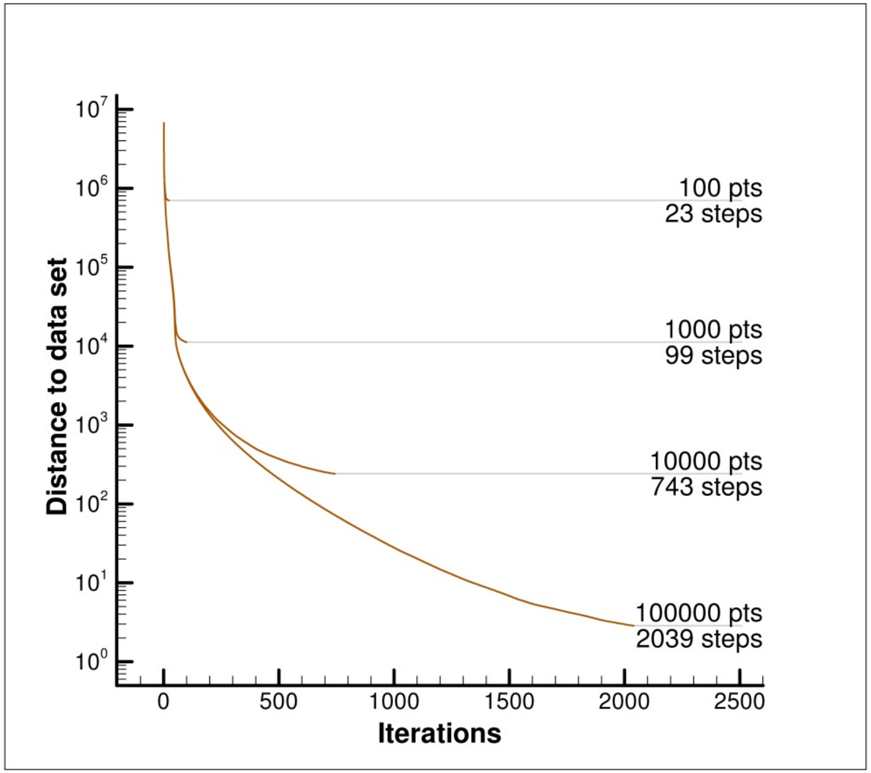
Numerical example: 3D Truss structure



Randomized material-data sets of increasing size



Convergence of fixed-point iteration

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

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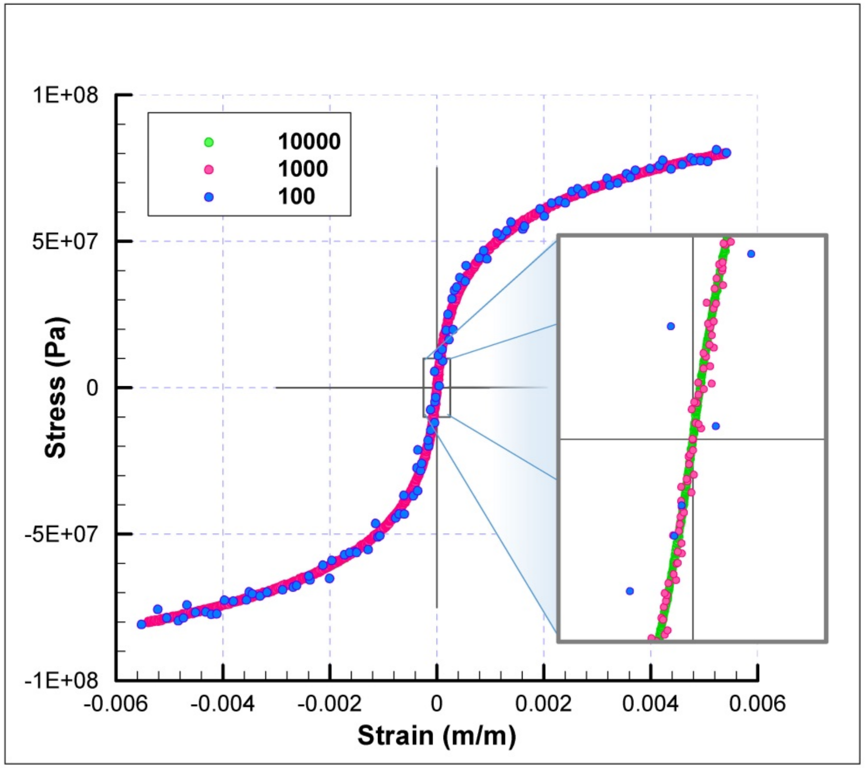
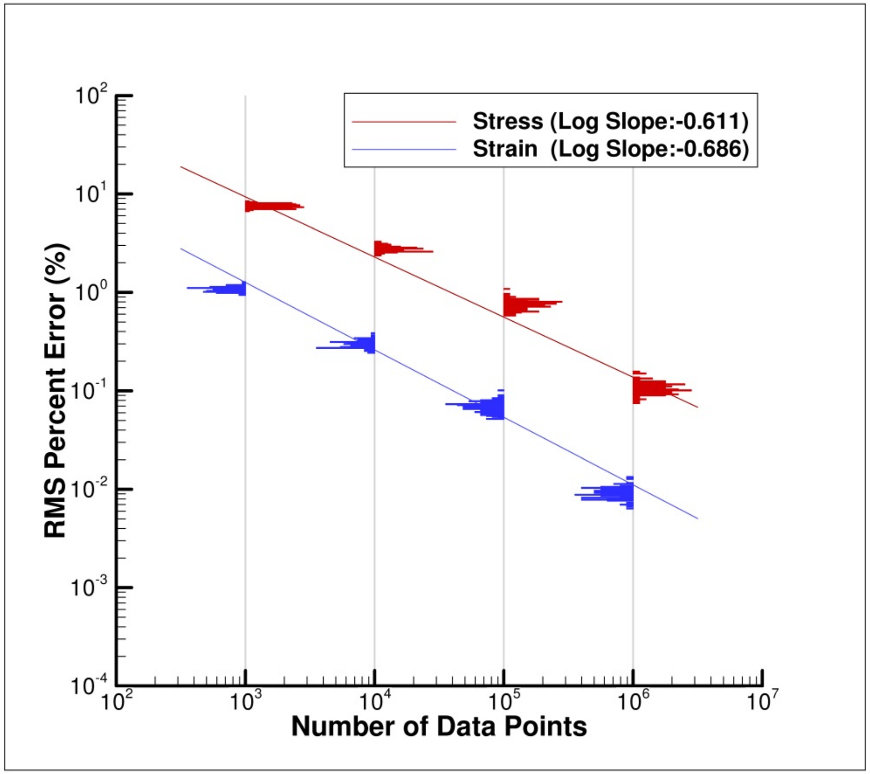
Numerical example: 3D Truss structure



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.

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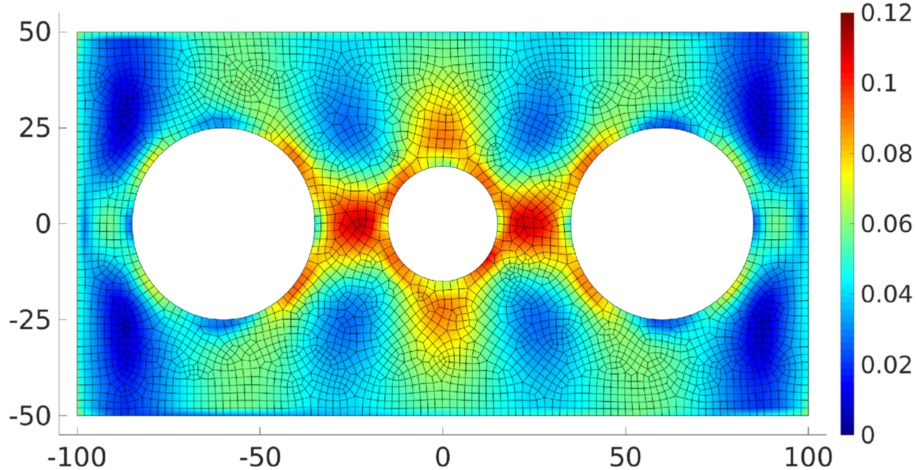
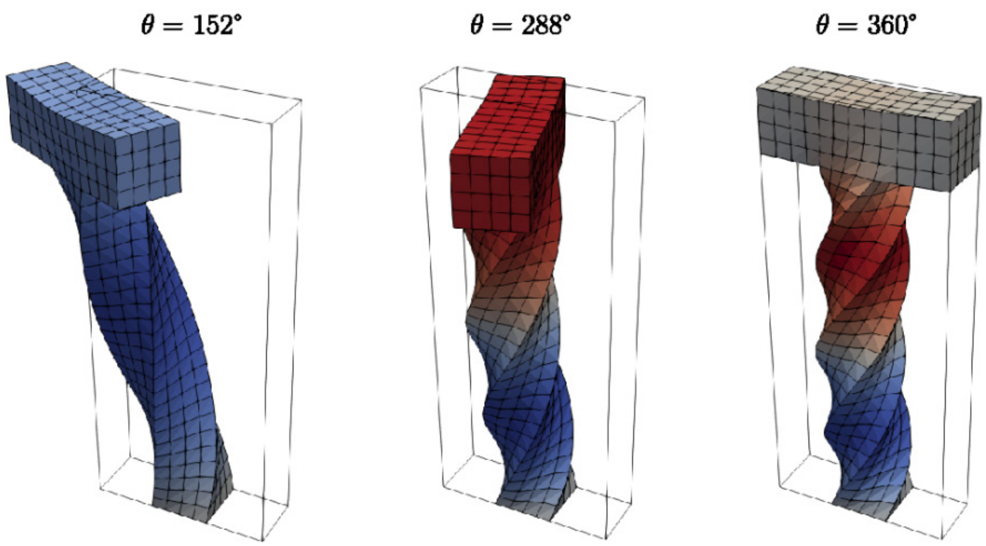
Data-Driven FE calculations



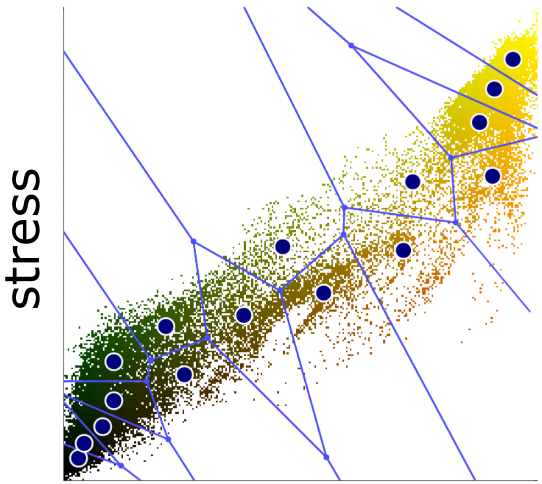
- DD FE calculations
- Linear elasticity
- Perforated plate
- Synthetic data

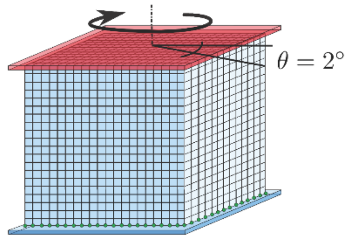


- DD FE calculations
- Finite elasticity
- Twisted elastic rod
- Random Green-S. Venant
- 10,000,000 data points

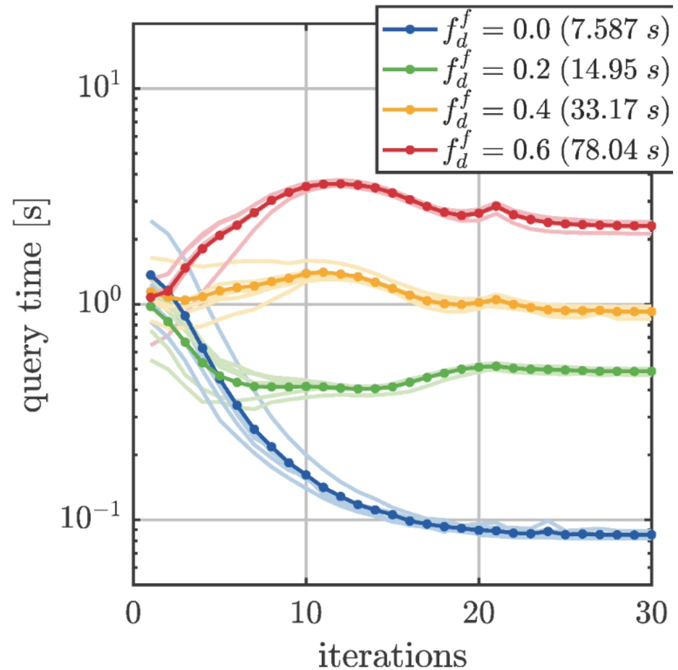
R. Eggersmann, S. Reese, RWTH Aachen (private communication)
A. Platzer, Doctoral Thesis, Ecole Centrale de Nantes, 2020.

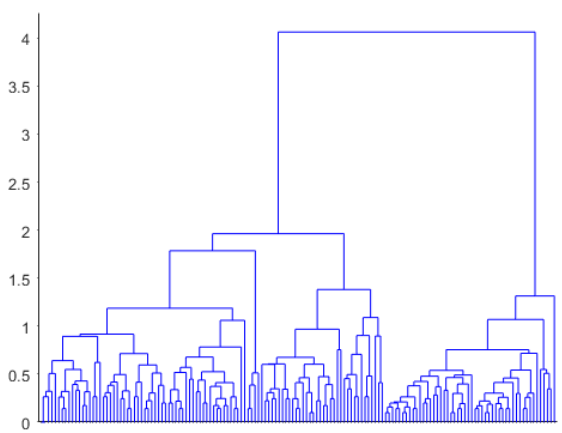
Connection with Machine Learning





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!*

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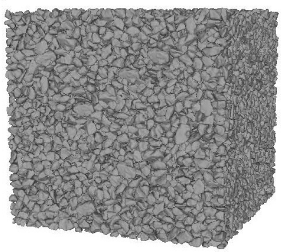
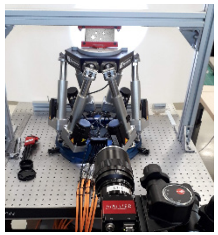
R. Eggersmann, L. Stainier, M. Ortiz & S. Reese, *CMAME*, **382** (2021) 113855.

Data mining, generation, upscaling

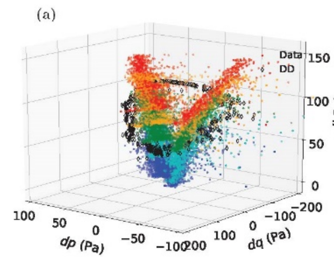


Sand RVE

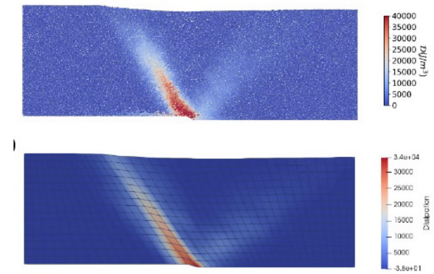
+



3D rig



Material data



DD calculations

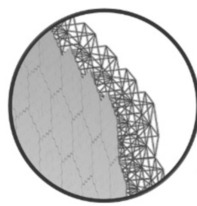
- Data can be *mined* from lower-scale calculations, then used in upper-scale calculations (*DD upscaling*)
- *DD queries* the microscale directly, *upscales data* directly to higher scales, bypasses the need to determine *effective material models* (e.g., by CoV)
- *DD sets forth new opportunities for synergism between experimental science and scientific computing, new multiscale analysis paradigms*

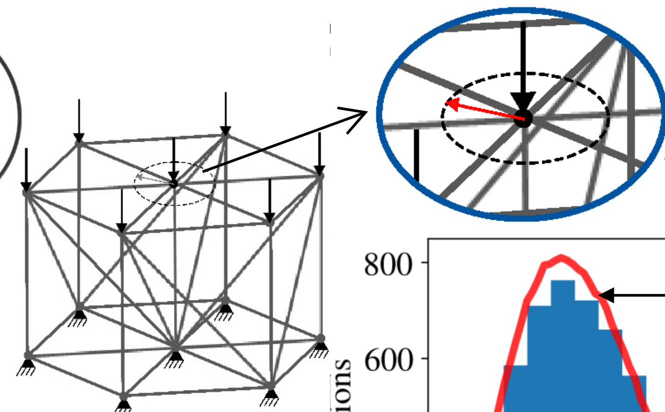
J. Rethore and A. Leygue, HAL Id: hal-01452494, Feb. 2017.
K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

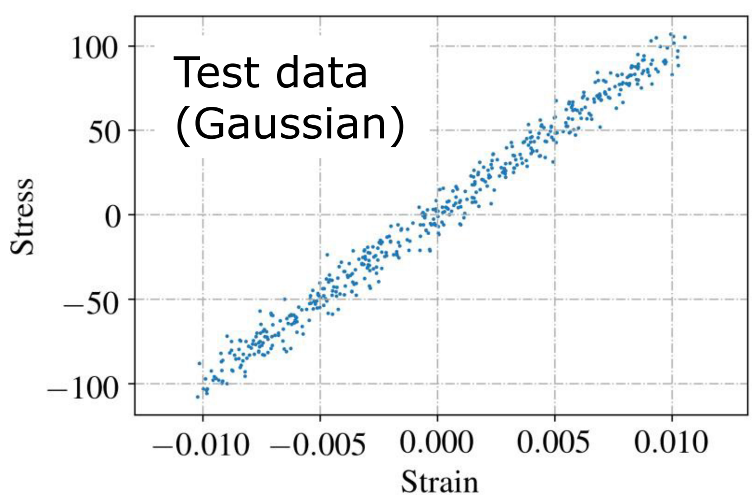
Extension to random materials

- Suppose that the *material behavior* is *truly random* (as opposed to experimental scatter, error, in the data)
- *Goal:* Infer system response directly from empirical data (*no modeling of priors, no modeling of material law*)
- *Data-Driven inference: Explicit expectations from data!*

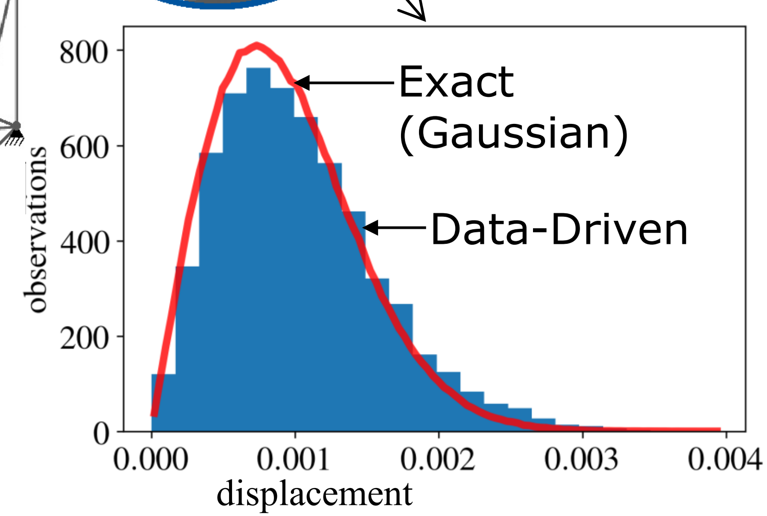
Space Telescope (ISTAR)
[Hogstrom *et al.*, 2014]





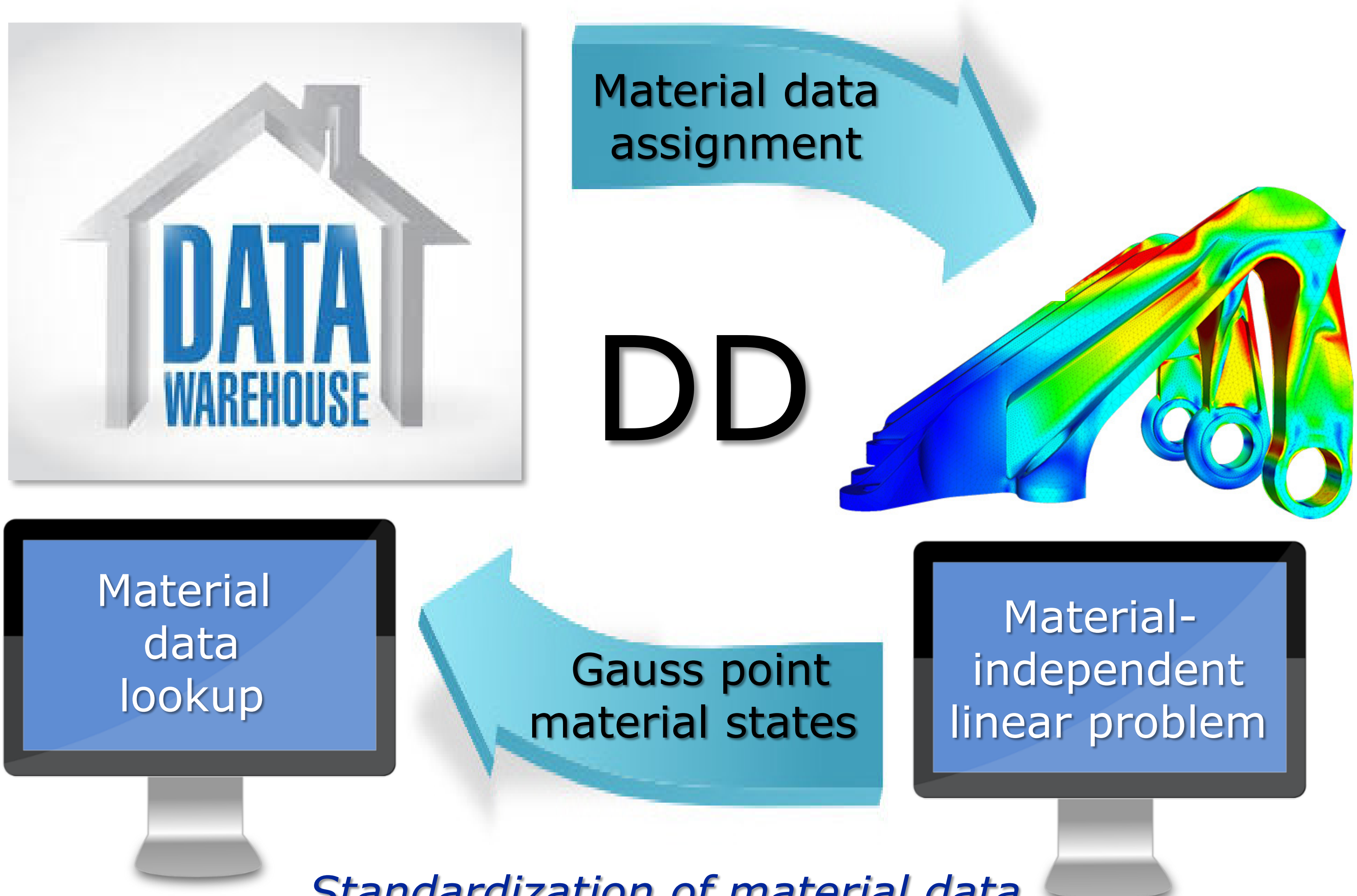


DD



Prume, E. & Reese, S., RWTH Aachen (private comm.)
Conti, S., Hoffmann, F. & MO, arXiv:2106.02728v1.

The Data-Driven information flow, cycle



Standardization of material data and solvers!

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Changing gears…
Analysis!

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?
- Random materials? Model-free DD inference?

Conti, S., Müller, S. & MO, *ARMA* **229,** 79–123 (2018).
Conti, S., Müller, S. & MO, *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: $\mathcal{Z} = \{(\epsilon, \sigma) \,:\, \epsilon \in L^2(\Omega, \mathbb{R}^{n\times n}_{\mathrm{sym}}),\ \sigma \in L^2(\Omega, \mathbb{R}^{n\times n}_{\mathrm{sym}})\}$

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

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)

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

are strongly (and weakly) closed in $L^2(\Omega,\mathbb{R}^{n\times n}_{\mathrm{sym}})$, $L^2(\Omega;\mathbb{R}^{n\times n}_{\mathrm{sym}}) = M\oplus N$ 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

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

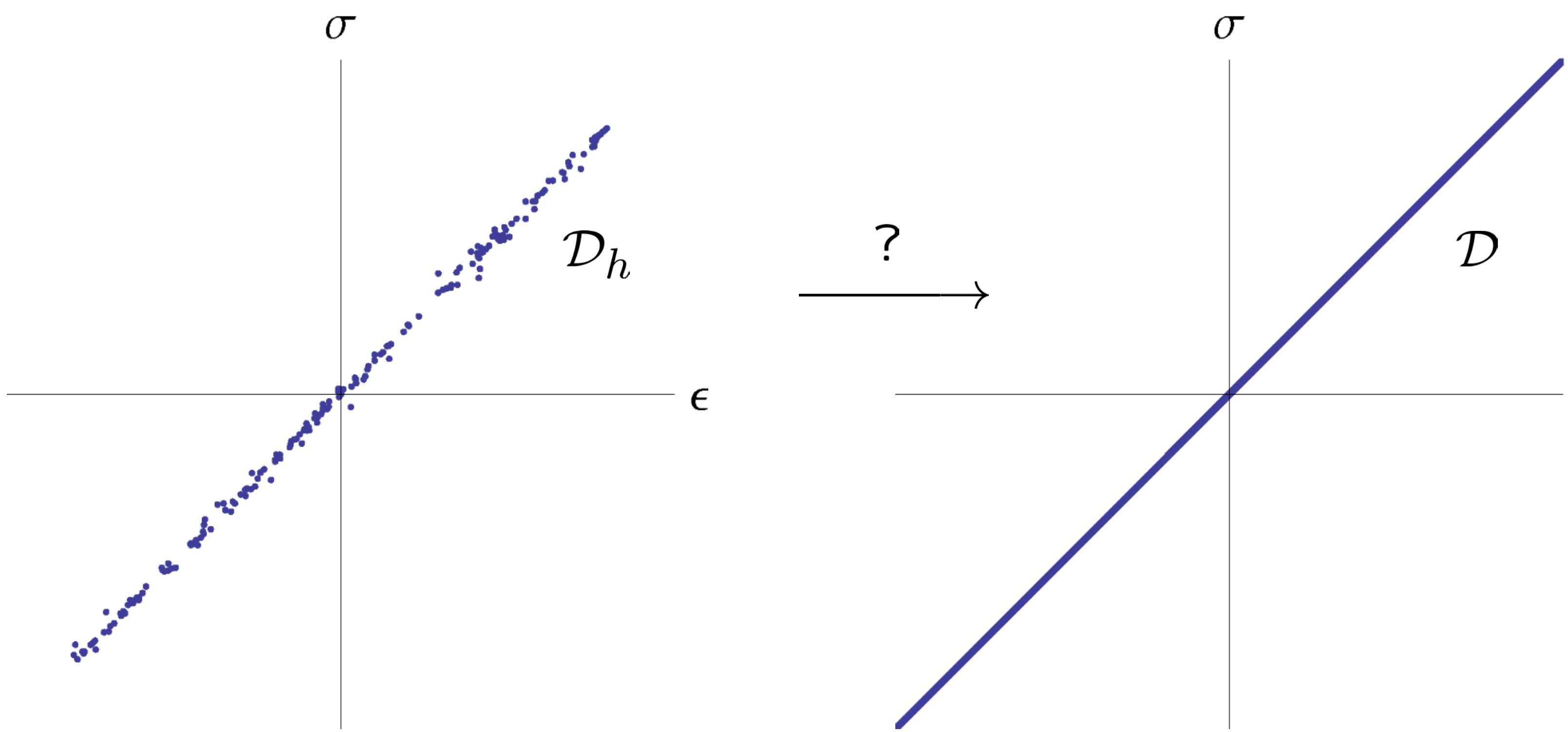
By the power identity, Korn, Poincaré and trace theorems, with $z \in \mathcal{E}$,

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

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.

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.

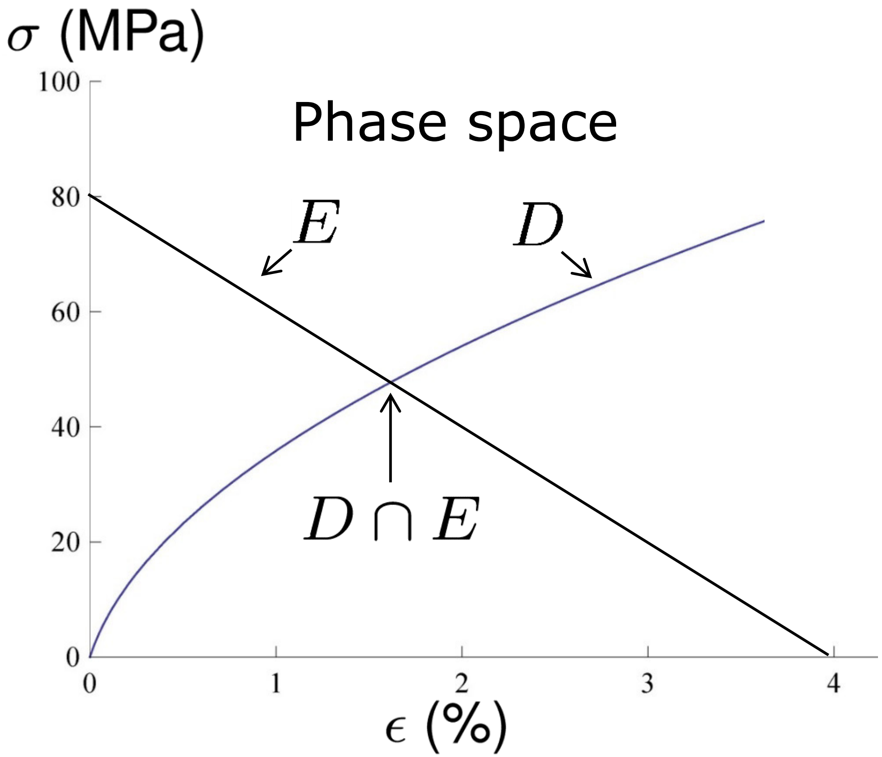
ii) *(Equi-transversality) There are constants* $c > 0$ *and* $b \geq 0$ *such that, for all* $y \in \mathcal{D}_h$ *and* $z \in \mathcal{E}$,

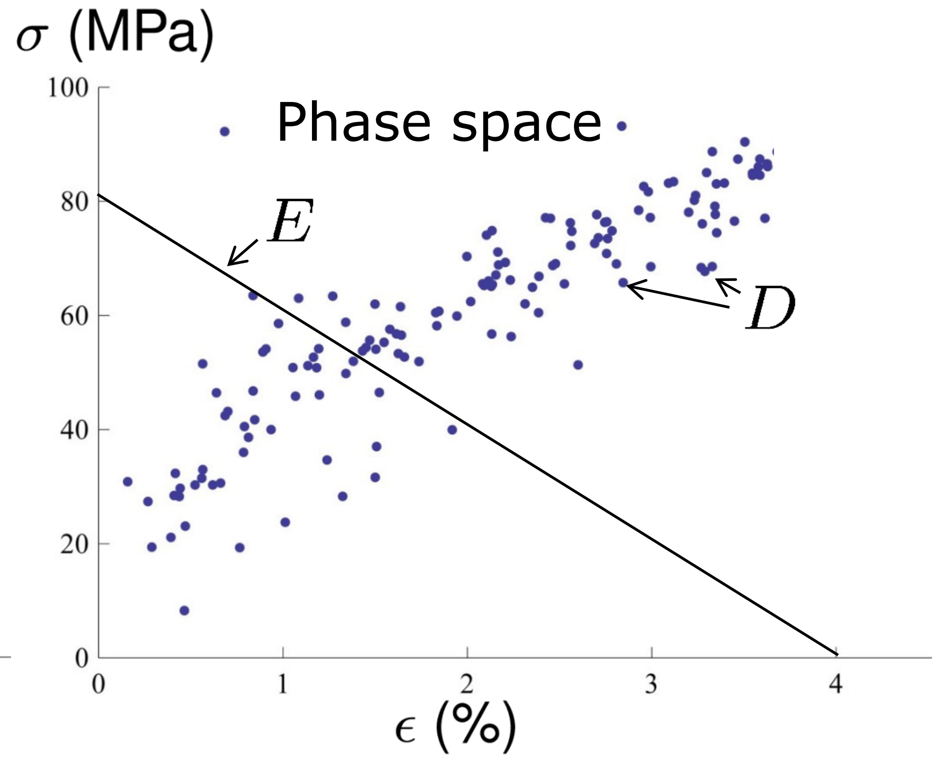
$$\|y - z\| \geq c(\|y\| + \|z\|) - b.$$

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





Transversality in the sense of *intersections* ensures existence of solutions $(D \cap E \neq \emptyset)$

What is the appropriate notion of transversality for *point data sets*?

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

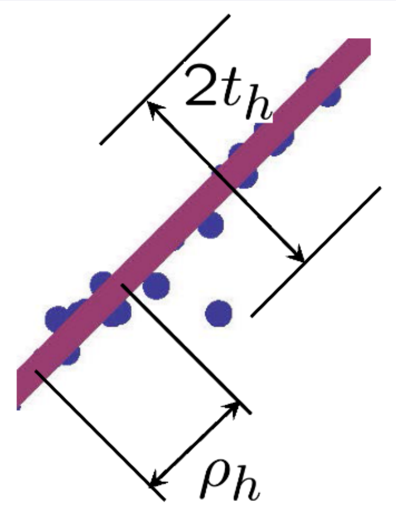
Theorem (Uniform approximation)

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

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

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

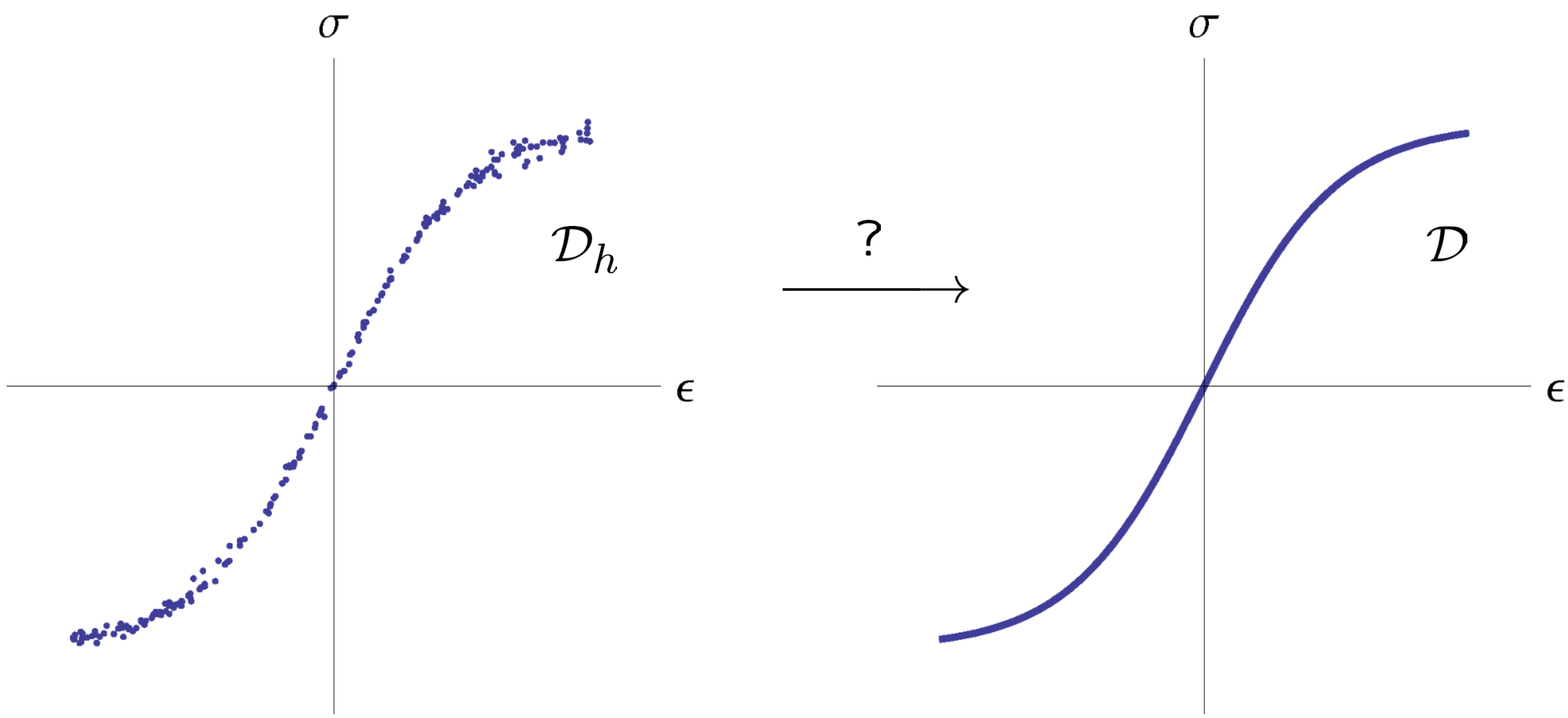
Then, $\mathcal{D} = M-\lim_{h\to\infty} \mathcal{D}_h$ *in* Z.



Proof.

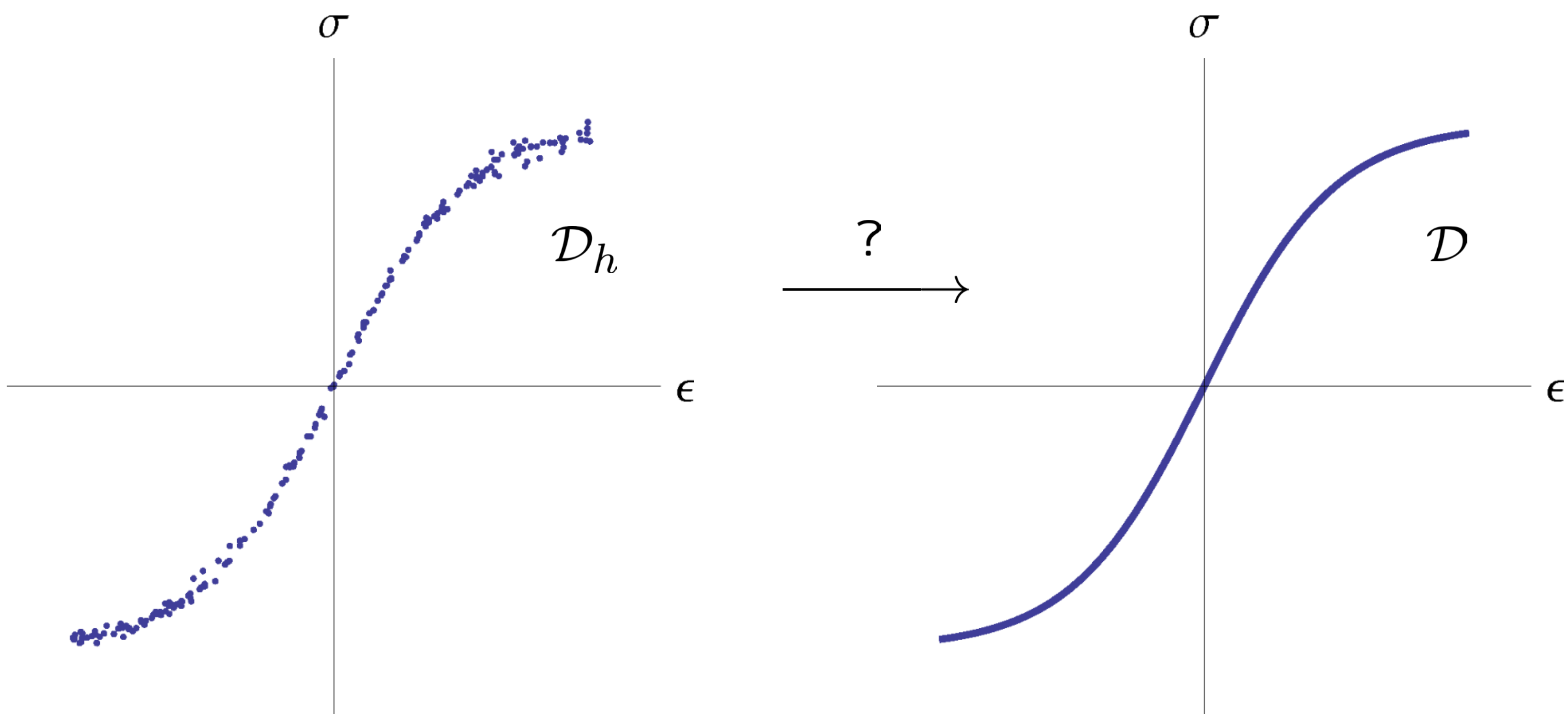
Equi-coercivity from (ii) and coercivity of the limit.
Lower bound from weak closedness of $\mathcal{D}$ and (ii).
Recovery sequence from (i). □

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?*

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 $y_h - z_h \to y - z$.

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 $z \in \mathcal{E}$,* $\|y-z\| \geq c(\|y\| + \|z\|) - b$.

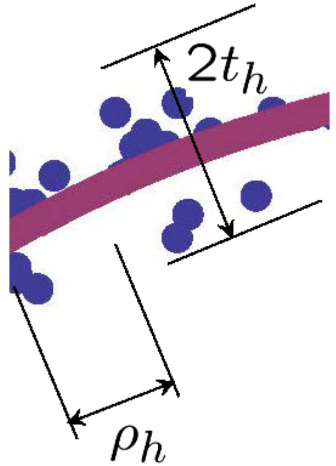
Then:

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

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* $d(\xi, \mathcal{D}_{\mathrm{loc},h}) < \rho_h$, $\forall \xi \in \mathcal{D}_{\mathrm{loc}}$.

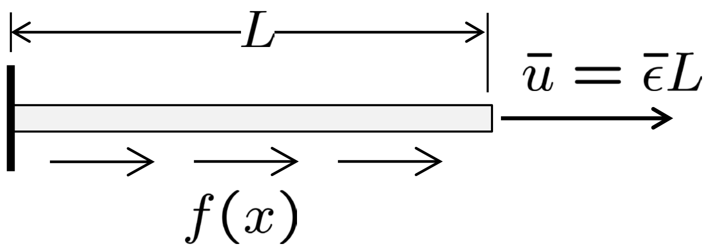
iii) *(Uniform approximation) There is a sequence* $t_h \downarrow 0$ *such that* $d(\xi, \mathcal{D}_{\mathrm{loc}}) < t_h$, $\forall \xi \in \mathcal{D}_{\mathrm{loc},h}$.

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

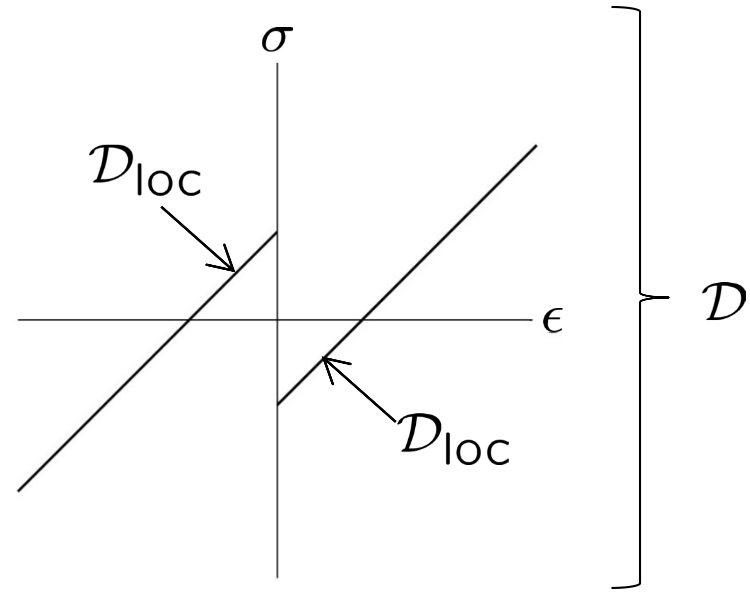
Then, $\overline{\mathcal{D}} \times \mathcal{E} = K(\Delta)-\lim_{h\to\infty}(\mathcal{D}_h \times \mathcal{E})$.

The topology of Δ-convergence: Relaxation

- Example of non-attainment: *Bistable bar*



$$\left.\begin{aligned} &\sigma'(x) + f(x) = 0 \\ &\bar{\epsilon} = \fint \epsilon(x)\, dx \end{aligned}\right\} \mathcal{E}$$

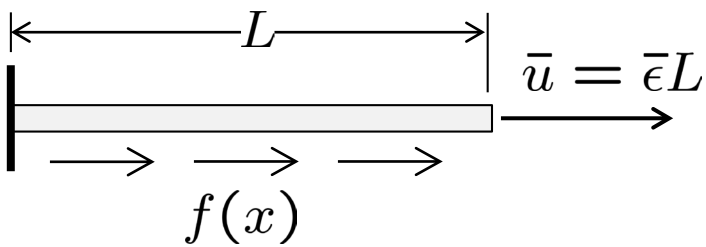


- Infimum not attained in general!
- Natural relaxation: $\bar{\mathcal{D}} \times \mathcal{E} = K(\Delta) - \lim_{h\to\infty} \mathcal{D} \times \mathcal{E}$

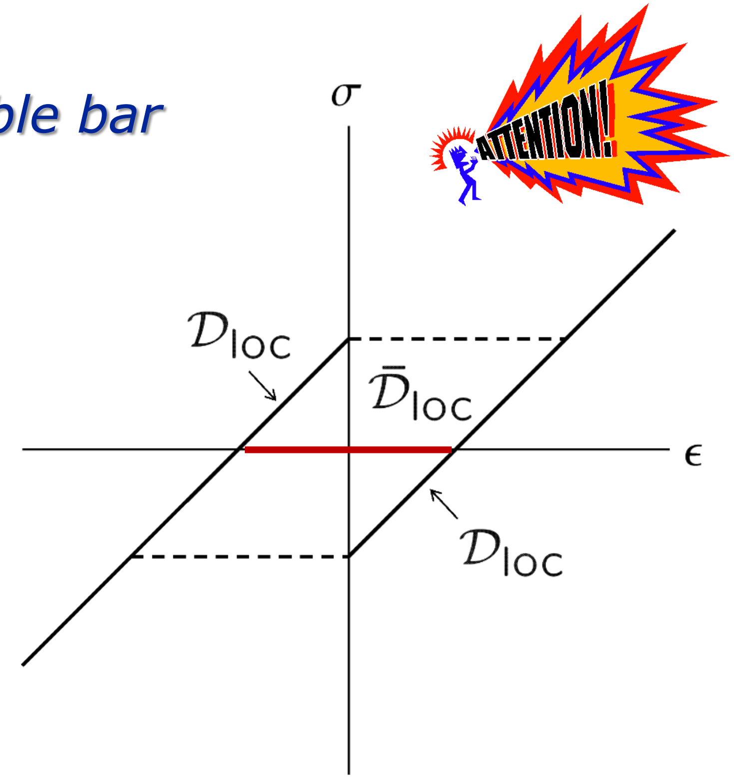
Conti, S., Müller, S. & Ortiz, M., *ARMA,* **229** (2018) 79-123.

The topology of Δ-convergence: Relaxation

- Example of non-attainment: *Bistable bar*



$$\left.\begin{array}{l}\sigma'(x) + f(x) = 0 \\ \bar{\epsilon} = \fint \epsilon(x)\, dx\end{array}\right\} \mathcal{E}$$



- Relaxed D is not a graph! (flag)
- Different from classical relaxation! (Maxwell line)

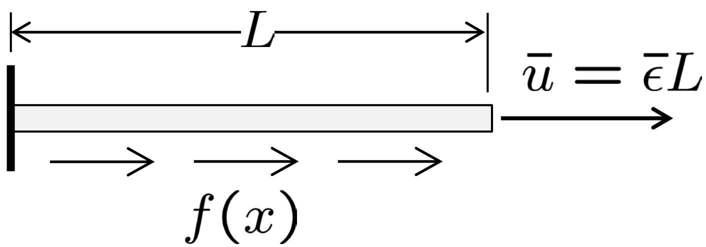
Theorem (One-dimensional bistable material)

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

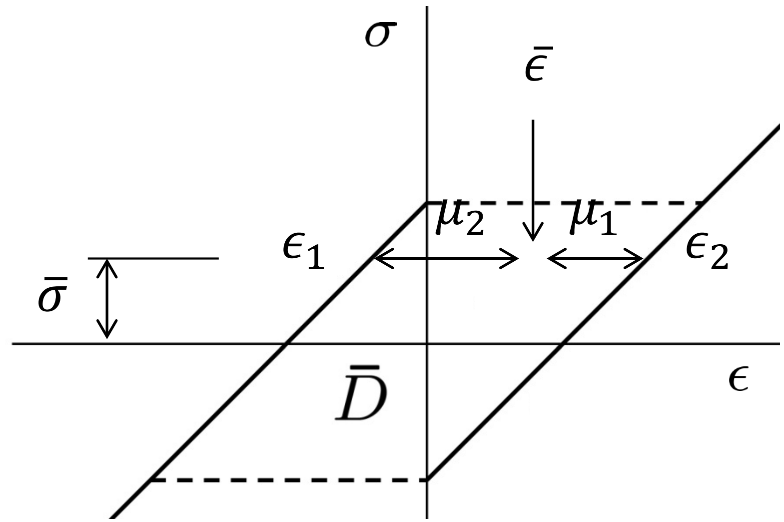
Conti, S., Müller, S. & Ortiz, M., *ARMA*, **229** (2018) 79-123.

The topology of Δ-convergence: Relaxation

- Example of non-attainment: *Bistable bar*



$$\left.\begin{aligned} &\sigma'(x) + f(x) = 0 \\ &\bar{\epsilon} = \textstyle{⨍} \epsilon(x)\, dx \end{aligned}\right\} \mathcal{E}$$



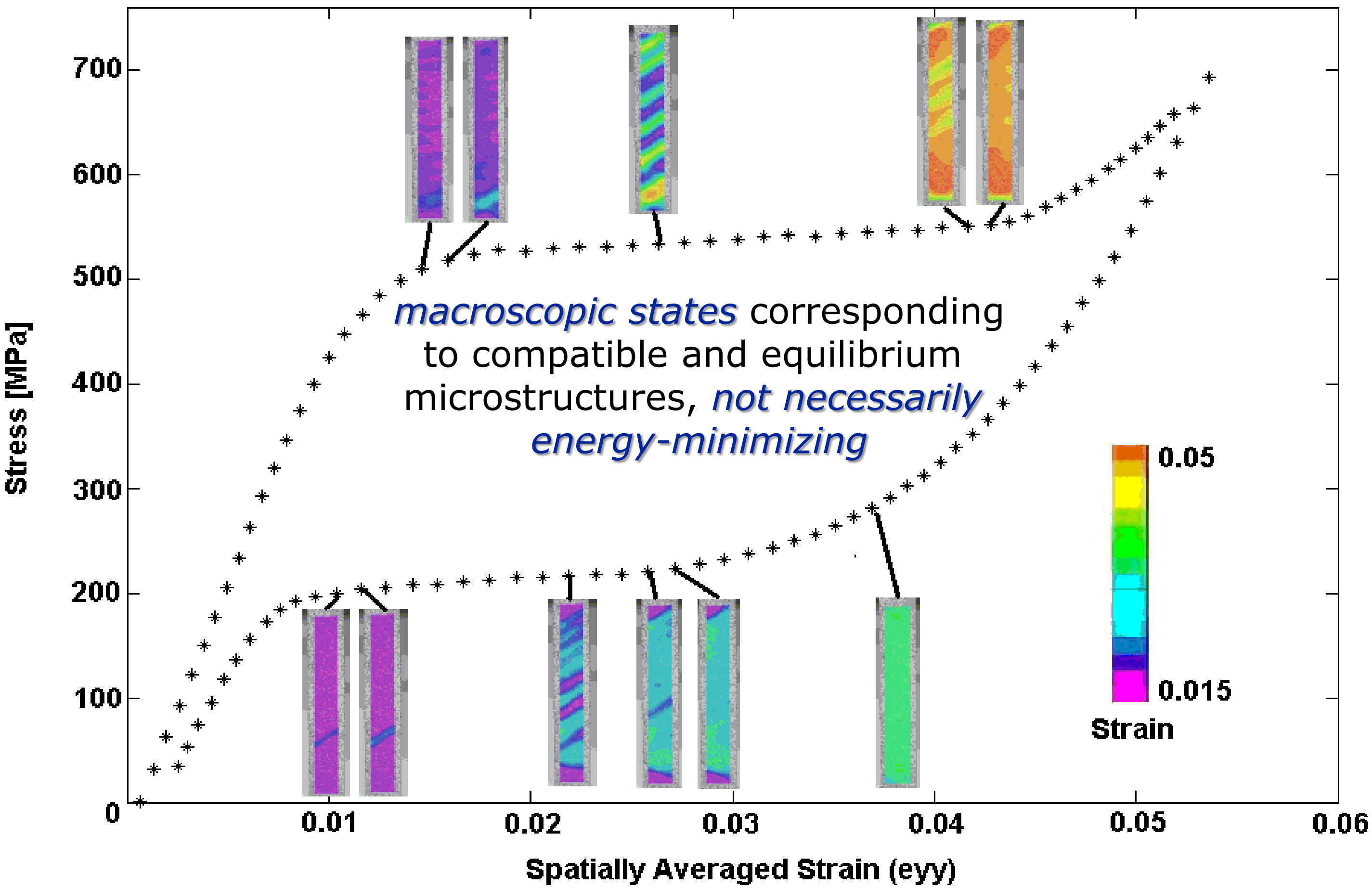
- Enough to consider case f = 0, stresses constant
- Add arbitrary strain oscillations matching mean strain

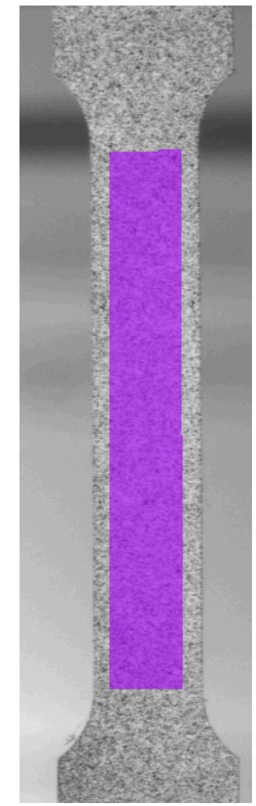
Theorem (One-dimensional bistable material)

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

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

The topology of Δ-convergence





Stress-induced martensitic phase transformation in thin sheets of Nitinol

S. Daly, G. Ravichandran and K. Bhattacharya, *Acta Mater.*, **55** (2007) 3593.

Extension to finite elasticity

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. $\exists u \in W^{1,p}$

$$\left.\begin{array}{llll} F = Du & \text{in } \Omega, & u = g_D & \text{on } \Gamma_D, \\ \operatorname{div} P + f = 0 & \text{in } \Omega, & P\nu = h_N & \text{on } \Gamma_N. \end{array}\right\} \text{Linear!}$$

Combine? $\mathcal{E} := \{(F,P) \in \mathcal{E}_0 : FP^T \text{symmetric a.e.}\}$

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

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

$J(F,P) = \int_\Omega \psi_{\mathcal{D}_{\text{loc}}}(F,P)\,dx$ Goal: minimize J in $\mathcal{E}$

Conti, S., Müller, S. & Ortiz, M.,*ARMA* **237,** 1–33 (2020).

Michael Ortiz
Warwick 2021

Extension to finite elasticity

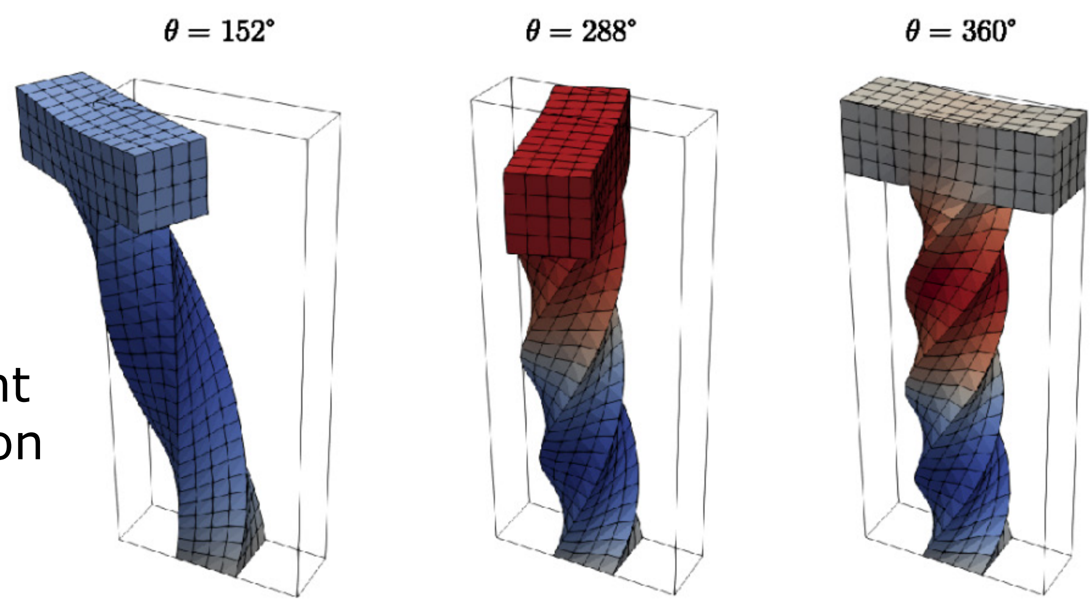
$$\psi_{\mathcal{D}_{\rm loc}}(F,P) := \inf\{\tfrac{1}{p}|F-F'|^p + \tfrac{1}{q}|P-P'|^q : (F',P') \in \mathcal{D}_{\rm loc}\}$$

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

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* $(F,P) \in \mathcal{E} \cap \mathcal{D}$.

Finite-element implementation



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)
- *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!*

Thank you!