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Data-Driven Mechanics: Constitutive Model-Free Approach

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

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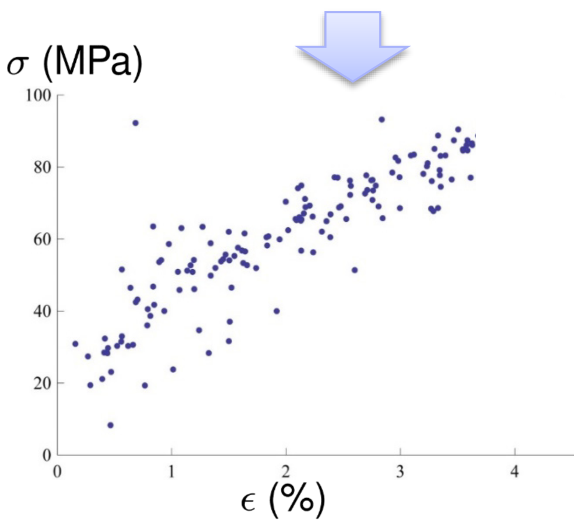
The anatomy of a field theory

- Scientific computing deals with the *field theories* of physics.

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	$\epsilon = \text{sym}\nabla u$	$\nabla \cdot \sigma + f = 0$	$\sigma = \mathbb{C}\,\epsilon$ (Hooke)
General	$\epsilon = \delta u$	$\partial\sigma + f = 0$	??

- Field equations are exactly known, *material law is determined from data*!

  - *Engineering predictions?*
  - *Mathematical solutions?*
  - *Numerical approximations?*



Example: Elastic bar

- *Phase space*, $Z = \{(\epsilon, \sigma)\}$.
- Note (ϵ, σ) work-conjugate
- Dimension of Z is even
- Compatibility: $\epsilon = u/L$
- Equilibrium: $\sigma A = k(u_0 - u)$
- Eliminate u: $\sigma A = k(u_0 - \epsilon L)$

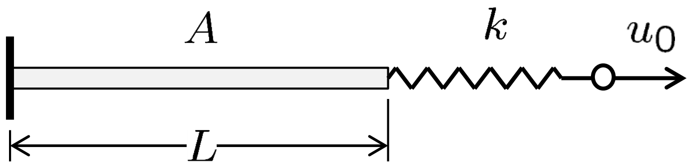
Definition (Constraint set)

The constraint set is the affine subspace of Z containing all admissible states (ϵ, σ) satisfying compatibility and equilibrium:

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

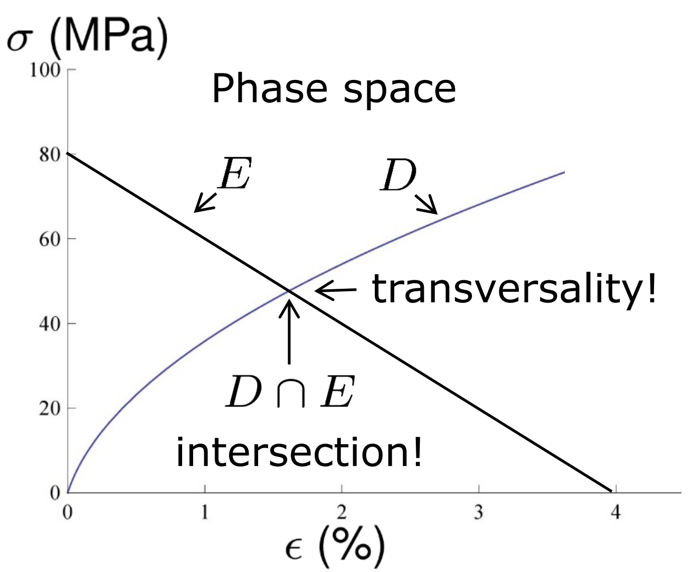
Definition (Material data set)

The material data set D is the subset of Z containing all the observed states (ϵ, σ).

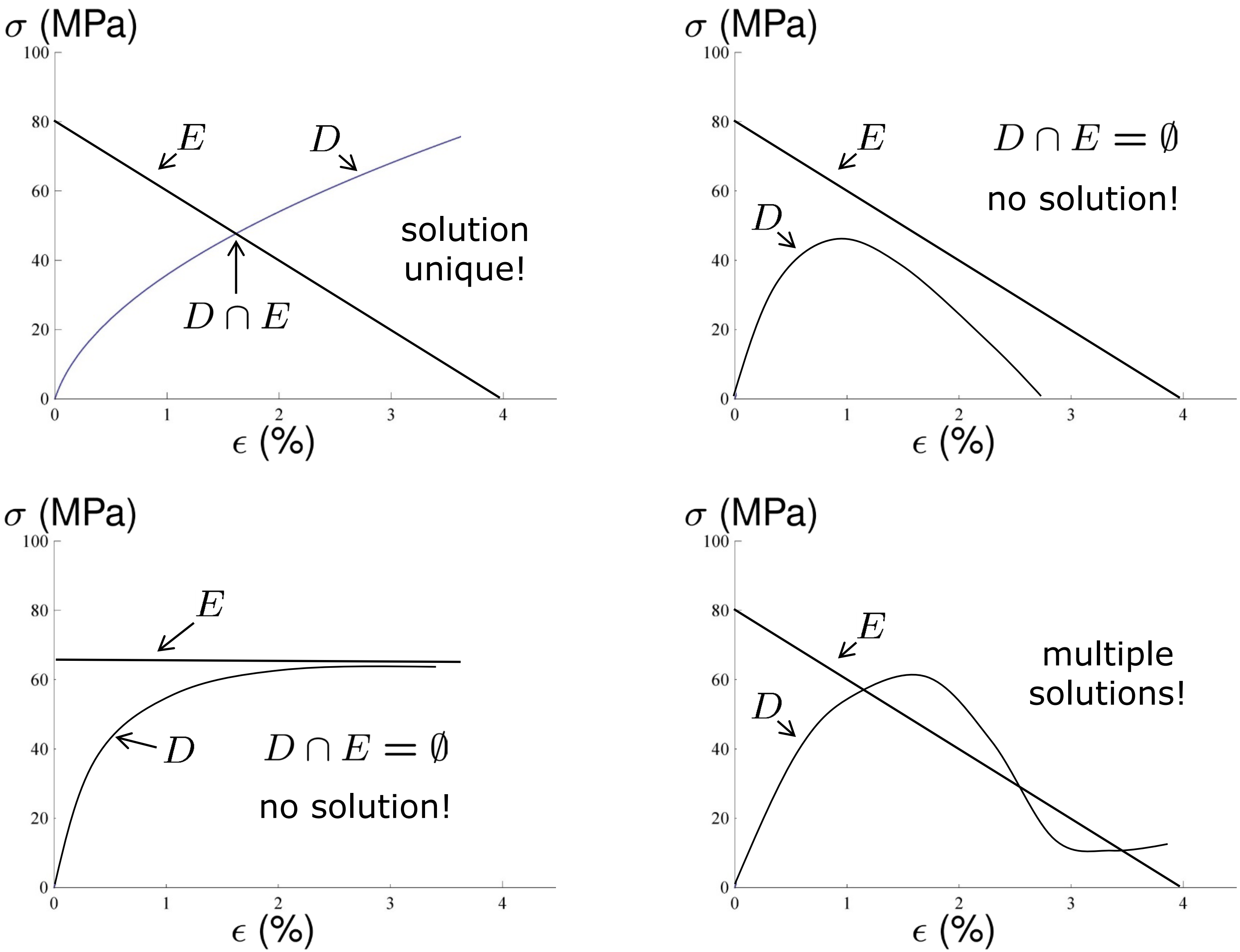


Definition (Classical solution)

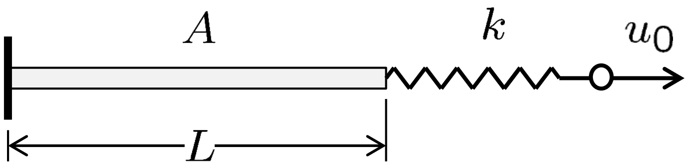
The classical solution is the intersection $D \cap E$, i. e., the set of all material states that are admissible.



Example: Elastic bar



Example: Elastic bar

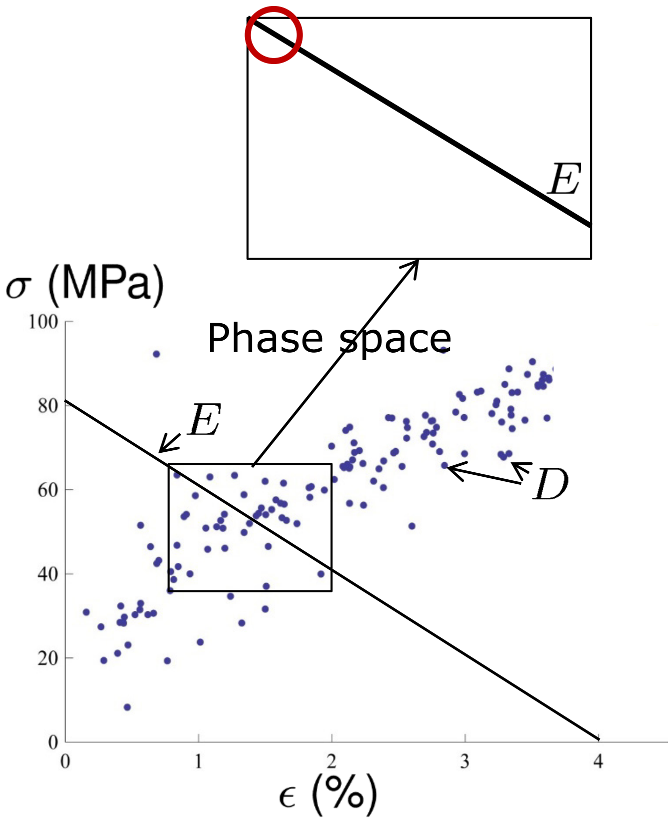


- Suppose that $D =$ point set
- Then, $D \cap E = \emptyset$
- No classical solutions! Must extend the concept of solution, classical approach is too rigid

Definition (Data-Driven solution)

An admissible state $z \in E$ is a Data-Driven solution if it minimizes the distance to the material data set D,

$$\mathrm{dist}(z, D) \to \min!, \quad z \in E$$

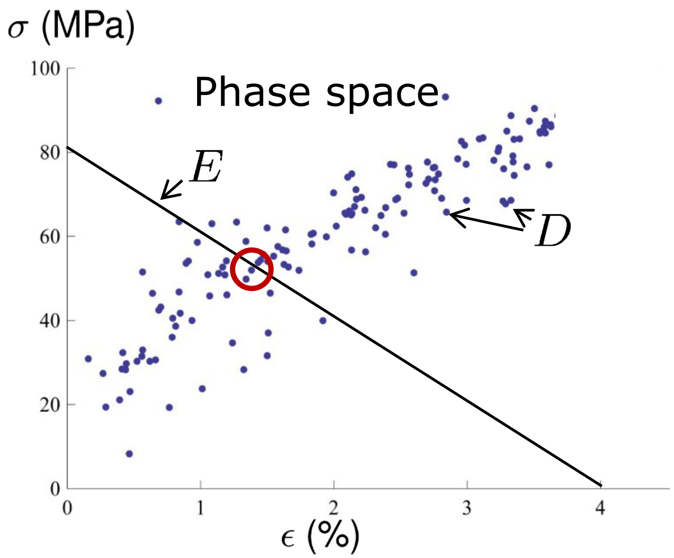


- Recall: $\mathrm{dist}^2(z, D) = \min_{y \in D} \|y - z\|^2$
- Data-Driven problem:

$$\min_{z \in E} \min_{y \in D} \|y - z\|^2 = \min_{y \in D} \min_{z \in E} \|y - z\|^2$$

- Find material state $y \in D$ and admissible state $z \in E$ closest to each other.

The Model-Free Data-Driven paradigm



Definition (Data-Driven Problem)

Given phase space $Z = \mathbb{R}^N \times \mathbb{R}^N$,

i) $D = \{\text{material data}\} \subset Z$,

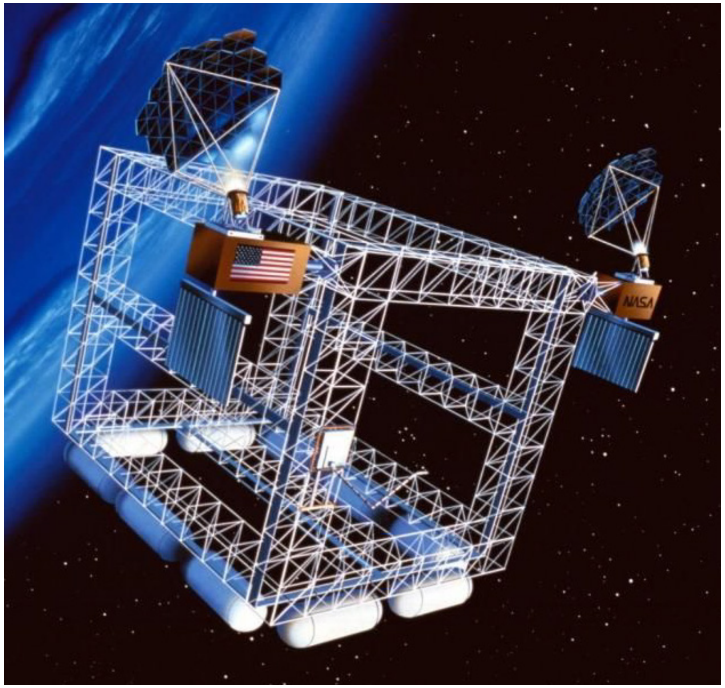
ii) $E = \{\text{field equations}\} \subset Z$,

Find: $\text{argmin}\{\|y - z\|^2 \ : \ y \in D, \ z \in E\}$

- Discussion:
  - Phase space Z determined by field equations (field-theory dependent)
  - Fundamental data (model-independent) $=$ Points in phase space
  - No material modeling, no loss of information, no biasing of the data
  - DD problem generalizes and subsumes classical field-theoretical problems

- Outlook:
  - Extensions to infinite dimensions? (e.g., linear elasticity)
  - Extensions to geometrically-nonlinear problems? (e.g., finite elasticity)
  - Well-posedness of Data-Driven problems? Convergence with respect to data?
  - Solvers? Computational performance? Scaling?

Structural/solid mechanics



- Finite-dimensional solids/structures
- m structural members or Gauss points
- Local phase spaces: For $e = 1, \dots, m$,

  $$Z_e = \{z_e := (\epsilon_e, \sigma_e)\} = \mathbb{R}^d \times \mathbb{R}^d$$

- Global phase space: With $N = md$,

  $$Z = \{z := (\epsilon, \sigma) = (\epsilon_e, \sigma_e)_{e=1}^m\} = \mathbb{R}^N \times \mathbb{R}^N$$

- Metric: With $\mathbb{C}_e^T = \mathbb{C}_e$, $\mathbb{C}_e > 0$, $w_e > 0$,

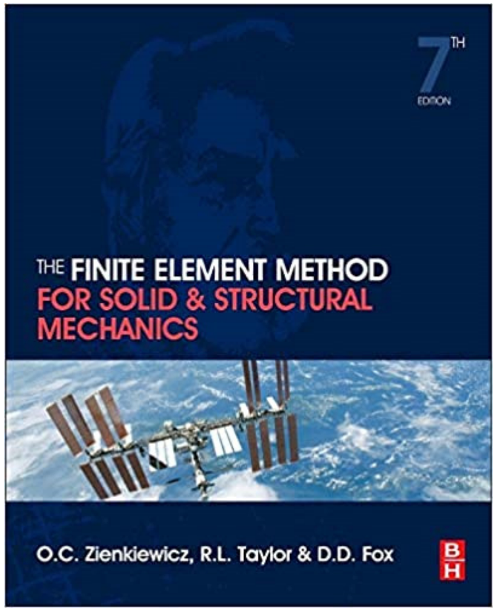
  $$\|z\|^2 = \sum_{e=1}^m w_e(\mathbb{C}_e \epsilon_e \cdot \epsilon_e + \mathbb{C}_e^{-1} \sigma_e \cdot \sigma_e).$$

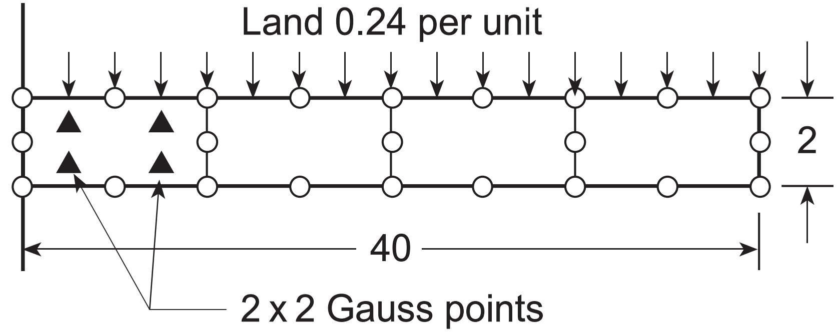
- Compatibility, equilibrium: For $e = 1, \dots, m$,

  $$\epsilon_e = B_e u + g_e, \qquad \sum_{e=1}^m w_e B_e^T \sigma_e = f$$

Structural/solid mechanics

- Finite-dimensional solids/structures





- Finite-element interpolation:

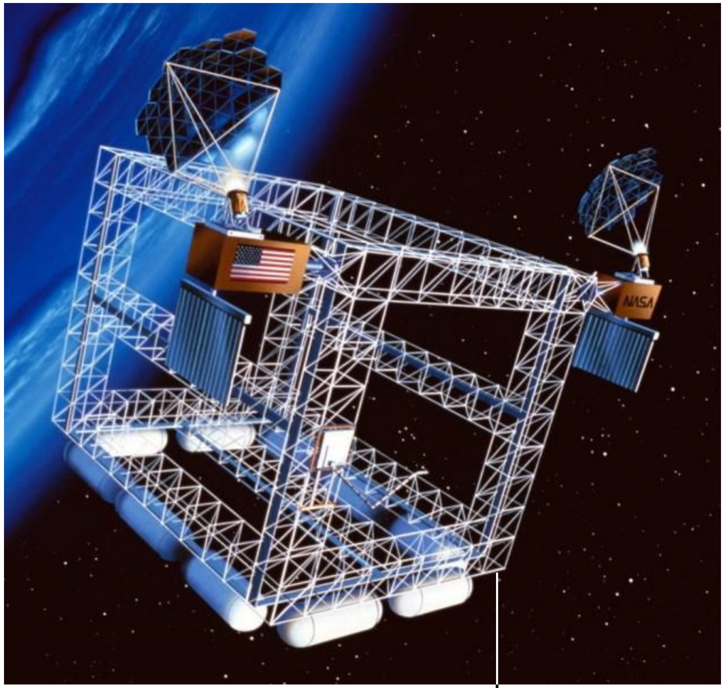
$$\mathbf{u} = \sum \mathbf{N}_i \mathbf{a}_i$$

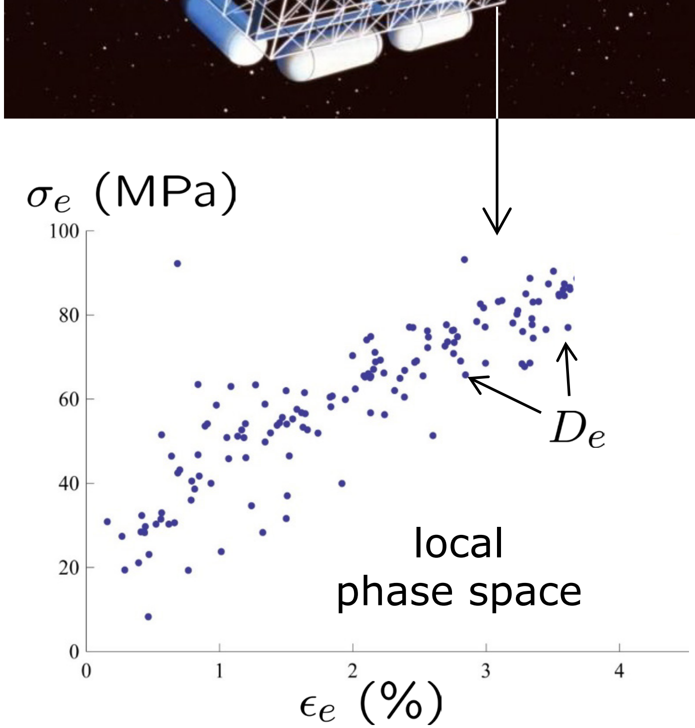
- Strains at Gauss quadrature points:

$$\boldsymbol{\varepsilon} = \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x}, & 0 \\ 0, & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial y}, & \frac{\partial}{\partial x} \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = \mathbf{S}\mathbf{u} \quad \Rightarrow \quad \mathbf{B}_i = \mathbf{S}N_i = \begin{bmatrix} \frac{\partial N_i}{\partial x}, & 0 \\ 0, & \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial y}, & \frac{\partial N_i}{\partial x} \end{bmatrix}$$

Structural/solid mechanics

- Finite-dimensional solids/structures
- m structural members or Gauss points
- Local phase spaces: For $e = 1, \dots, m$,
  $Z_e = \{z_e := (\epsilon_e, \sigma_e)\} = \mathbb{R}^d \times \mathbb{R}^d$
- Global phase space: With $N = md$,
  $Z = \{z := (\epsilon, \sigma) = (\epsilon_e, \sigma_e)_{e=1}^m\} = \mathbb{R}^N \times \mathbb{R}^N$
- Metric: With $\mathbb{C}_e^T = \mathbb{C}_e$, $\mathbb{C}_e > 0$, $w_e > 0$,
  $\|z\|^2 = \sum_{e=1}^m w_e(\mathbb{C}_e \epsilon_e \cdot \epsilon_e + \mathbb{C}_e^{-1} \sigma_e \cdot \sigma_e)$.
- Compatibility, equilibrium: For $e = 1, \dots, m$,
  $\epsilon_e = B_e u + g_e, \quad \sum_{e=1}^m w_e B_e^T \sigma_e = f$
- Admissible space: Given $f \in \mathbb{R}^n$, $g \in \mathbb{R}^N$,
  $E = \{(\epsilon, \sigma) \in Z \; : \; \epsilon = Bu + g, \; B^T W \sigma = f\}$
- Local material sets: $D_e \subset Z_e$, $e = 1, \dots, m$,
- Global material set: $D = D_1 \times \cdots \times D_m \subset Z$
- Data-Driven problem: Given Z, D and E, find
  $\mathrm{argmin}\{\|y - z\|^2, \; y \in D, \; z \in E\}$





Field-theoretical structure of constraint spaces

Definition (Constraint set)

The constraint subspace E is the set of points $(\epsilon, \sigma) \in Z = \mathbb{R}^N \times \mathbb{R}^N$ such that

$$\epsilon = Bu + g, \quad B^T \sigma = f, \qquad \text{(field eqs)}$$

with $B \in L(\mathbb{R}^n, \mathbb{R}^N)$, $n \leq N$, $f \in \mathbb{R}^n$, $g \in \mathbb{R}^N$.

Theorem (Constraint sets)

Let $Z = \mathbb{R}^N \times \mathbb{R}^N$ and $B \in L(\mathbb{R}^n, \mathbb{R}^N)$, $n \leq N$. Then,

i) *The system of equations (field eqs) has solutions (u, ϵ, σ) if and only if*

$$f^T v = 0, \quad \forall v \in \mathrm{Ker}(B).$$

ii) *The solutions of (field eqs) satisfy the work-energy identity*

$$f^T u = \sigma^T (\epsilon - g).$$

iii) *If condition (i) is satisfied, then the set E of all solutions of (field eqs) is an affine subspace of Z of dimension N and co-dimension N.*

Field-theoretical structure of constraint spaces

Proof.

i) The equations in (field eqs) are decoupled. The first is always soluble. By the Fredholm alternative theorem of linear algebra, the second is soluble iff (i) holds.

ii) Suppose that (i) holds and let (u, ϵ, σ) be a solution of (field eqs). Then,

$$f^T u = \sigma^T B u = \sigma^T (\epsilon - g).$$

iii) If (i) holds, then there exists $\sigma_0 \in \mathbb{R}^N$ such that $f = B^T \sigma_0$, and the affine space E defined by (field eqs) is a translate of the linear subspace E_0 defined by the homogeneous constraints

$$\epsilon = Bu, \quad B^T \sigma = 0, \qquad \text{(hom field eqs)}$$

Evidently, $E_0 = E_\epsilon \times E_\sigma$, where E_ϵ is the linear subspace defined by the first of (hom field eqs) and E_σ is the linear subspace defined by the second. Therefore, we have

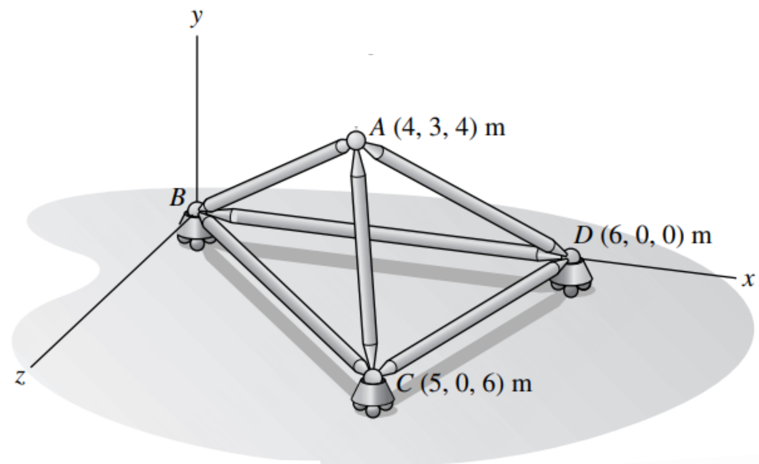
$$\dim(E_0) = \dim(E_\epsilon) + \dim(E_\sigma) = \dim(\mathrm{Im}(B)) + \dim(\mathrm{Ker}(B^T)) = N.$$

Since $Z = \mathbb{R}^N \times \mathbb{R}^N$, it follows that the constraint set E is an affine subspace of Z of dimension N and co-dimension N. □

Field-theoretical structure of constraint spaces

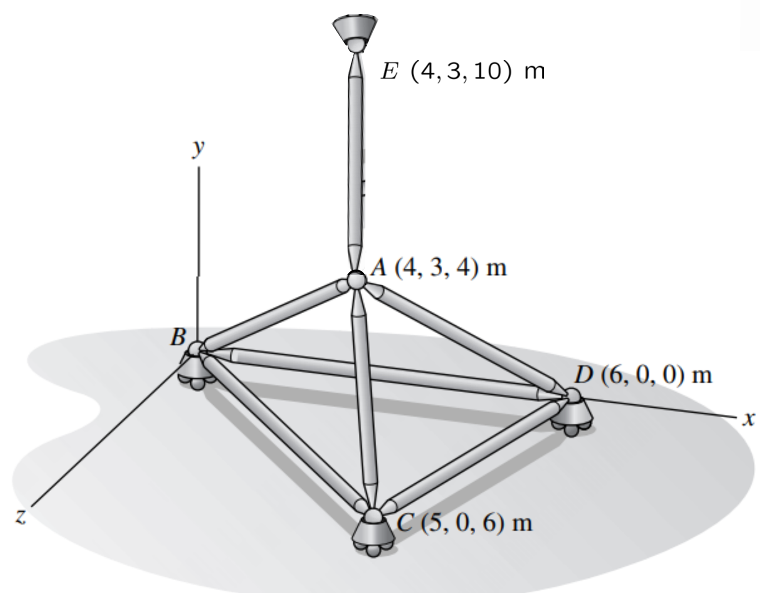
Example

- $m = 6$, $d = 1$, $N = md = 6$.
- Suppose $f = 0 \Rightarrow B^T\sigma = 0$.
- From A: $\sigma_{\rm AB} = \sigma_{\rm AB} = \sigma_{\rm AB} = 0$.
- From B, C, D: $\sigma_{\rm BC} = \sigma_{\rm CD} = \sigma_{\rm DB} = 0$.
- Together: ${\rm Ker}(B^T) = 0 \Rightarrow {\rm Im}(B) = \mathbb{R}^6$,
- $\dim(E) = \dim {\rm Ker}(B^T) + \dim {\rm Im}(B) = N$.

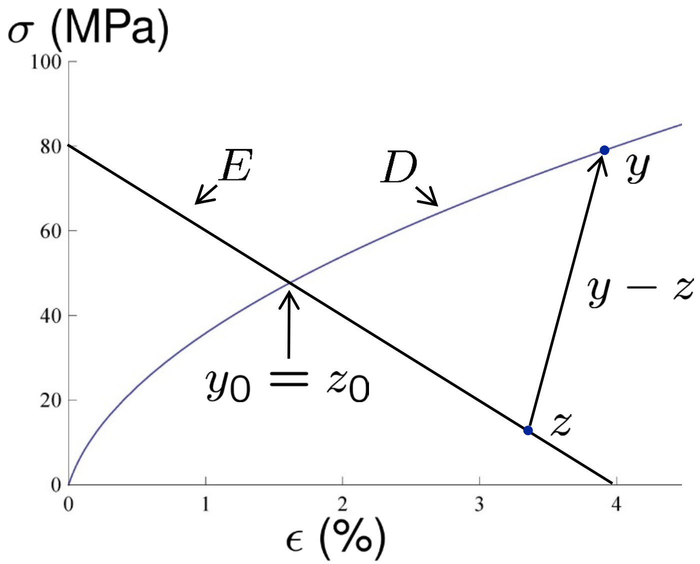


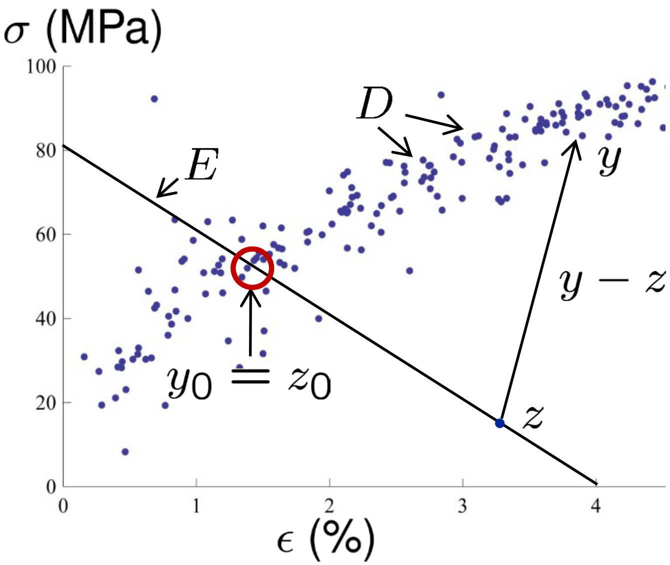
Example

- $m = 7$, $d = 1$, $N = md = 7$.
- Suppose $f = 0 \Rightarrow B^T\sigma = 0$. Fix $\sigma_{\rm AE}$.
- From $A \Rightarrow \{\sigma_{\rm AB}, \sigma_{\rm AB}, \sigma_{\rm AB}\}$.
- From B, C, $D \Rightarrow \{\sigma_{\rm BC}, \sigma_{\rm CD}, \sigma_{\rm DB}\}$.
- Together: ${\rm Ker}(B^T) = \mathbb{R} \Rightarrow {\rm Im}(B) = \mathbb{R}^6$,
- $\dim(E) = \dim {\rm Ker}(B^T) + \dim {\rm Im}(B) = N$.



The Model-Free Data-Driven paradigm





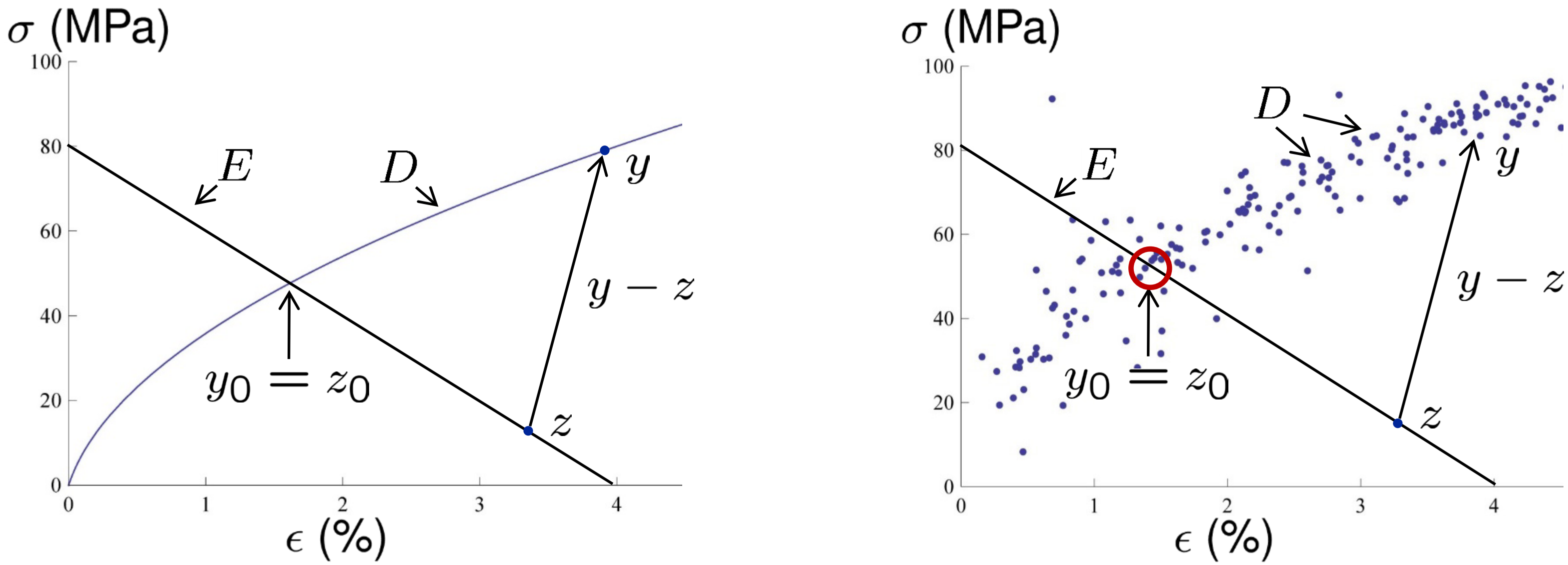
Theorem (Existence of DD solutions)

Let $Z = \mathbb{R}^N \times \mathbb{R}^N$, E an affine subspace of Z and D a non-empty closed subset of Z. Suppose that the transversality condition

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

holds for all $y \in D$, $z \in E$, with constants $c > 0$ and $b \geq 0$. Then, the DD problem has at least one solution.

The Model-Free Data-Driven paradigm

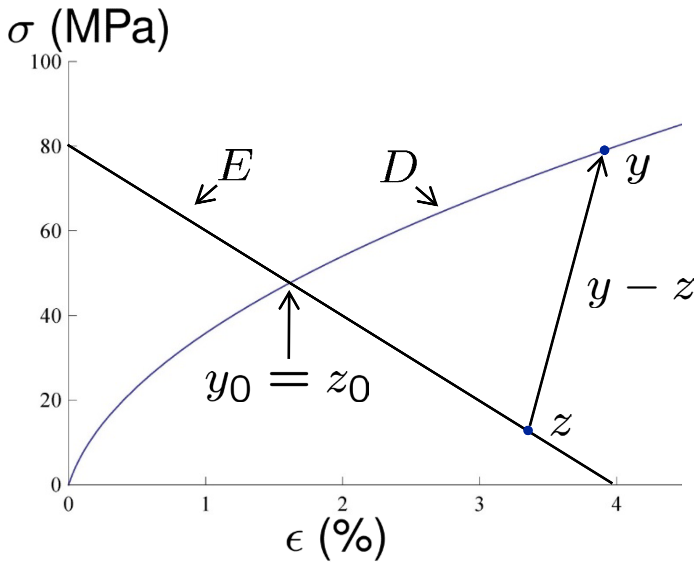


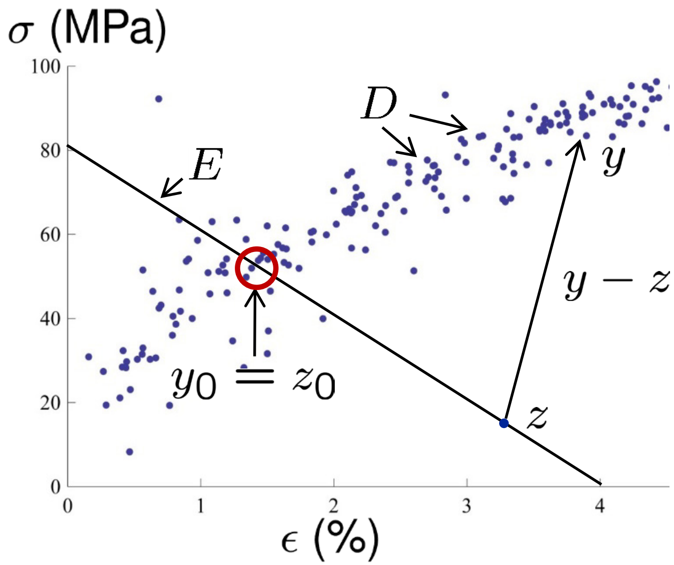
- Transversality between D and E is a necessary condition for existence.
- Transversality requires D and E to increasingly separate from each other:

$$\|y - z\| \to +\infty \quad \text{if:} \quad \|y - y_0\| \to +\infty, \quad \text{or} \quad \|z - z_0\| \to +\infty.$$

- Transversality condition makes sense for general (non-manifold) material data sets, including point sets.

The Model-Free Data-Driven paradigm





Proof.

Let $(y_h, z_h) \subset D \times E$ be a minimizing sequence. By transversality, (y_h) and (z_h) are bounded in Z. Passing to subsequences, there is $(y, z) \in Z \times Z$ such that $(y_h, z_h) \to (y, z)$. By the closedness of E and D, it follows that $(y, z) \in D \times E$. By the continuity of the norm,

$$\inf_{(y',z')\in D\times E} \|y' - z'\|^2 \leq \|y - z\|^2 = \lim_{h\to\infty} \|y_h - z_h\|^2 = \inf_{(y',z')\in D\times E} \|y' - z'\|^2,$$

and (y, z) is a DD solution. □

Classical solutions are recovered from DD solutions

Lemma (Elastic structures, transversality)

Let $Z = \mathbb{R}^N \times \mathbb{R}^N$, E *affine subspace of* Z, $\dim(E) = N$, $D = \{\sigma = \mathbb{C}\epsilon\}$. *Suppose that* $B^T \mathbb{C} B > 0$. *Then,* E *and* D *are transversal.*

Proof. *(reading assignment)*

Recall $E_0 = \mathrm{Im}(B) \times \mathrm{Ker}(B^T)$. We claim that there is $c > 0$ such that

$$\|y - z'\| \geq c(\|y\| + \|z'\|), \qquad \forall y \in D,\ z' \in E_0.$$

With $z' = (\epsilon', \sigma')$, $\epsilon' \in \mathrm{Im}(B)$ and $\sigma' \in \mathrm{Ker}(B^T)$, we have

$$\|y - z'\|^2 \geq \mathrm{dist}^2(z', D) = \frac{1}{2}\mathbb{C}^{-1}(\sigma' - \mathbb{C}\epsilon') \cdot (\sigma' - \mathbb{C}\epsilon').$$

By the orthogonality: $\|y - z'\|^2 \geq \frac{1}{2}\mathbb{C}^{-1}\sigma' \cdot \sigma' + \frac{1}{2}\mathbb{C}\epsilon' \cdot \epsilon' = \frac{1}{2}\|z'\|^2$, and

$$\|y - z'\| \geq \frac{1}{2}\|y - z'\| + \frac{1}{2}\mathrm{dist}(z', D) \geq \frac{1}{2}\|y - z'\| + \frac{1}{2\sqrt{2}}\|z'\| \geq c(\|y\| + \|z'\|).$$

Let z_0 be the unique elastic solution, $y \in D$, $z \in E$, $z' = z - z_0 \in E_0$. Then,

$$\|z'\| \geq \|z\| - \|z_0\| \text{ and } \|y - z\| \geq c(\|y\| + \|z\|) - c\,\|z_0\|. \qquad \square$$

Classical solutions are recovered from DD solutions

Theorem (Elastic structures)

Let $Z = \mathbb{R}^N \times \mathbb{R}^N$, E *affine subspace of* Z, $\dim(E) = N$, $D = \{\sigma = \mathbb{C}\epsilon\}$, $B^T \mathbb{C} B > 0$. *Then, there is a unique DD solution such that* $\sigma = \mathbb{C}\epsilon$.

Proof. *(reading assignment)*

By the transversality lemma and the existence theorem, it follows that there are DD solutions. Let $z = (\epsilon, \sigma) \in E$ be a DD solution. By minimality of the distance,

$$\frac{1}{2}\mathbb{C}^{-1}(\sigma - \mathbb{C}\epsilon) \cdot (\sigma' - \mathbb{C}\epsilon') = 0, \text{ for all } z' = (\epsilon', \sigma') \in E_0.$$

Choosing $\epsilon' = 0$ and $\sigma' \in \mathrm{Ker}(B^T)$: $\quad \mathbb{C}^{-1}\sigma - \epsilon \in \mathrm{Ker}(B^T)^\perp = \mathrm{Im}(B)$.

Hence, there is $u \in \mathbb{R}^n$ such that: $\quad \mathbb{C}^{-1}\sigma - \epsilon = Bu$.

Choosing $\sigma' = 0$ and $\epsilon' \in \mathrm{Im}(B)$: $\quad \sigma - \mathbb{C}\epsilon \in \mathrm{Im}(B)^\perp = \mathrm{Ker}(B^T)$.

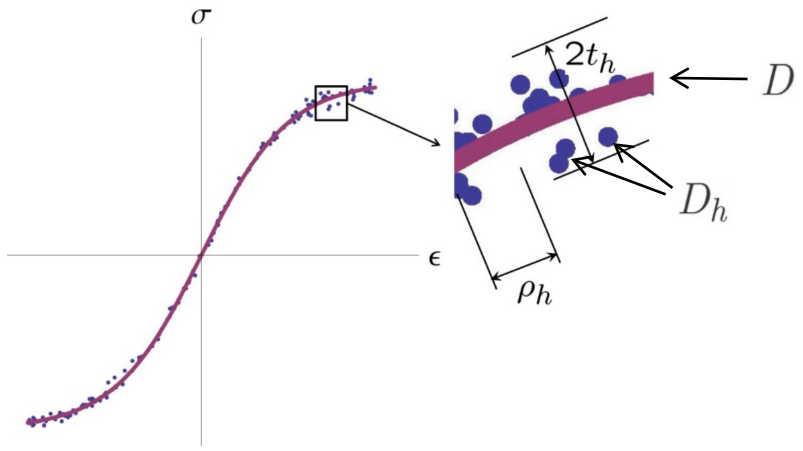
Hence: $B^T(\sigma - \mathbb{C}\epsilon) = B^T \mathbb{C} B u = 0 \Rightarrow u = 0$, and $\sigma = \mathbb{C}\epsilon$.

To prove uniqueness, let z' and z'' be two DD solutions. Then, by linearity, $z' - z'' \in D \cap E_0$ is a DD solution with zero forcing. It follows that

$$\|z' - z''\|^2 = 2\mathrm{dist}^2(z' - z'', D) = 0 \Rightarrow z' = z''.$$

□

The topology of Data Convergence



Theorem

Let (D_h) be a sequence of subsets of Z, D a subset of Z and E an affine subspace. Let z be an isolated point of $D \cap E$ and let $y_h, z_h \in Z$ be such that

$$(y_h, z_h) \in \operatorname{argmin}\{|y' - z'|,\ y' \in D_h,\ z' \in E\}.$$

Suppose that:

i) *There is a sequence $\rho_h \downarrow 0$ such that:* $\operatorname{dist}(y, D_h) \leq \rho_h, \quad \forall y \in D.$

ii) *There is a sequence $t_h \downarrow 0$ such that:* $\operatorname{dist}(y, D) \leq t_h, \quad \forall y \in D_h.$

iii) *(Transversality) There is a constant $0 \leq \lambda < 1$ s. t., for all $y \in D$,*

$$\|P_E y - z\| \leq \lambda \|y - z\|,$$

Then: $$\|z_h - z\| \leq \frac{t_h + \lambda(t_h + \rho_h)}{1 - \lambda} \quad \text{and} \quad \lim_{h \to \infty} \|z_h - z\| = 0.$$

The topology of Data Convergence

Proof. *(reading assignment)*

By assumption (i), we can find $\xi_h \in D_h$ such that $\|\xi_h - z\| \leq \rho_h$

By optimality: $\text{dist}(y_h, E) \leq \text{dist}(\xi_h, E)$

Then, we have: $\|y_h - z_h\| = \text{dist}(y_h, E) \leq \text{dist}(\xi_h, E) \leq \|\xi_h - z\| \leq \rho_h$

By assumption (ii), we can find $\eta_h \in D$ such that: $\|y_h - \eta_h\| \leq t_h$

By the triangle inequality: $\|z_h - z\| \leq \|z_h - P_E\eta_h\| + \|P_E\eta_h - z\|$

By the contractivity of projections:

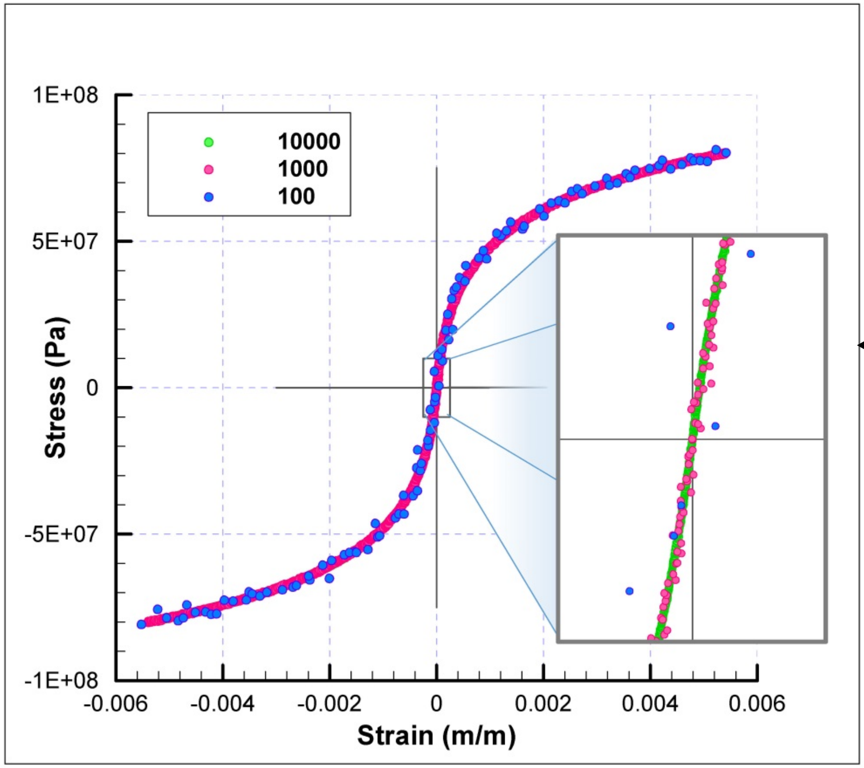
$$\|z_h - P_E\eta_h\| = \|P_E y_h - P_E\eta_h\| = \|P_E(y_h - \eta_h)\| \leq \|y_h - \eta_h\| \leq t_h$$

By transversality, with $0 \leq \lambda < 1$: $\|P_E\eta_h - z\| \leq \lambda\|\eta_h - z\|$

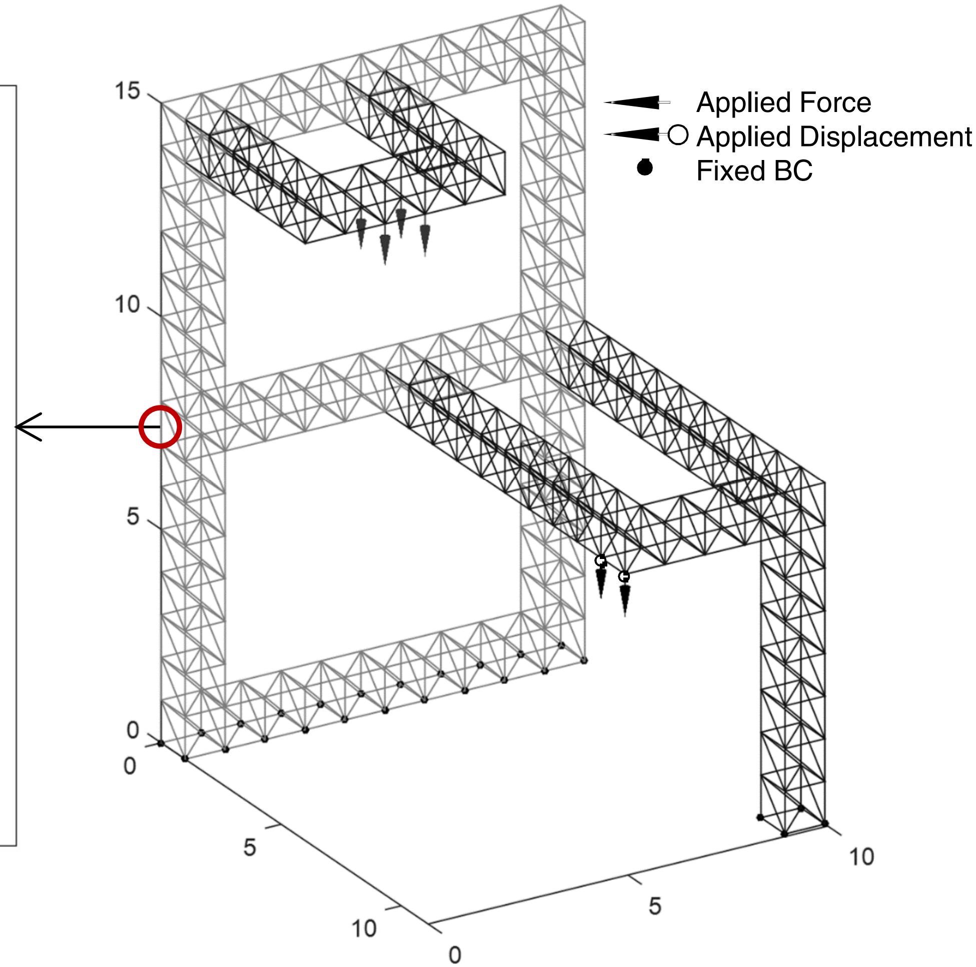
Triangulating again: $\|\eta_h - z\| \leq \|\eta_h - y_h\| + \|y_h - z_h\| + \|z_h - z\|$

Collecting estimates: $\|z_h - z\| \leq t_h + \lambda(t_h + \rho_h + \|z_h - z\|)$ $\square$

The topology of Data Convergence



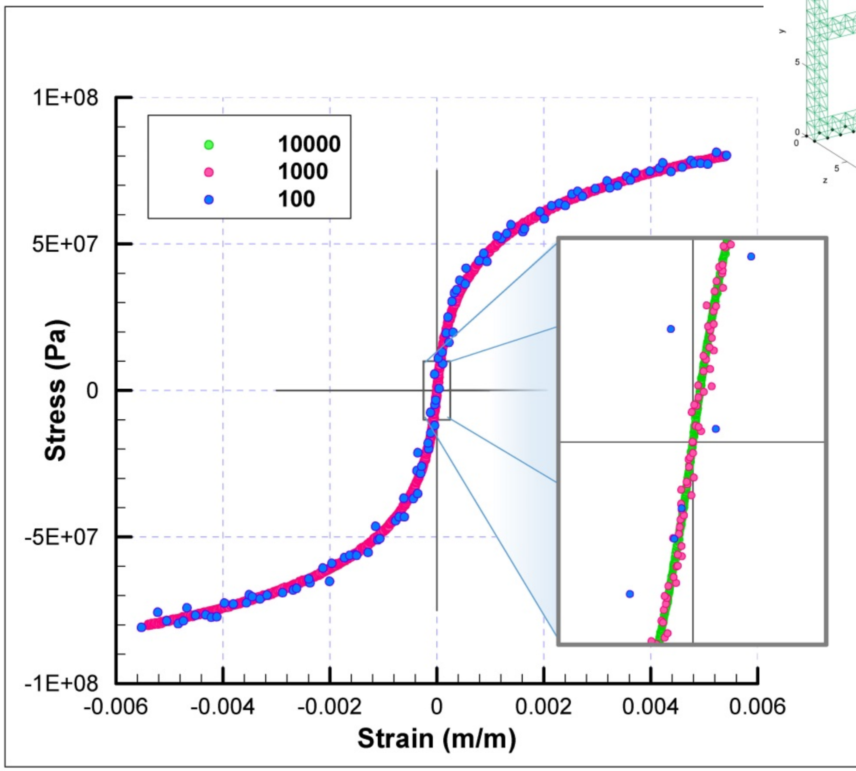
Sequence of
uniformly converging data sets
(increasing number of points, decreasing scatter)

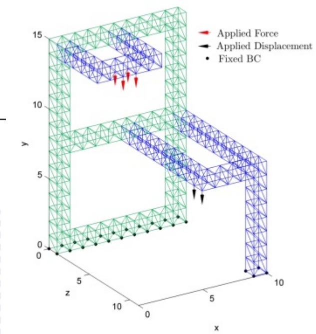


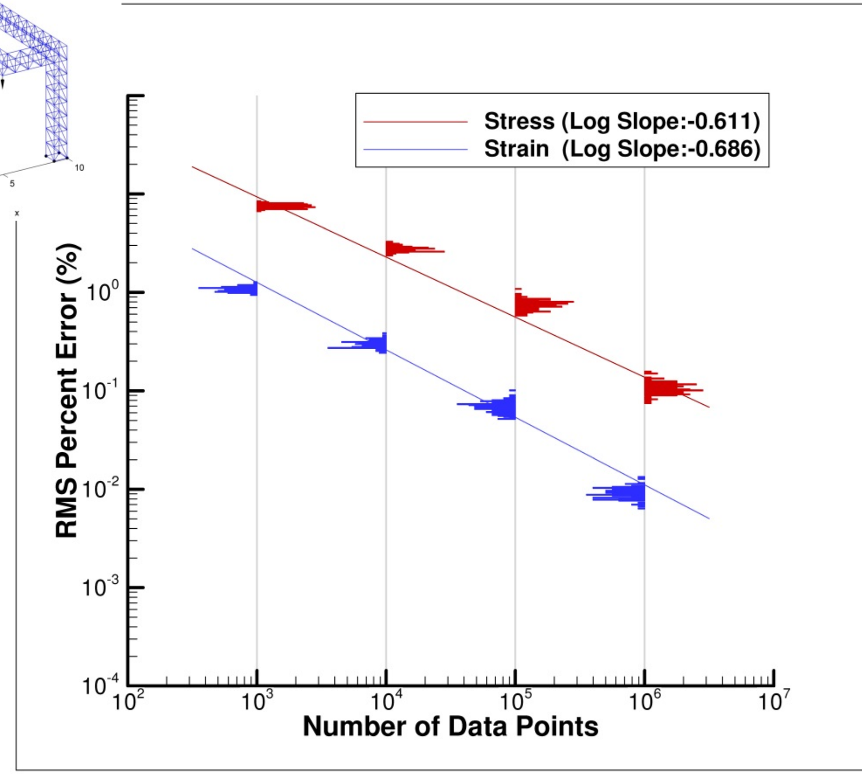
3D truss structure

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

The topology of Data Convergence







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

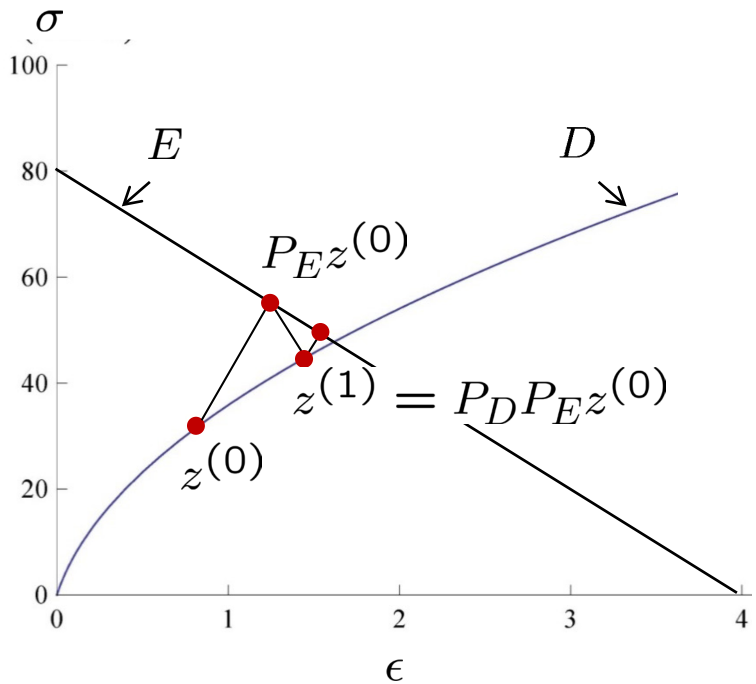
Convergence with respect to material data set towards solution of limiting problem (nonlinear elasticity)

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

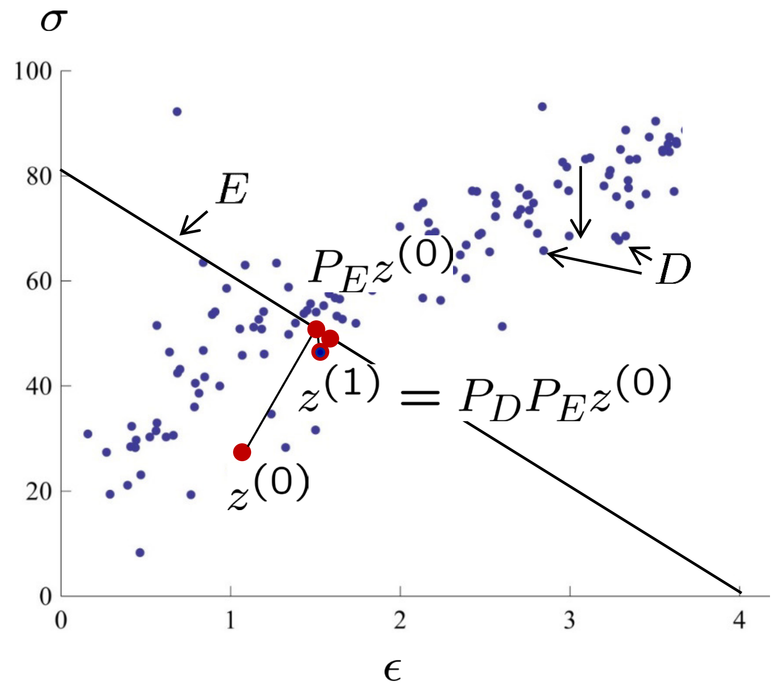
Solvers: Fixed-point iteration

- Find: $\text{argmin}\{\text{dist}(z, D),\ z \in E\}$
- Solver: $z^{(k)} = P_D \circ P_E z^{(k-1)}$
  - $P_D :=$ closest-point projection onto D.
  - $P_E :=$ closest-point projection onto E.

- *Implementation?*
- *Convergence?*



Fixed-point iteration, manifold data set D

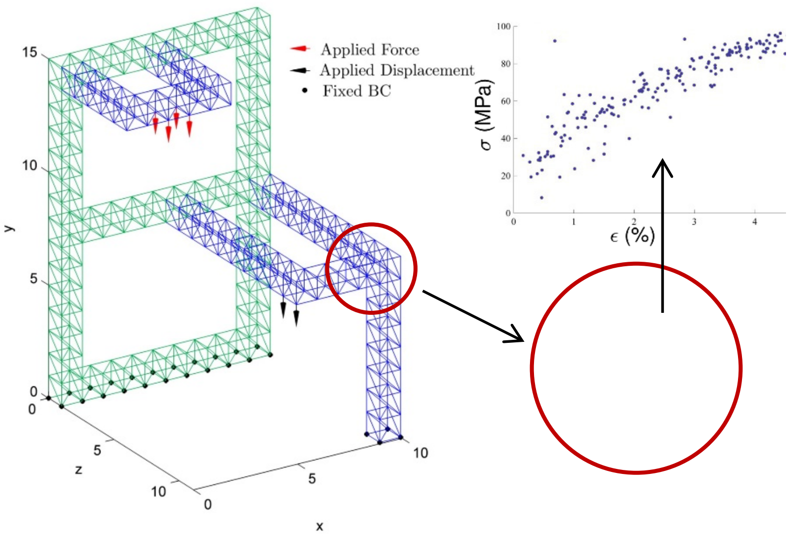


Fixed-point iteration, point data set D

Solvers: Fixed-point iteration

- Degrees of freedom: $(u_i)_{i=1}^n$
- Phase space: $Z = \{(\epsilon_e, \sigma_e)_{e=1}^m\}$
- Norm: $\|(\epsilon, \sigma)\|^2 = \sum_{e=1}^m w_e \left(\mathbb{C}_e \epsilon_e^2 + \mathbb{C}_e^{-1} \sigma_e^2\right.$
- Constraint set: $E = \{\epsilon = Bu,\ B^T W \sigma = f\}$
- Data-Driven problem:

$$\min_{(\epsilon', \sigma') \in D} \left(\min_{(\epsilon, \sigma) \in E} \|(\epsilon - \epsilon', \sigma - \sigma')\|^2 \right)$$



- Projection to E (inner minimization at fixed (ϵ', σ')): i) Enforce compatibility directly by writing $\epsilon = Bu$; ii) Enforce equilibrium through a Lagrange multiplier v,

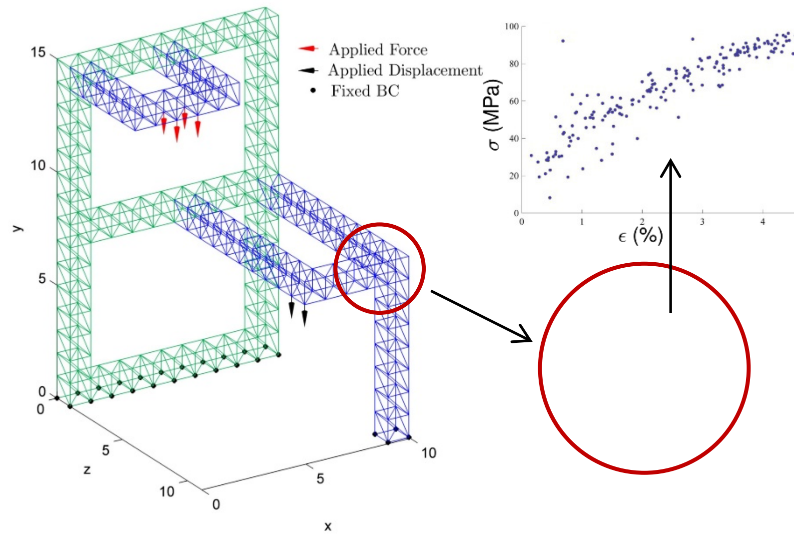
$$\delta\Big(\|(Bu - \epsilon', \sigma - \sigma')\|^2 - (B^T W \sigma - f) \cdot v \Big) = 0$$

- Euler-Lagrange equations: $(B^T \mathbb{C} W B) u = B^T \mathbb{C} \epsilon'$, $\quad (B^T \mathbb{C} W B) v = f - B^T \sigma'$.
- State update: $\quad \epsilon = Bu; \quad \sigma = \sigma' + \mathbb{C} B v$.
- Two standard linear problems! (regardless of material behavior).
- DD leads to (material-independent) standardization of solvers.

Solvers: Fixed-point iteration

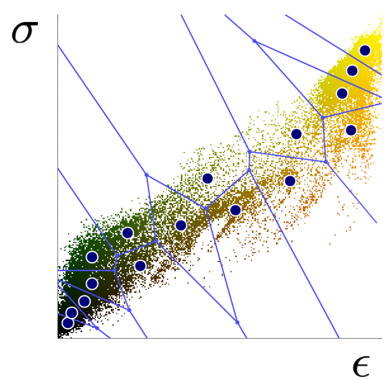
- Degrees of freedom: $(u_i)_{i=1}^n$
- Phase space: $Z = \{(\epsilon_e, \sigma_e)_{e=1}^m\}$
- Norm: $\|(\epsilon, \sigma)\|^2 = \sum_{e=1}^m w_e \big(\mathbb{C}_e \epsilon_e^2 + \mathbb{C}_e^{-1} \sigma_e^2$
- Constraint set: $E = \{\epsilon = Bu,\ B^T W \sigma = f\}$
- Data-Driven problem:

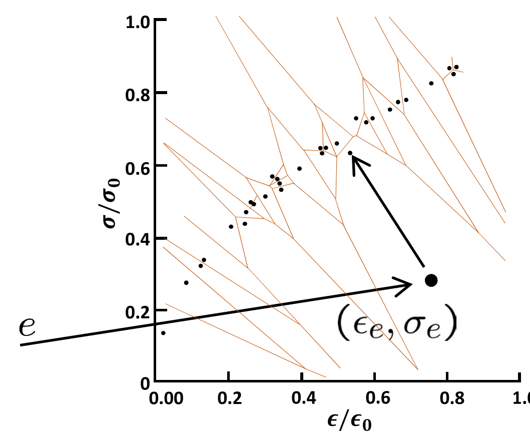
$$\min_{(\epsilon',\sigma')\in D} \left(\min_{(\epsilon,\sigma)\in E} \|(\epsilon - \epsilon', \sigma - \sigma')\|^2 \right)$$



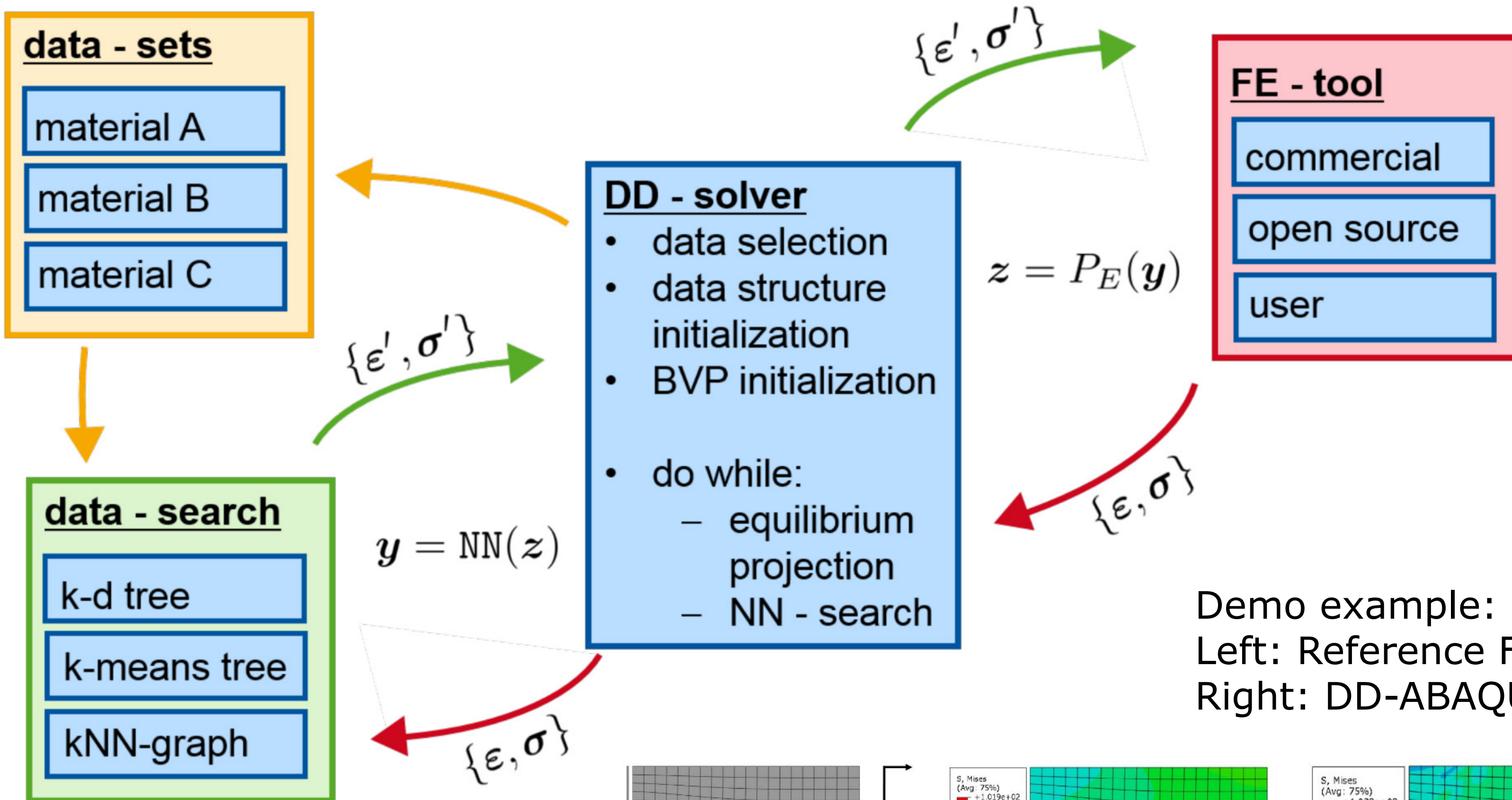
- Outer minimization: Projection onto (closest point in the) material data set D
- Fast searching algorithm
- Requires data structures
- 'Learning' structure of D
- Set-oriented (lossless) ML!

cf. S. Reese's lecture!
Wednesday 12, 14:00-14:45

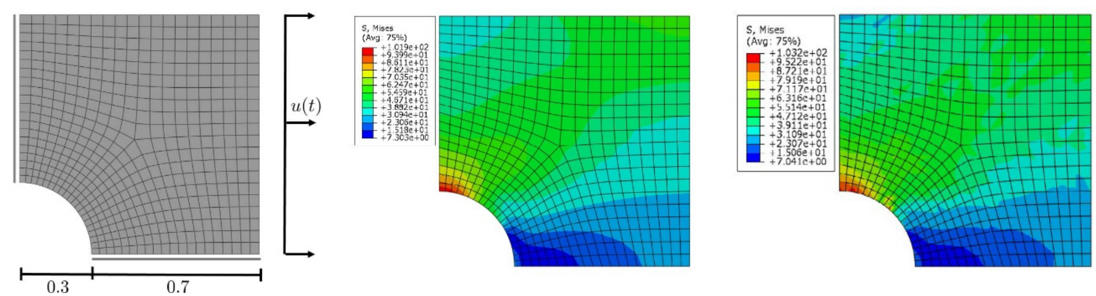




Solvers: Fixed-point iteration – Using commercial software

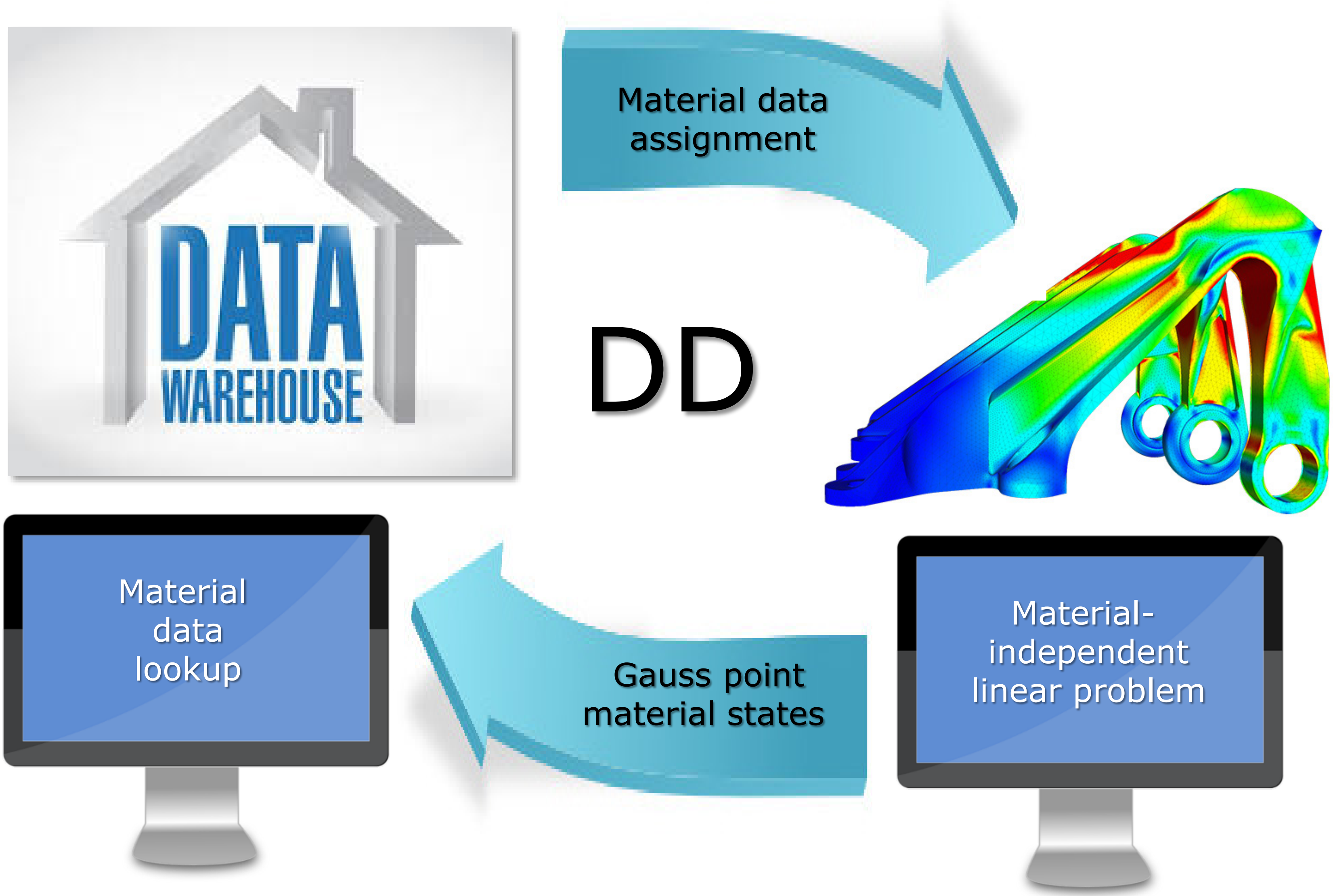


Demo example:
Left: Reference FE
Right: DD-ABAQUS



E. Prume, L. Stainier, M. Ortiz, and S. Reese,
Proc. Appl. Math. Mech., 5 October 2022.

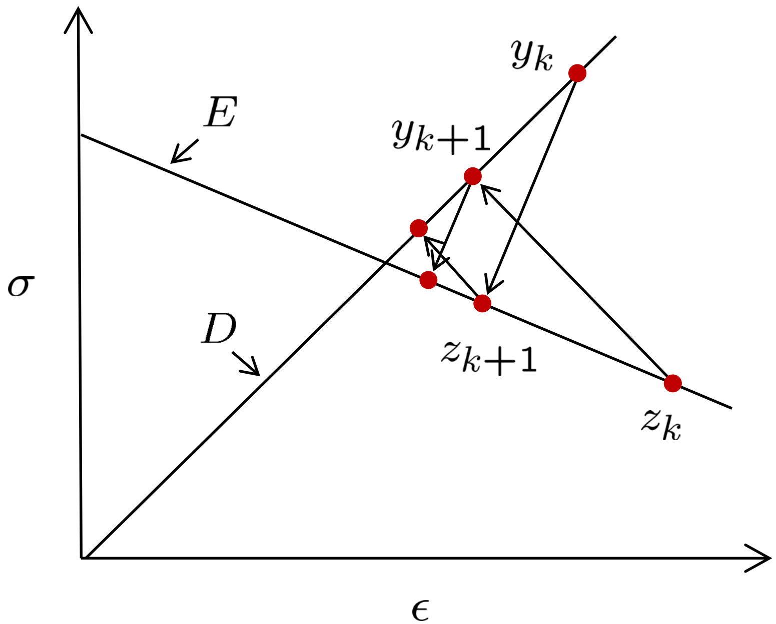
Solvers: Fixed-point iteration – Data flow



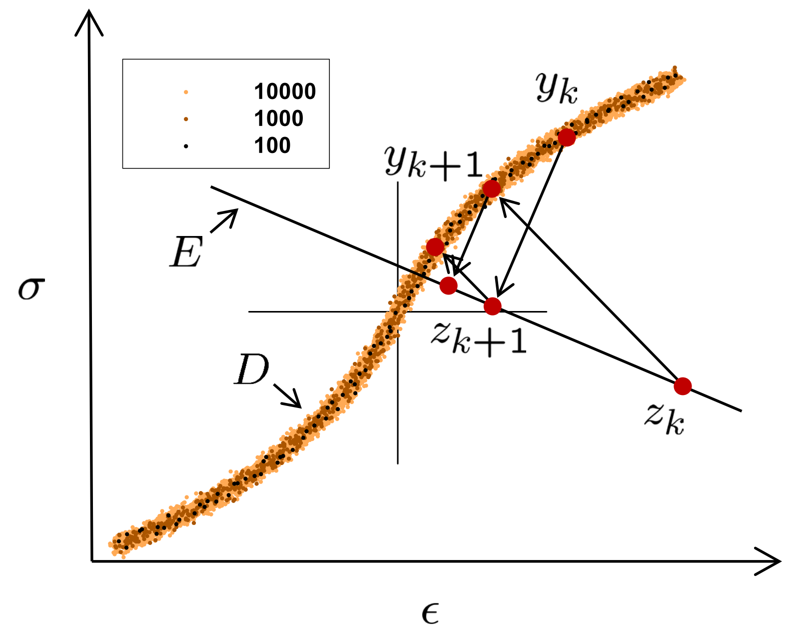
Fixed-point iteration

Theorem

Let $Z = \mathbb{R}^N \times \mathbb{R}^N$, D and E transversal affine subspaces of dimension N. Then, the fixed-point iteration converges to the unique solution of the Data-Driven problem.

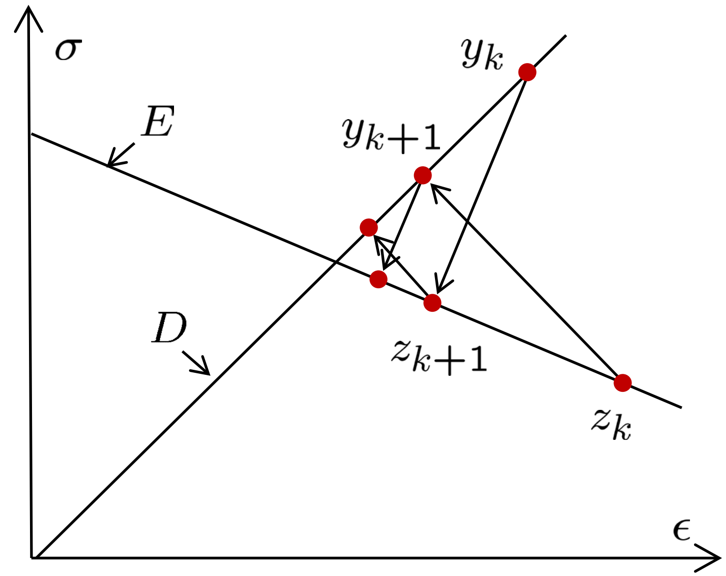


Fixed-point iteration,
affine data set D



Fixed-point iteration,
point data set D

Fixed-point iteration



Proof.

By translation, D, $E \equiv$ linear spaces.
Consider the fixed-point iteration

$$(y_k, z_k) \mapsto (y_{k+1}, z_{k+1}) = (P_D z_k, P_E y_k).$$

By the orthogonality of the projections,

$$\|z_k\|^2 = \|y_{k+1}\|^2 + \|y_{k+1} - z_k\|^2, \quad \|y_k\|^2 = \|z_{k+1}\|^2 + \|z_{k+1} - y_k\|^2.$$

By transversality, for some $c > 0$,

$$\|y_{k+1} - z_k\|^2 + \|z_{k+1} - y_k\|^2 \geq c(\|y_{k+1}\|^2 + \|z_{k+1}\|^2) + c(\|y_k\|^2 + \|z_k\|^2).$$

Combining, rearranging,

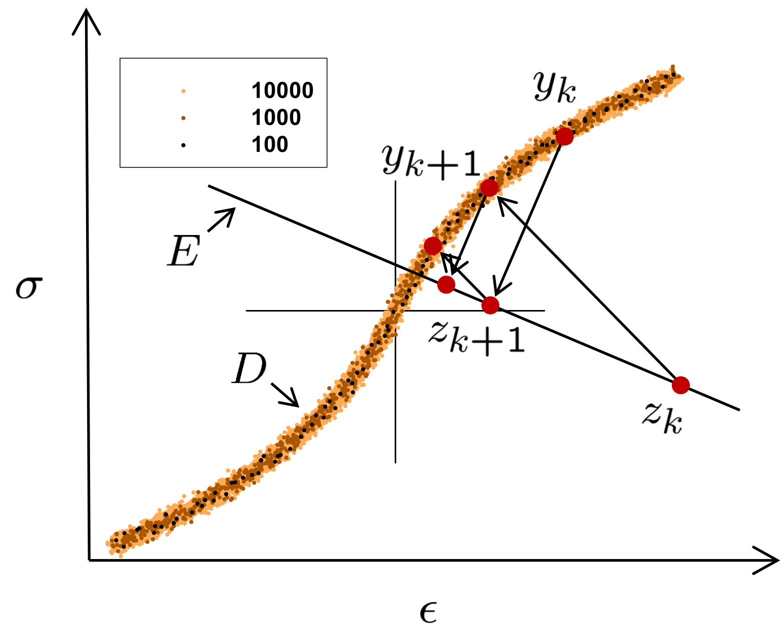
$$\|y_{k+1}\|^2 + \|z_{k+1}\|^2 \leq \frac{1-c}{1+c}(\|y_k\|^2 + \|z_k\|^2).$$

Hence, $(y_k, z_k) \mapsto (y_{k+1}, z_{k+1})$ is a contraction and $(y_k, z_k) \to (0, 0)$. □

Fixed-point iteration

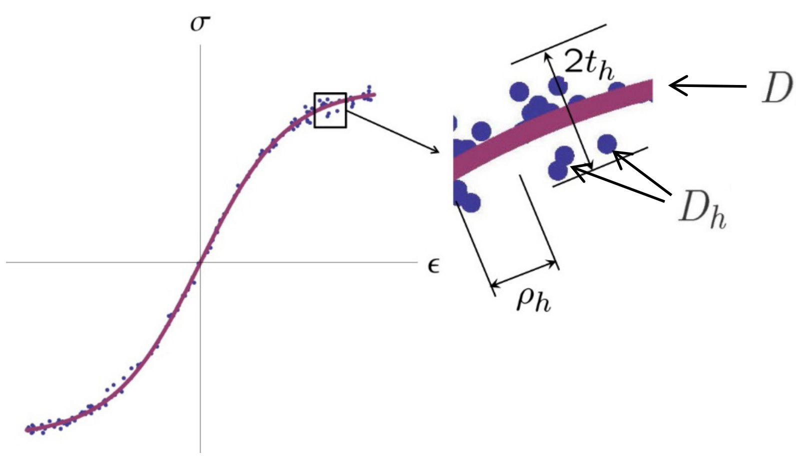
Theorem

Let E be an affine subspace of Z and (D_h) an equi-transversal sequence of point subsets of Z converging uniformly to D. Let (y_h, z_h) be a fixed point of $(y_k, z_k) \mapsto (P_{D_h} z_k, P_E y_h)$. Then, (y_h, z_h) converges to a solution (y, z) of the D Data-Driven problem.

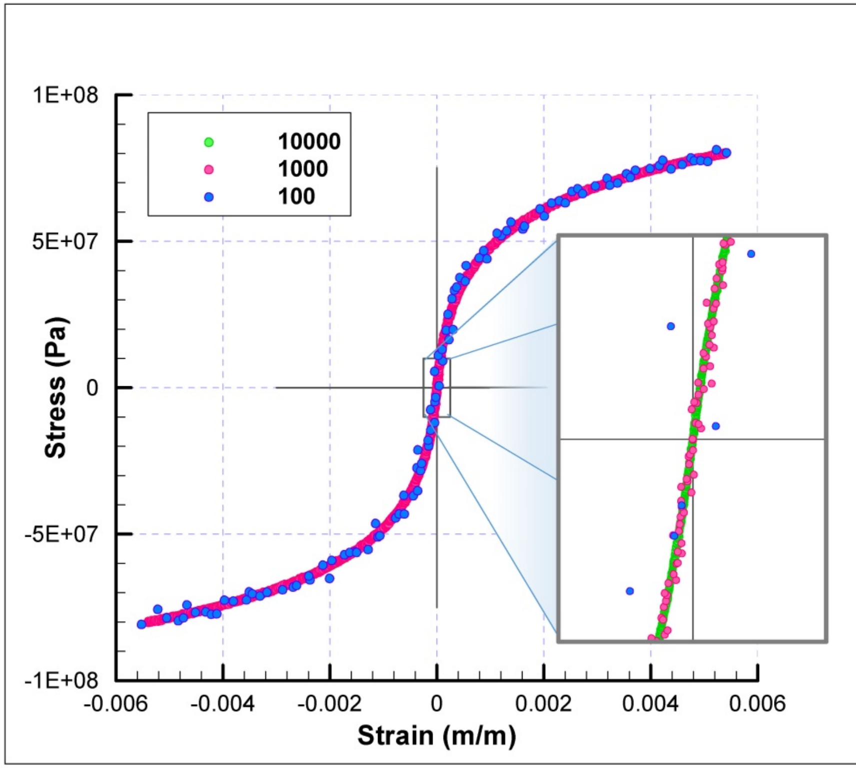


Proof.

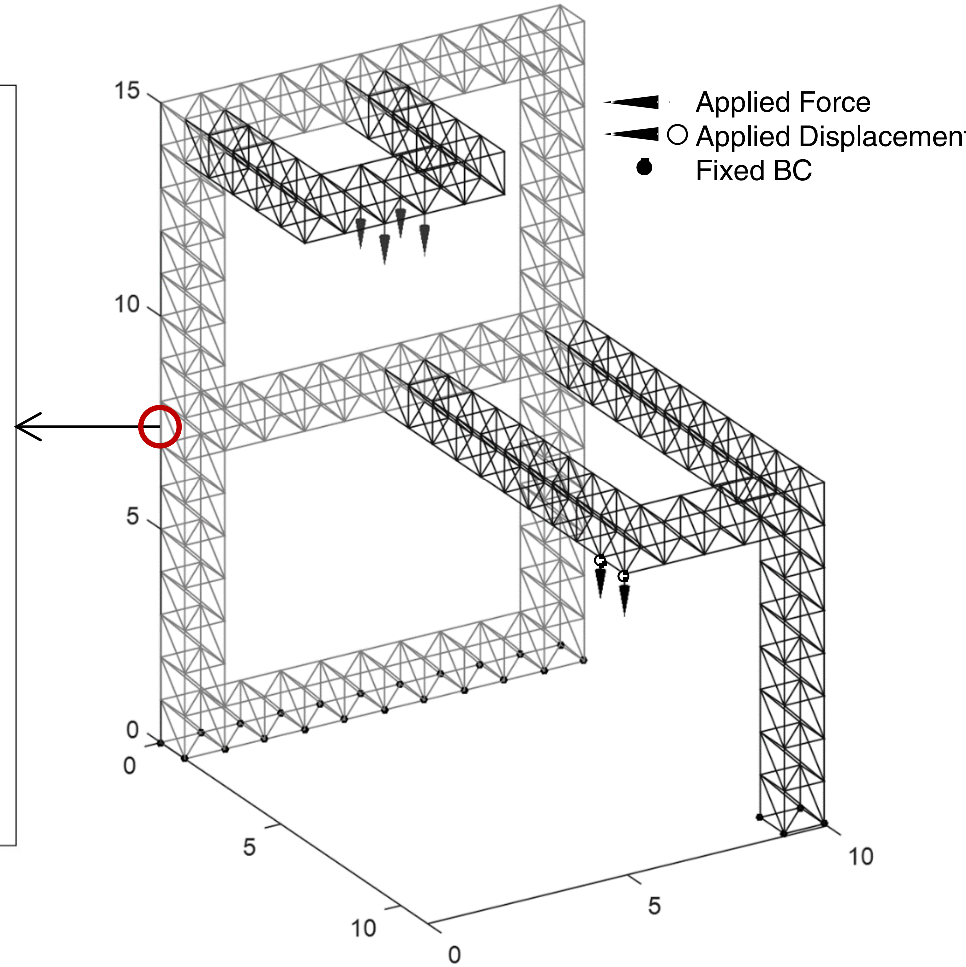
If (y_h, z_h) is a fixed point of the iteration, $y_h = P_{D_h} z_h$ and $z_h = P_E y_h$. By uniform convergence, $\|y_h - z_h\| \to 0$. By equi-transversality, $y_h \to y \in D$, $z_h \to z \in E$ and $y = z$, hence a solution of the D Data-Driven problem. □



The topology of Data Convergence



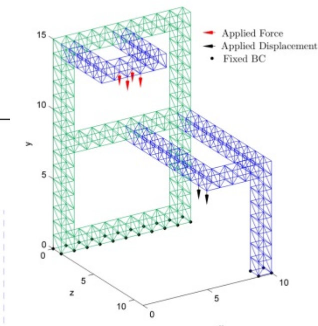
Sequence of
uniformly converging data sets
(increasing number of points,
decreasing scatter)

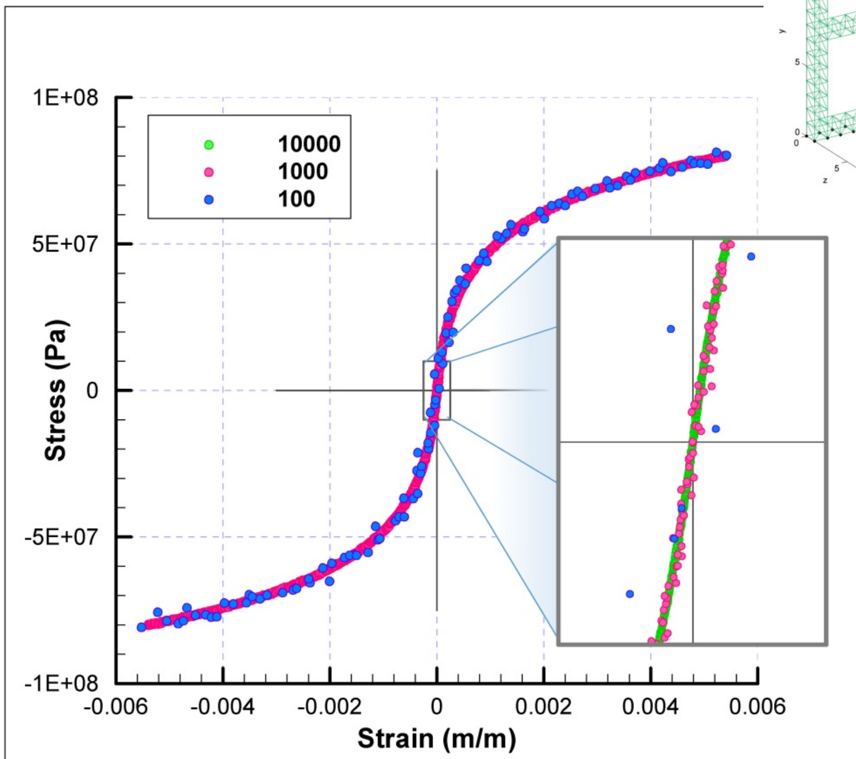


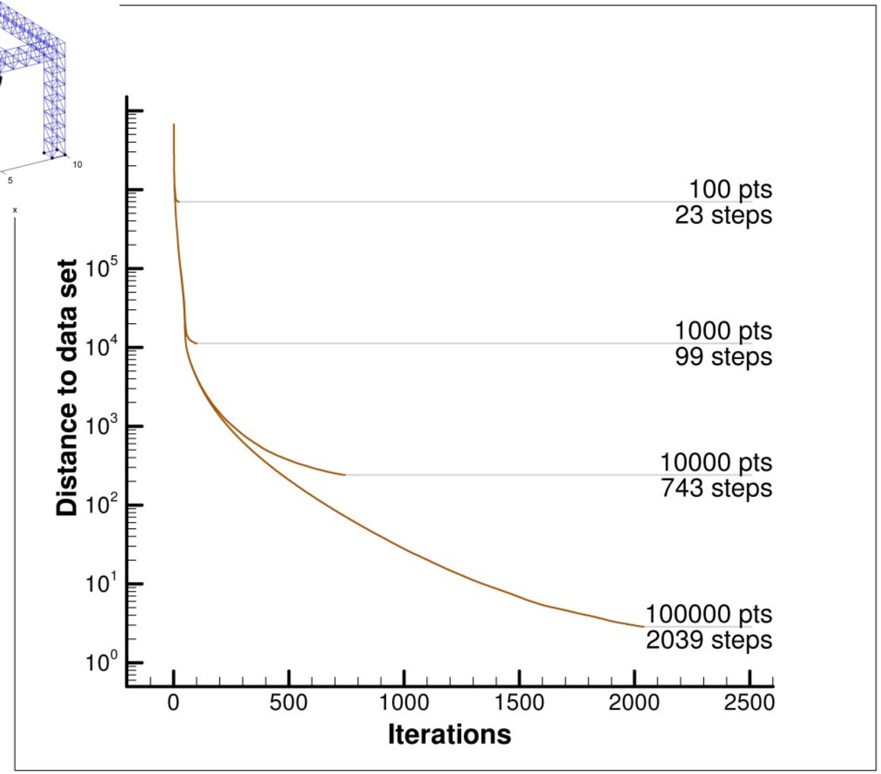
3D truss structure

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

The topology of Data Convergence





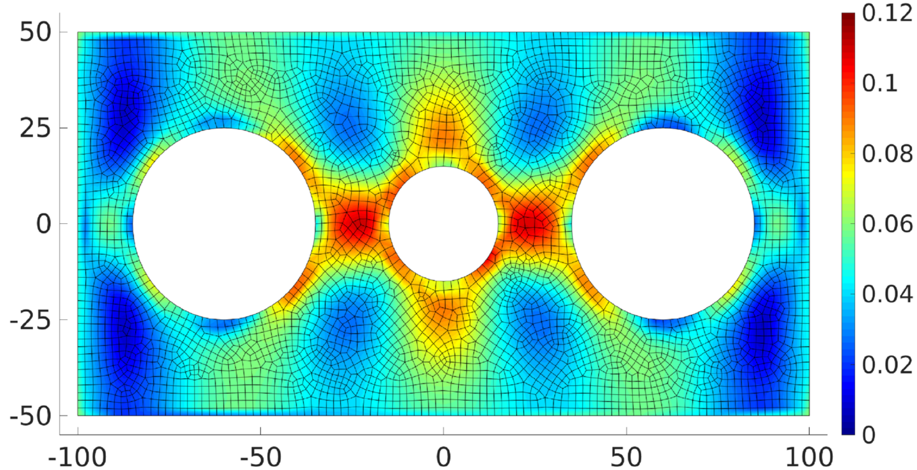


Sequence of
uniformly converging data sets
(increasing number of points, decreasing scatter)

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.

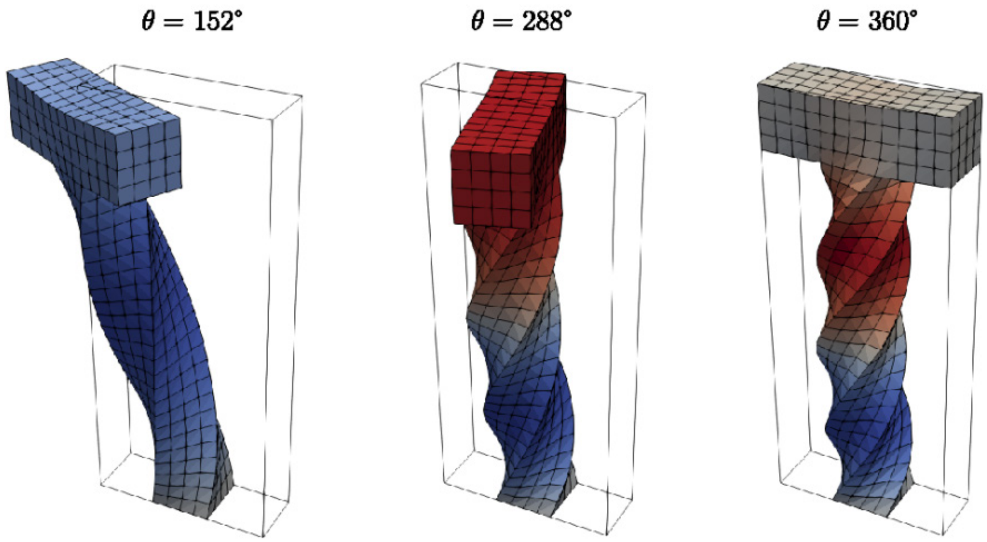
Model-free Data-Driven finite-elements



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

R. Eggersmann, S. Reese
RWTH Aachen (2019) .

cf. S. Reese's lecture!
Wednesday 12, 14:45-15:30



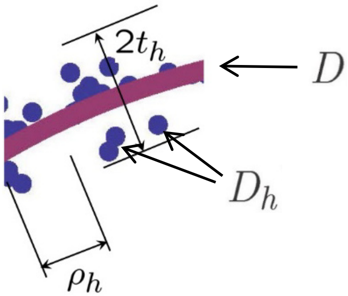
- DD FE calculations
- Finite elasticity
- Twisted elastic rod
- Random Green-S. Venant
- 10,000,000 data points

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

cf. L. Stainier's lecture!
Thursday 13, 11:00-11:45

Model-free Data-Driven finite-elements

- Sequence of FE discretizations of size h_k.
- Sequence of admissible sets (E_{h_k}).
- Sequence of material-data sets (D_k).
- $z \equiv$ solution of (D, E)-problem.
- $z_{h_k} \equiv$ solution of (D, E_{h_k})-problem.
- $z_{k,h_k} \equiv$ solution of (D_k, E_{h_k})-problem.



Theorem *Assume:*

i) *(Equi-transversality) There is* $0 \leq \lambda < 1$ *s. t.,*

$$\|P_{E_{h_k}} y - z\| \leq \lambda \|y - z\|, \quad \text{for all } y \in D_k,$$

ii) *(Finite-element convergence). There is* $C > 0$ *and* $\alpha > 0$ *s. t.* $\|z_{h_k} - z\| \leq C h_k^\alpha$.

iii) *(Equi-uniform data convergence).* $D_k \to D$ *uniformly and* $\rho_k < C h_k^\alpha$, $t_k < C h_k^\alpha$.

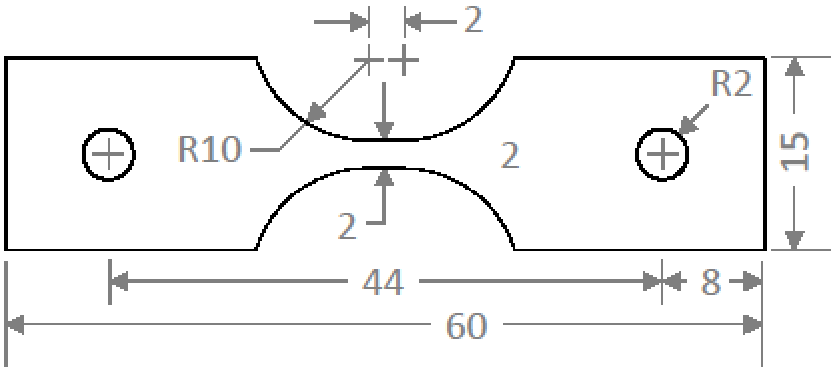
Then, $\|z_{k,h_k} - z\| \leq C h_k^\alpha$ *and, in particular,* $z_{k,h_k} \to z$.

Proof. By finite-element convergence and equi-transversality,

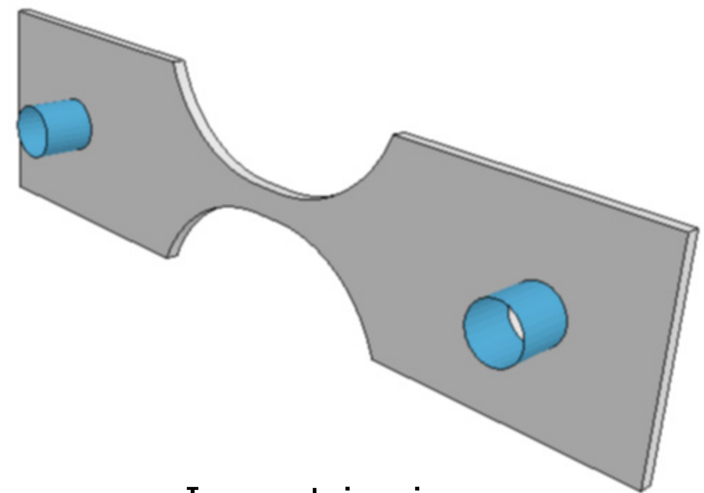
$$\|z_{k,h_k} - z\| \leq \|z_{k,h_k} - z_{h_k}\| + \|z_{h_k} - z\| \leq \frac{t_k + \lambda(t_k + \rho_k)}{1 - \lambda} + C h_k^\alpha,$$

and the claim follows by the equi-uniform convergence of the data. □

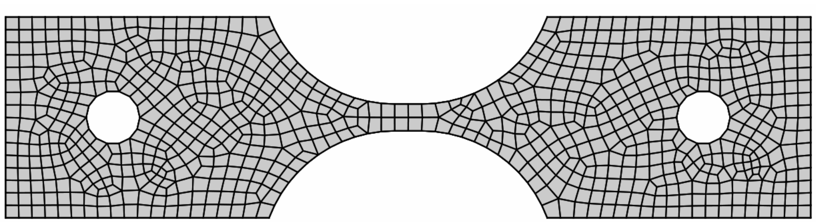
Model-free Data-Driven finite-elements



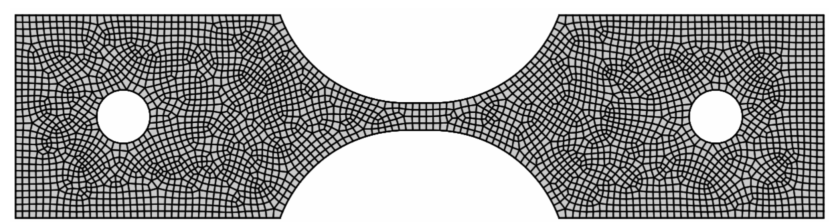
Sketch of thin dog-bone tensile specimen loaded in tension. The thickness of the sample is 1mm, plane stress is assumed.



Isometric view of simulation set-up in 3D consisting of two rigid pins and the tensile specimen

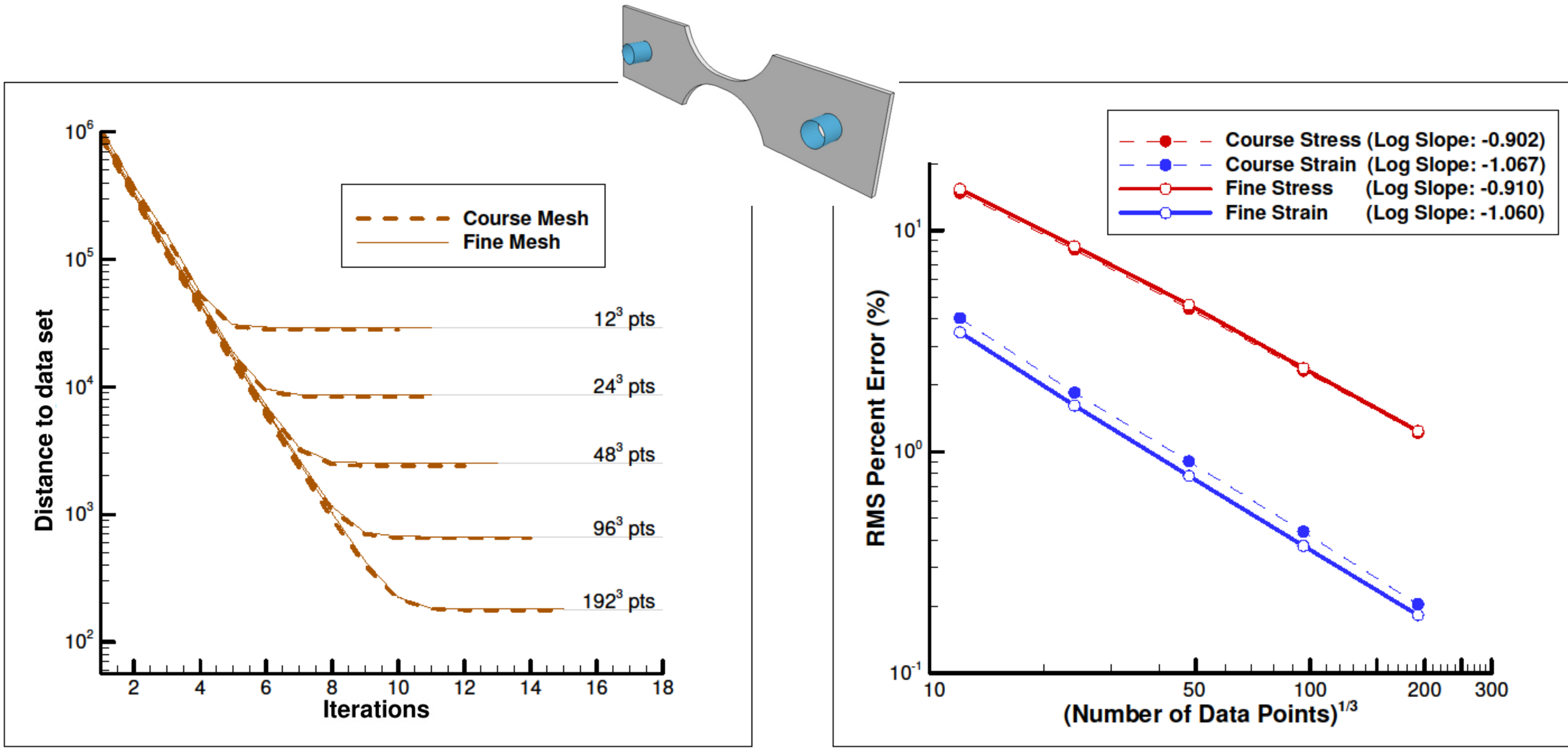


Coarse mesh with 811 hexes, h 1mm



Fine mesh with 6428 hexes, h 0.5mm

Model-free Data-Driven finite-elements



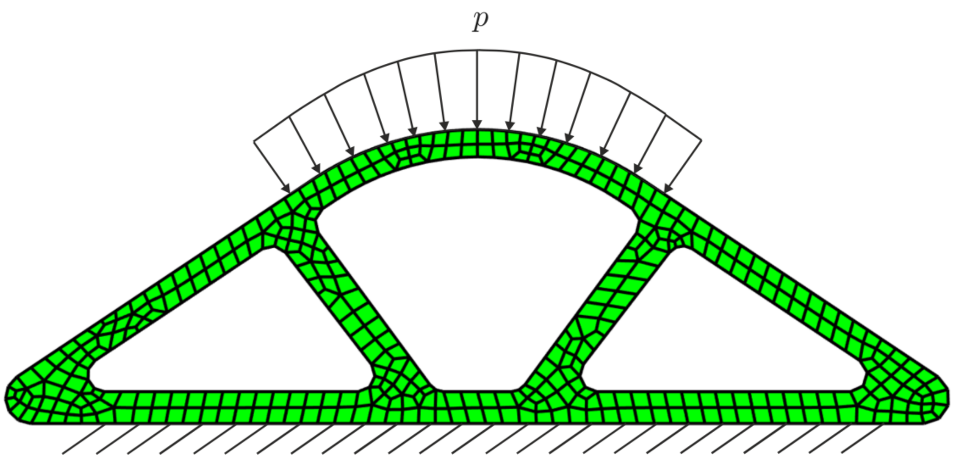
Convergence of fixed-point solver: Each iteration requires two back-substitutions for standard linear systems and one material data search/member

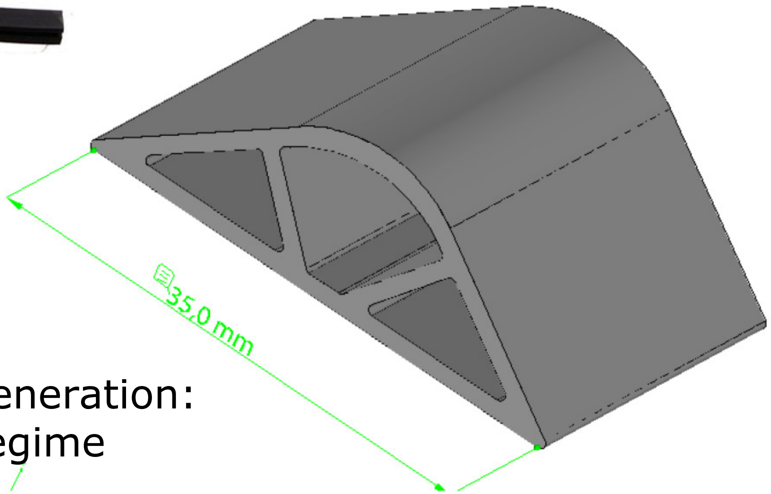
Convergence with respect to material data set, uniformly sampled cube in $(\sigma_{11}, \sigma_{22}, \sigma_{12})$ space

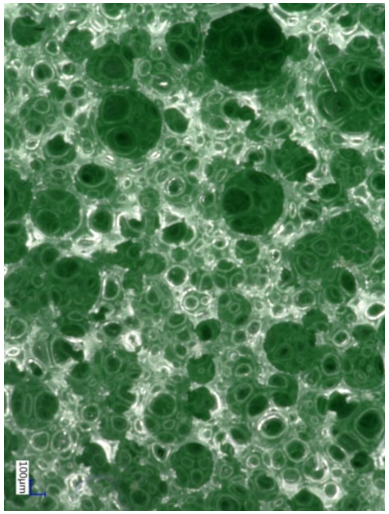
T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81-101.

Model-free Data-Driven finite-elements – Rubber sealing

- Application: *Rubber sealing*
- Sealing for doors, windows
- Self adhesive, loaded by pressure







- Open-cell foam
- isotropic material
- 3D computation
- Microscopic data generation: linear/non-linear regime

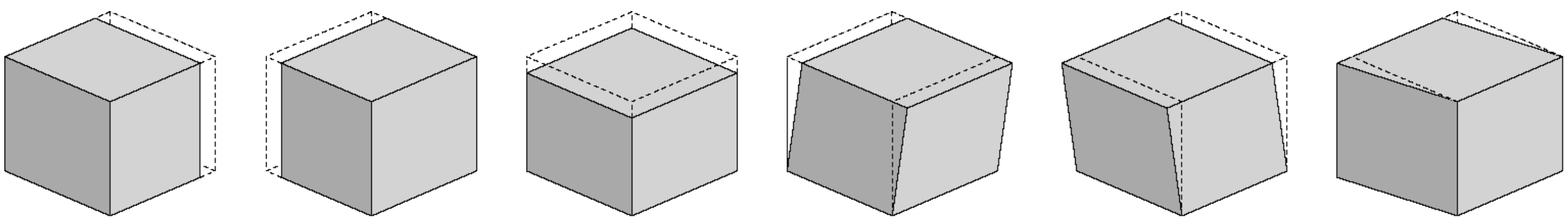
T.F. Korzeniowski and K. Weinberg, *CMAME*, **400** (2022) 115487.

Model-free Data-Driven finite-elements – Rubber sealing

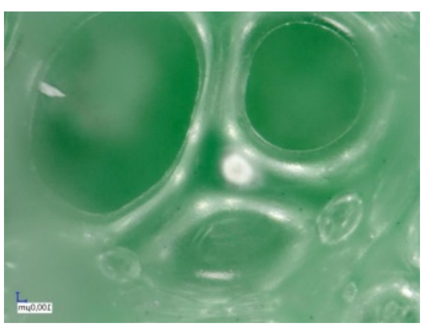
- Data sets: $\mathcal{D} = \{\epsilon_i - \sigma_i\}$ or $\mathcal{D} = \{F_i - P_i\}$ or $\mathcal{D} = \{C_i - S_i\}$

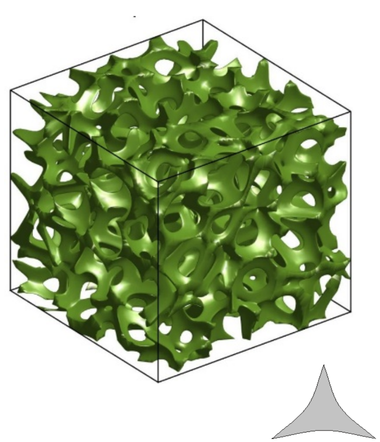
1. apply deformation
2. compute RVE and determine average stress
3. collect data pairs

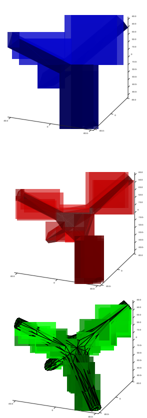
- Case D: non-linear, isotropic
- superpose 6 different loading scenarios (unit loads)

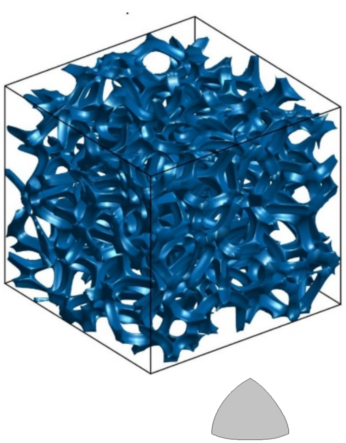


- 3D open-cell foam RVEs:





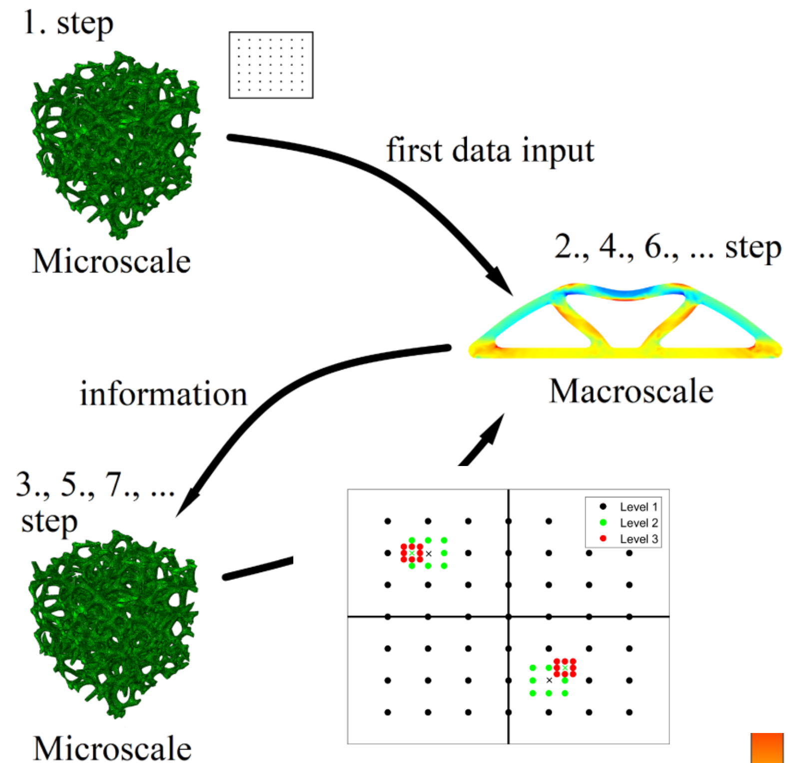


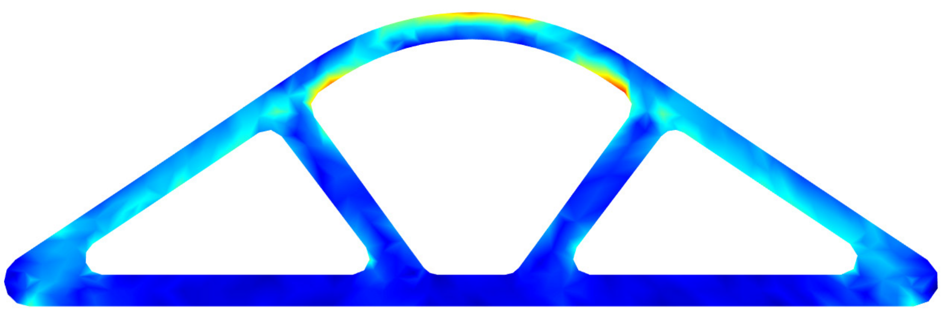


T.F. Korzeniowski and K. Weinberg, *CMAME*, **400** (2022) 115487.

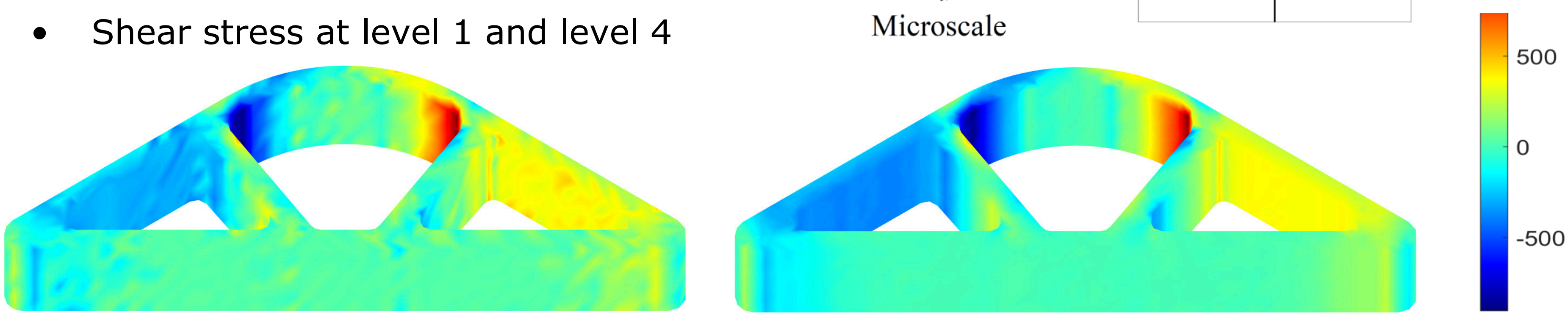
Model-free Data-Driven finite-elements – Rubber sealing

- Cauchy stress distribution (vertical)
- Start with a coarse level of data
- Identify data points of interest
- Do additional RVE calculations
- Redo computation at finer level till TOL





- Shear stress at level 1 and level 4



T.F. Korzeniowski and K. Weinberg, *CMAME*, **400** (2022) 115487.

to be continued…