(Model-Free) Data-Driven Computing

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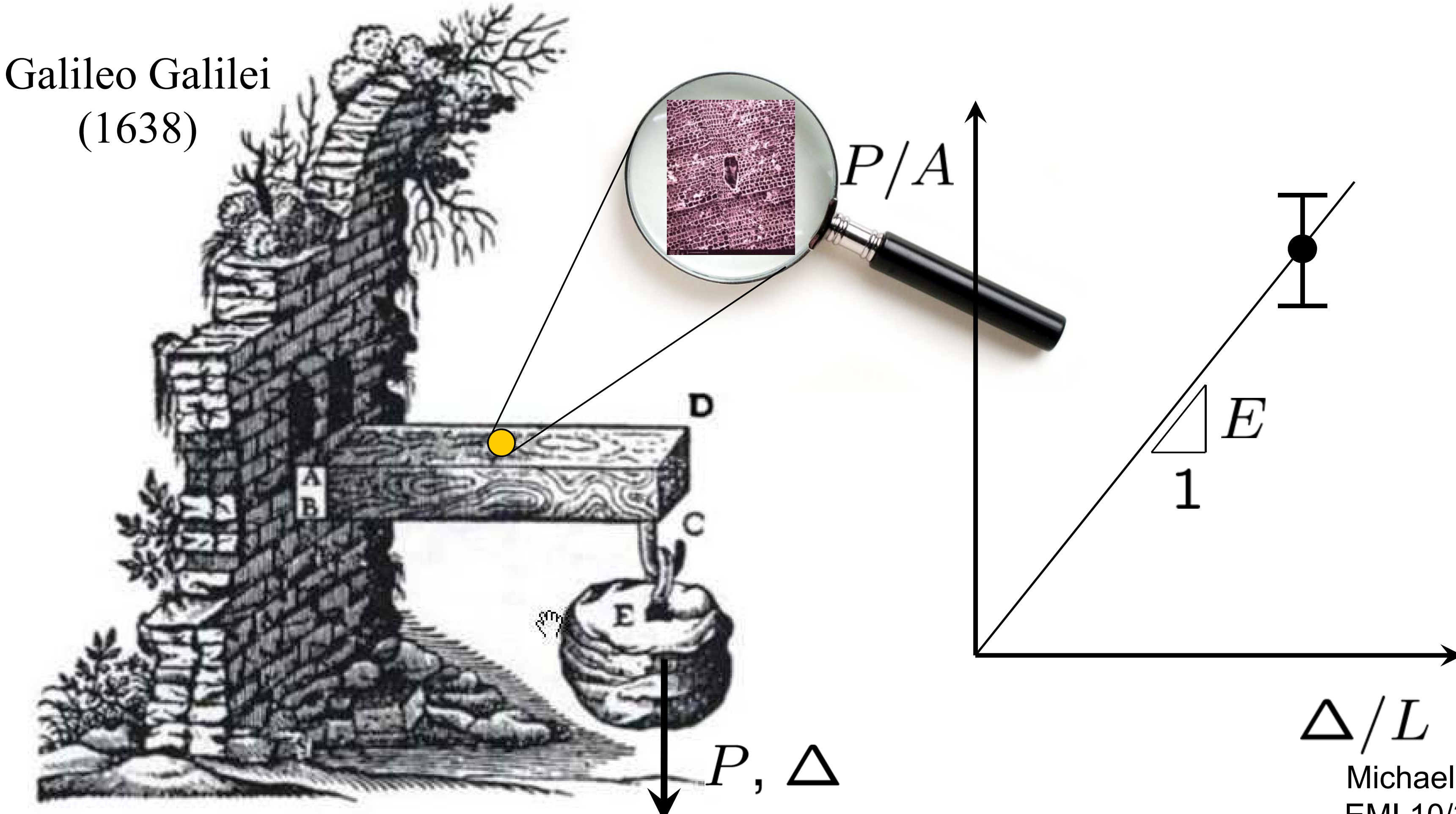
Ernst Mach Institute, EMI
Freiburg, Germany, October 31, 2018

Materials data through the ages…

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



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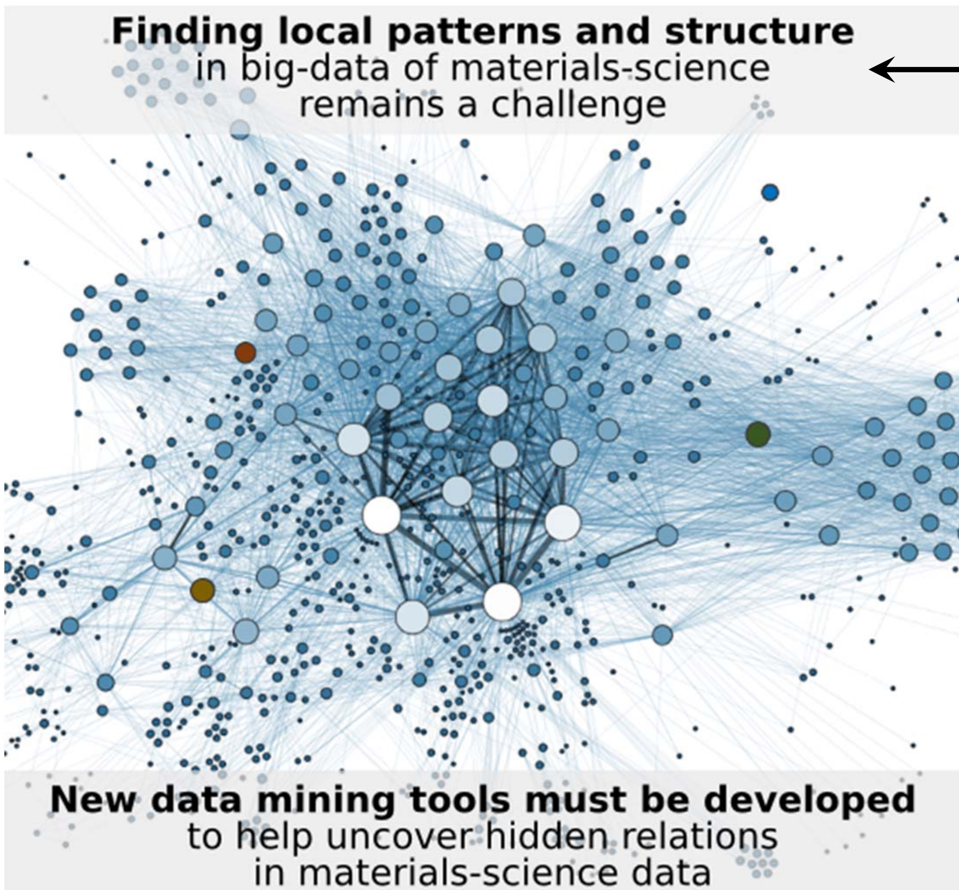
Material data through the ages…

At present, mechanics of materials is *data rich!*



(E. Munch, 1893)

NOMAD
https://www.nomad-coe.eu/

Data Science, Big Data…

http://olap.com/forget-big-data-lets-talk-about-all-data/

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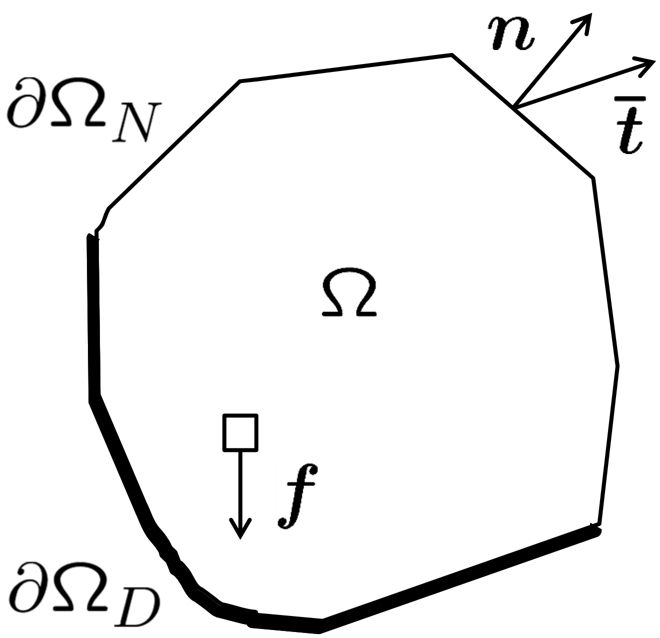
Data Science, Big Data…

- *Data Science* is the extraction of '*knowledge*' from large volumes of unstructured data[1]
- Data science requires sorting through *big-data* sets and extracting '*insights*' from these data
- Data science uses data management, statistics and machine learning to derive *mathematical models* for subsequent use in decision making
- Data science influences (*non-STEM*) fields such as marketing, advertising, finance, social sciences, security, policy, medical informatics…
- *But… What's in it for us? (STEM folk)*

[1]Dhar, V., *Communications of the ACM*, **56**(12) (2013) p. 64.

Where does Data Science intersect with (computational) mechanics?

- Anatomy of a field-theoretical *STEM* problem:



i) Kinematics + Dirichlet:

$$\left.\begin{aligned} \epsilon(\boldsymbol{u}) &= 1/2(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \\ \boldsymbol{u} &= \bar{\boldsymbol{u}}, \quad \text{on } \partial\Omega_D \end{aligned}\right\}$$

ii) Equilibrium + Neumann:

$$\left.\begin{aligned} \operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} &= \boldsymbol{0} \\ \boldsymbol{\sigma} \boldsymbol{n} &= \bar{\boldsymbol{t}}, \quad \text{on } \partial\Omega_N \end{aligned}\right\}$$

iii) Material law: $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}\Big(\epsilon(\boldsymbol{x})\Big)$

Where does Data Science intersect with (computational) mechanics?

- Anatomy of a field-theoretical *STEM* problem:

Universal laws!
(Newton's laws,
Schrodinger's eq.,
Maxwell's eqs.,
Einstein's eqs...)
Exactly known!
Uncertainty-free!
(epistemic)

i) Kinematics + Dirichlet:

$$\begin{rcases} \epsilon(\boldsymbol{u}) = 1/2(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \\ \boldsymbol{u} = \bar{\boldsymbol{u}}, \quad \text{on } \partial\Omega_D \end{rcases}$$

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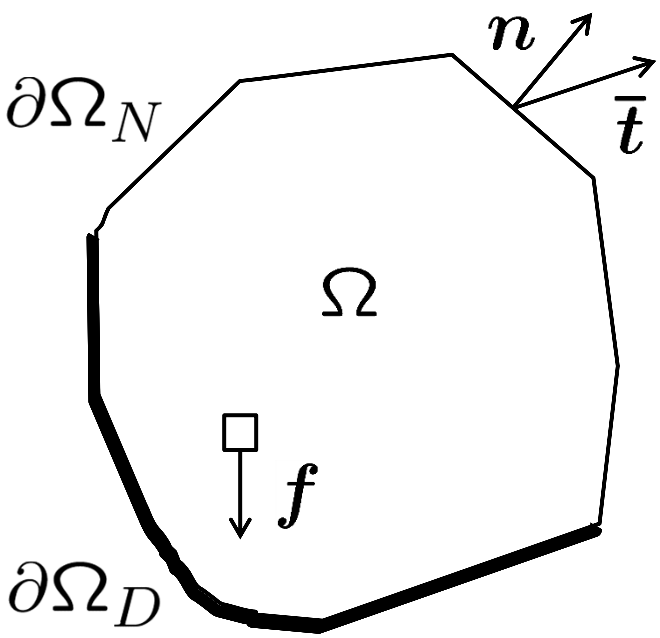

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iii) Material law: $\underbrace{\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}\big(\epsilon(\boldsymbol{x})\big)}$

Unknown! Epistemic uncertainty!

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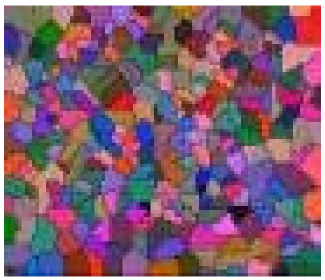
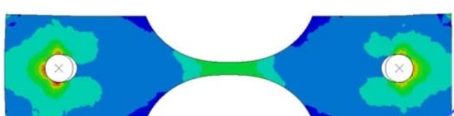
Classical Modeling & Simulation

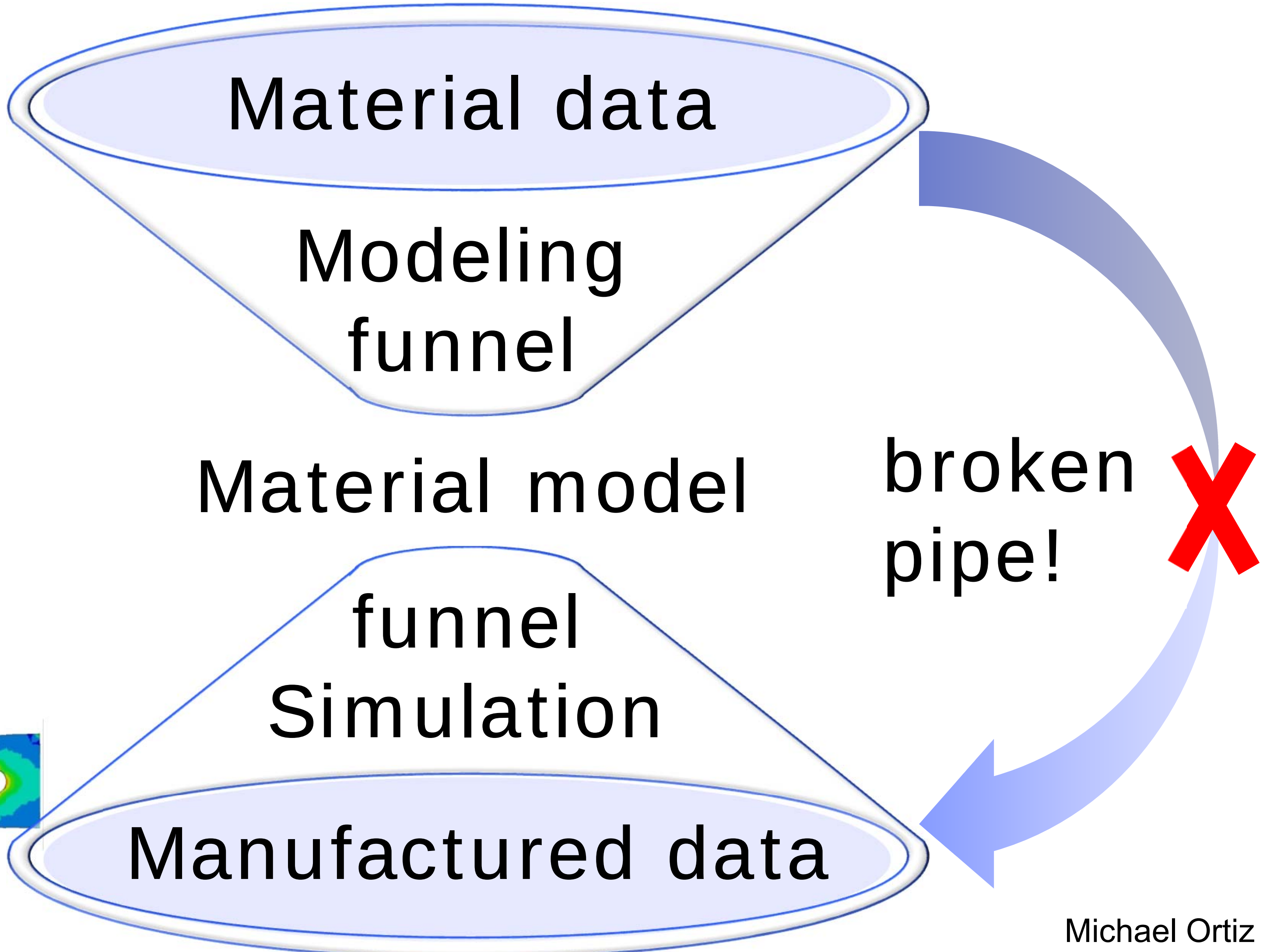
- Need to generate (epistemic) '*knowledge*' about material behavior to close BV problems...
- Traditional *modeling paradigm*: Fit data (a.k.a. regression, machine learning, model reduction, central manifolds...), use calibrated empirical models in BV problems

Classical Modeling & Simulation



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

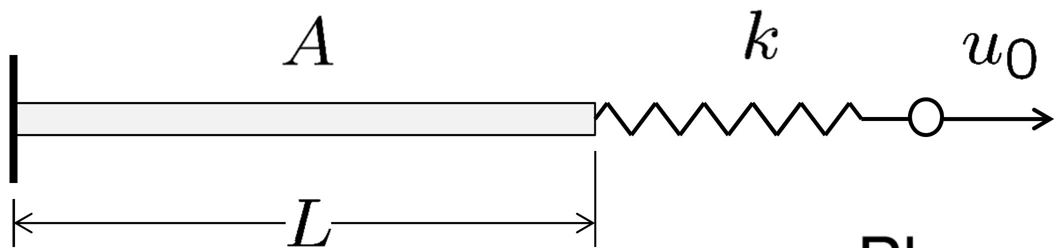


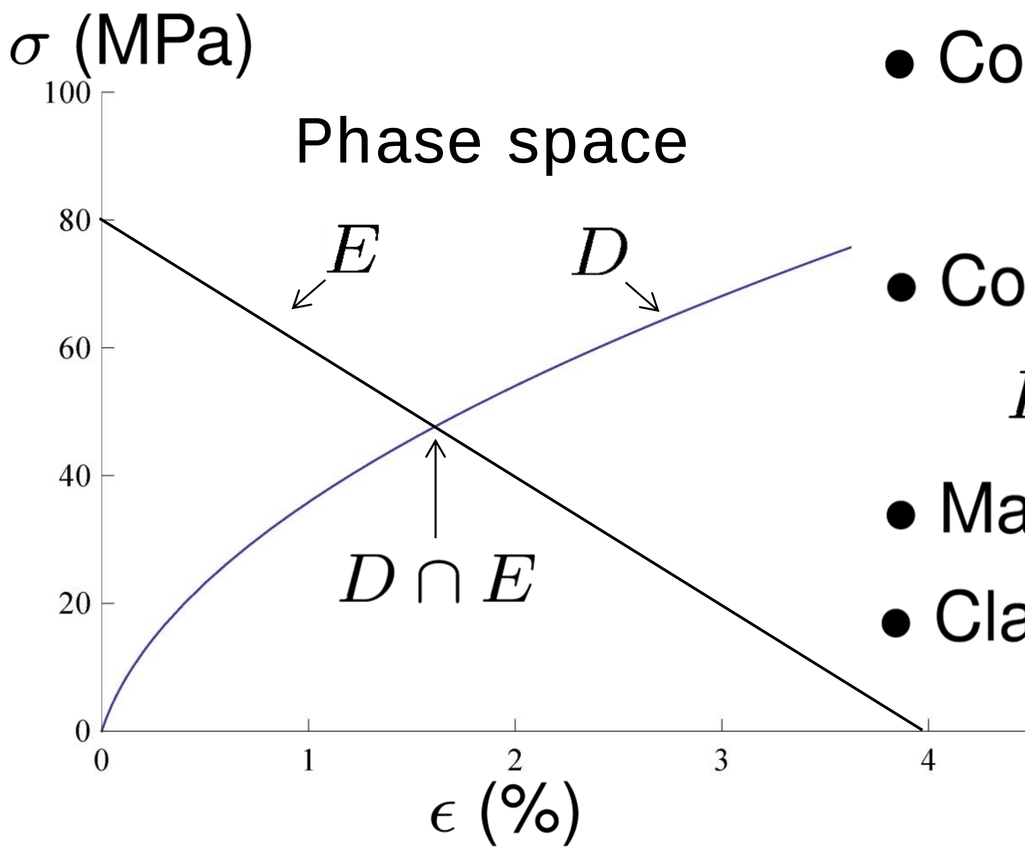


Data-Driven (model-free) mechanics

- Need to generate (epistemic) '*knowledge*' about material behavior to close BV problems…
- Traditional *modeling paradigm*: Fit data (a.k.a. regression, machine learning, model reduction, central manifolds…), use calibrated empirical models in BV problems
- *But:* We live in a *data-rich world* (full-field diagnostics, data mining from first principles...)
- *Extreme Data-Driven paradigm* (*model-free!*): Use material data directly in BVP (no fitting by any name, no loss of information, no broken pipe between material and manufactured data)
- *How?*

Elementary example: Bar and spring





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

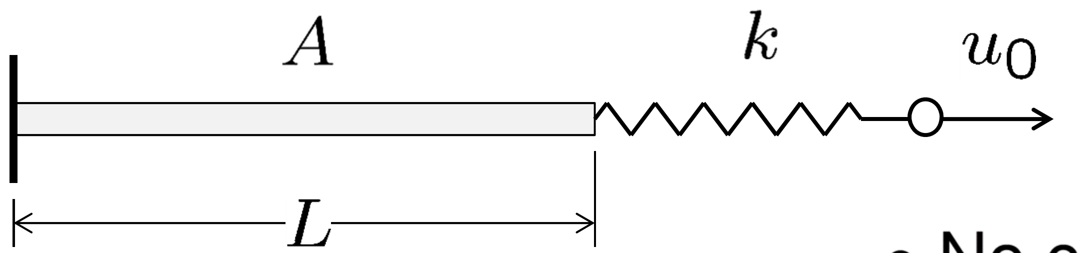
$$\sigma A = k(u_0 - \epsilon L)$$

- Constraint set:

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

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

Elementary example: Bar and spring

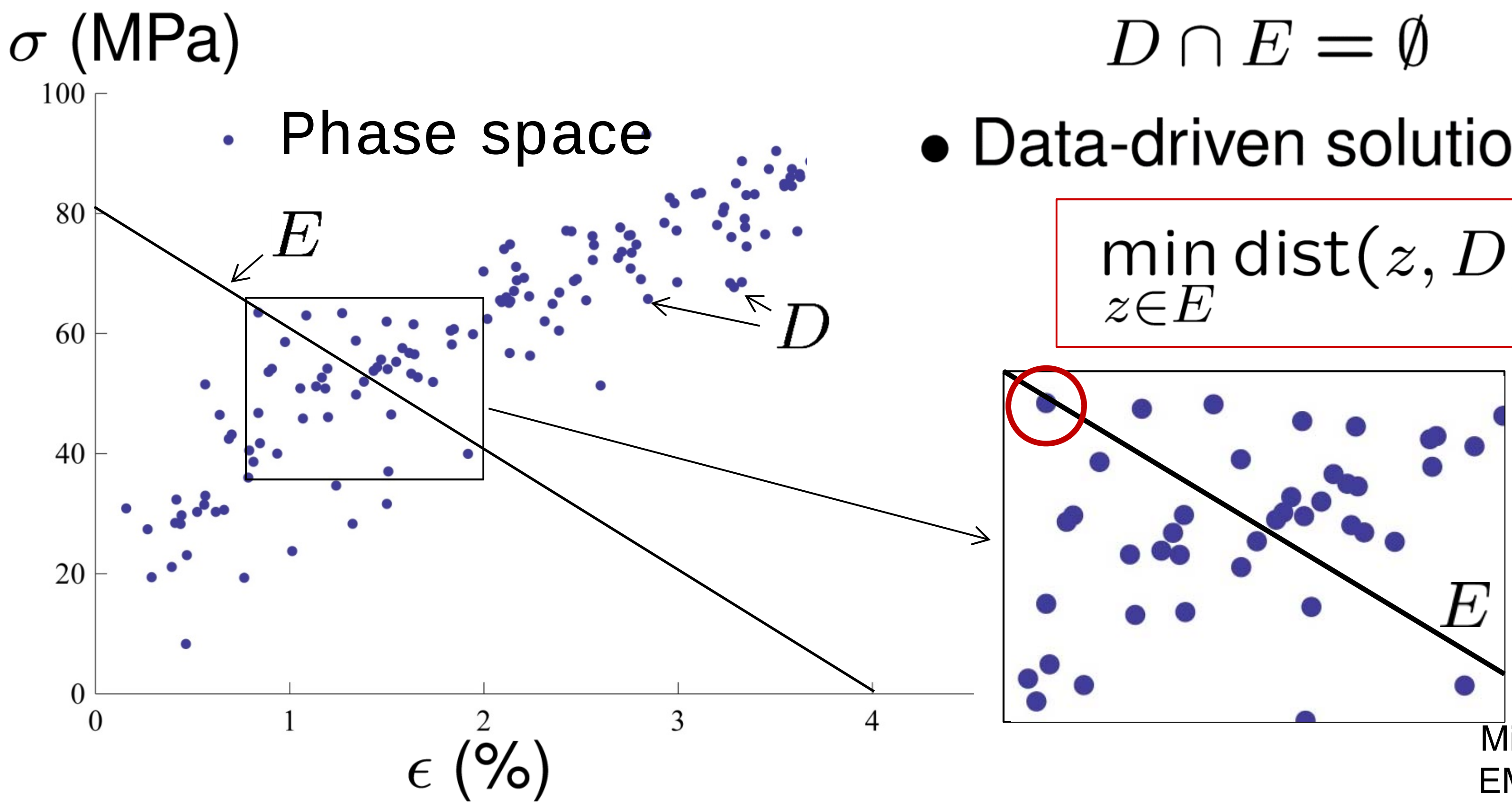


- No classical solutions!

$$D \cap E = \emptyset$$

- Data-driven solution:

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



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The general Data-Driven (DD) problem

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

  Find: $\text{argmin}\{d(z, D),\ z \in E\}$
- *The aim of Data-Driven analysis is to find the compatible strain field and the equilibrated stress field closest to the material data set*
- No material modeling, no data fitting, no V&V…
- Raw *fundamental* (stress *vs* strain) material data is used (unprocessed) in calculations
- No assumptions, artifacts, loss of information…

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

Data-Driven Computing: Issues

- *Data-driven (model-free!) computing: Use material data sets directly in calculations!*
- Is the Data-Driven reformulation of classical BVPs (possibly off of noisy data) *well-posed*?
- Implementation of *Data-Driven solvers*?
- *Numerical convergence* (iterative solvers, mesh size, time step…)
- Convergence with respect to *material data set*
- Extension to *time-dependent* problems
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- *Phase-space sampling* in high dimension
- *Data management*, repositories, outlook…

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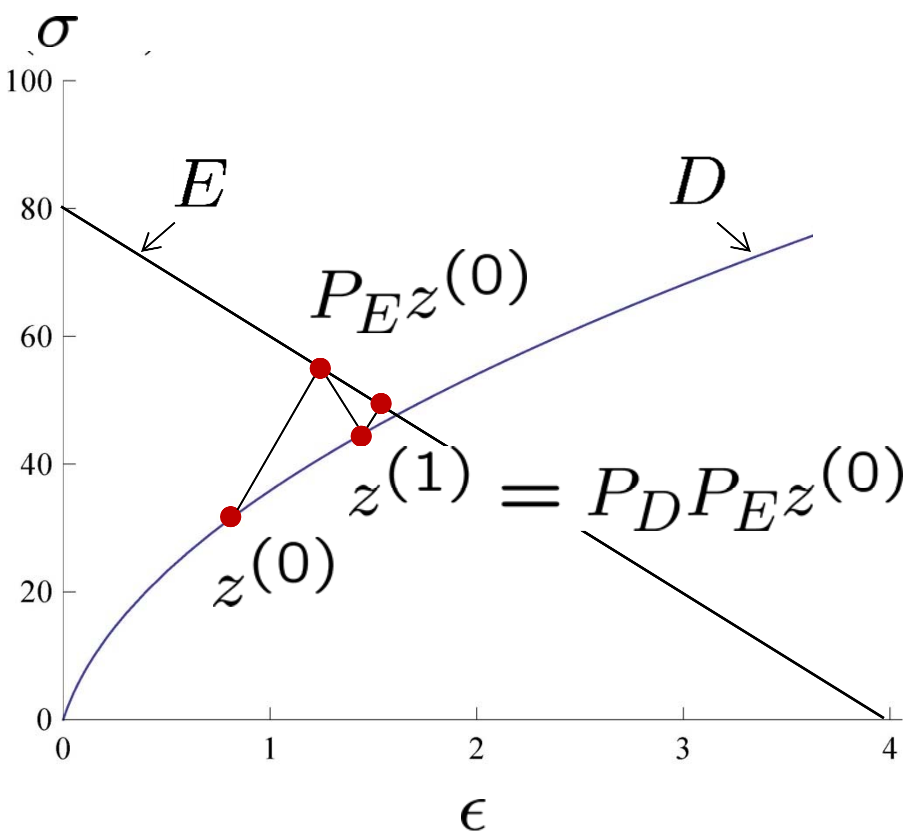
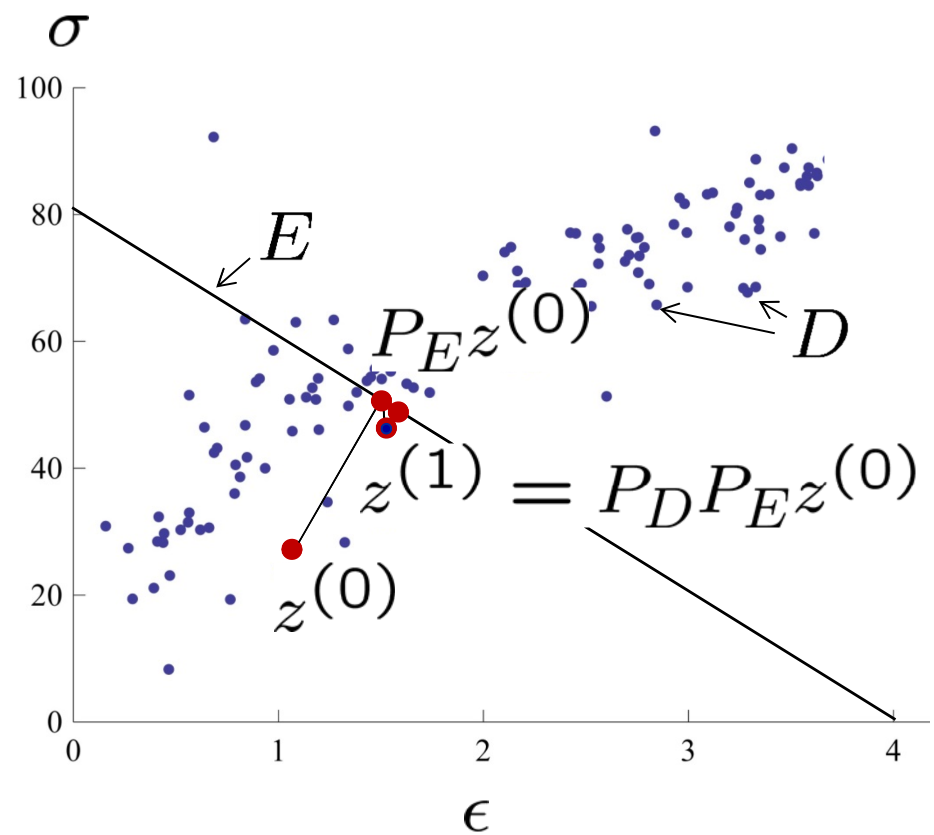
DD solvers: Fixed-point iteration

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





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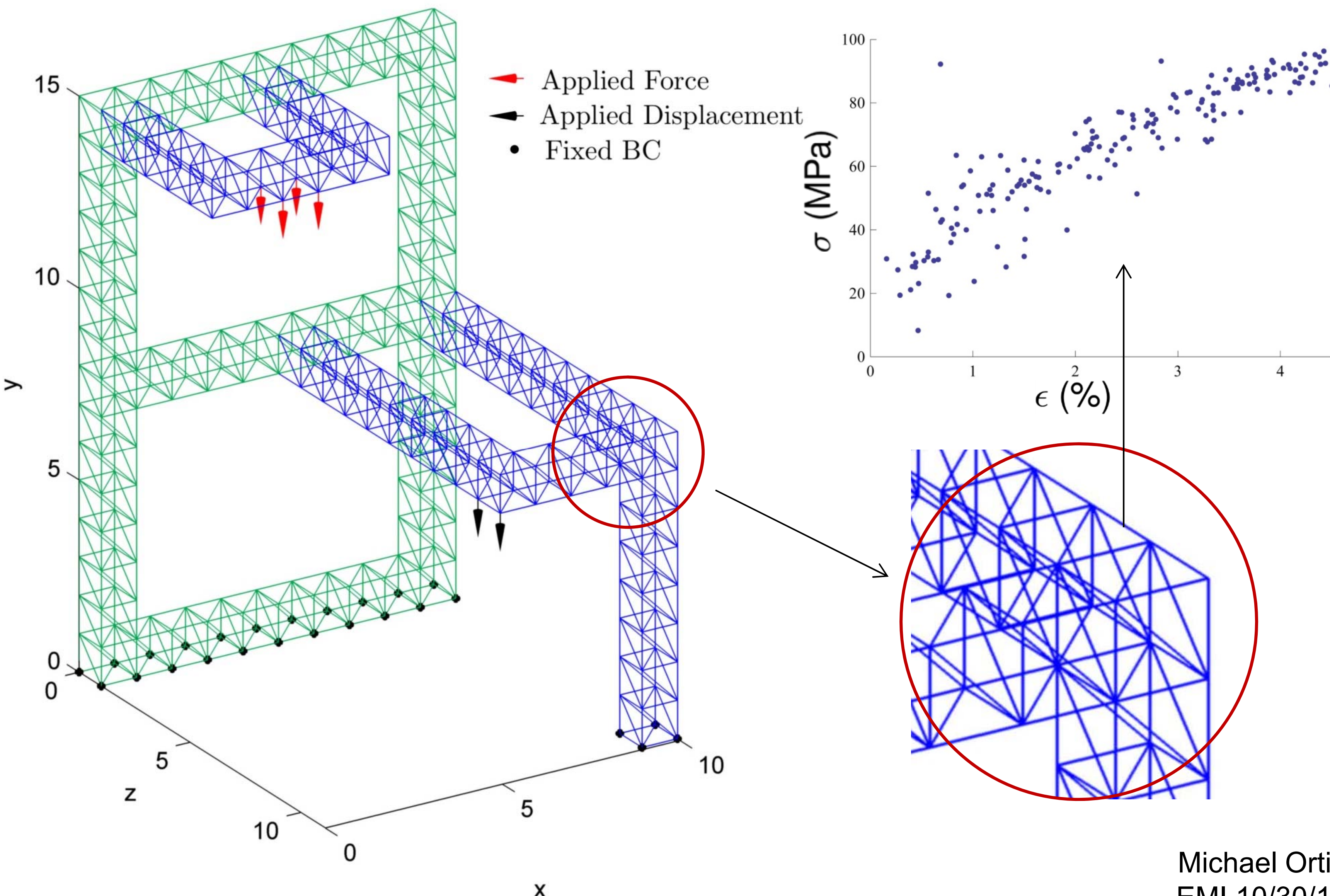
Test case: 3D Truss



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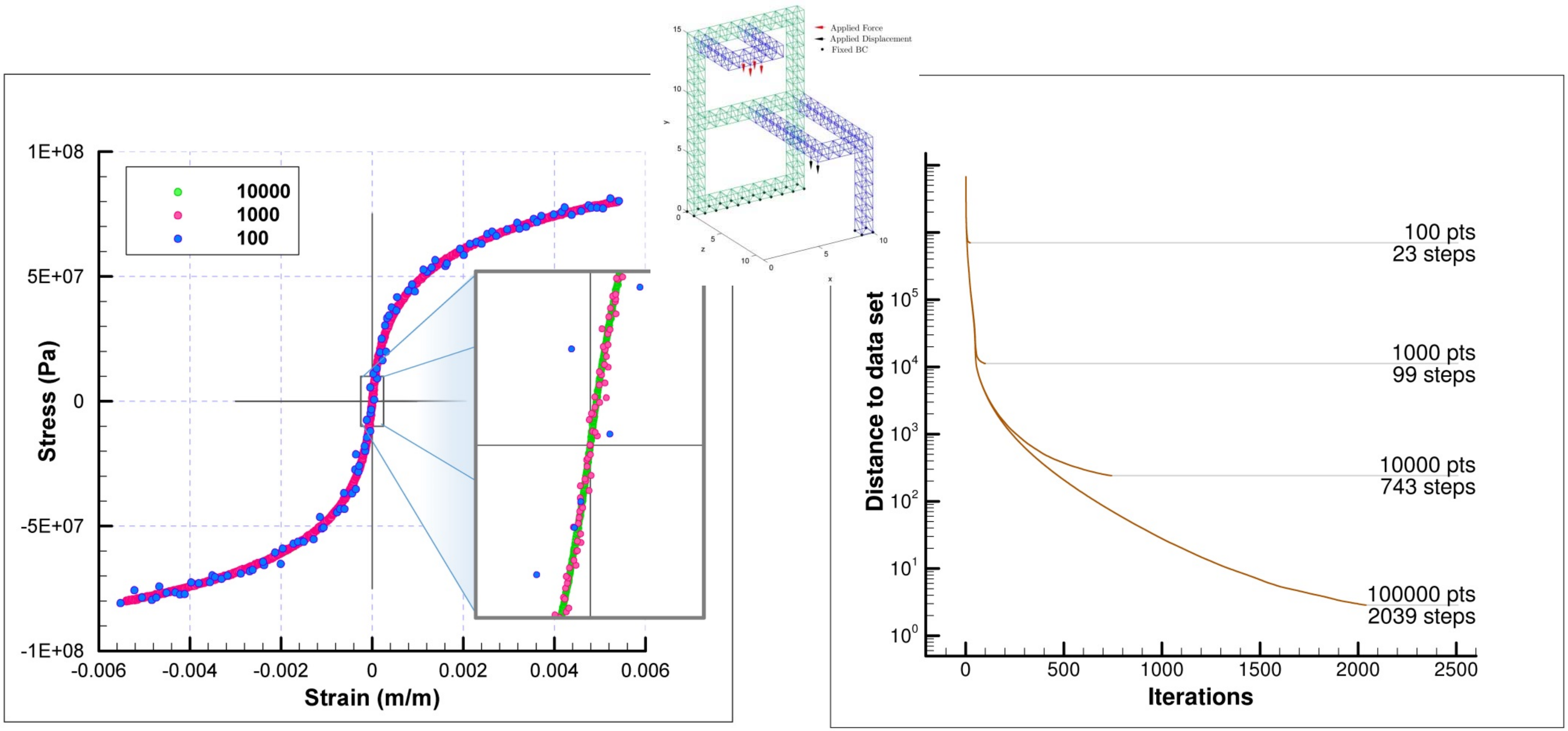
Truss test: Convergence of solver

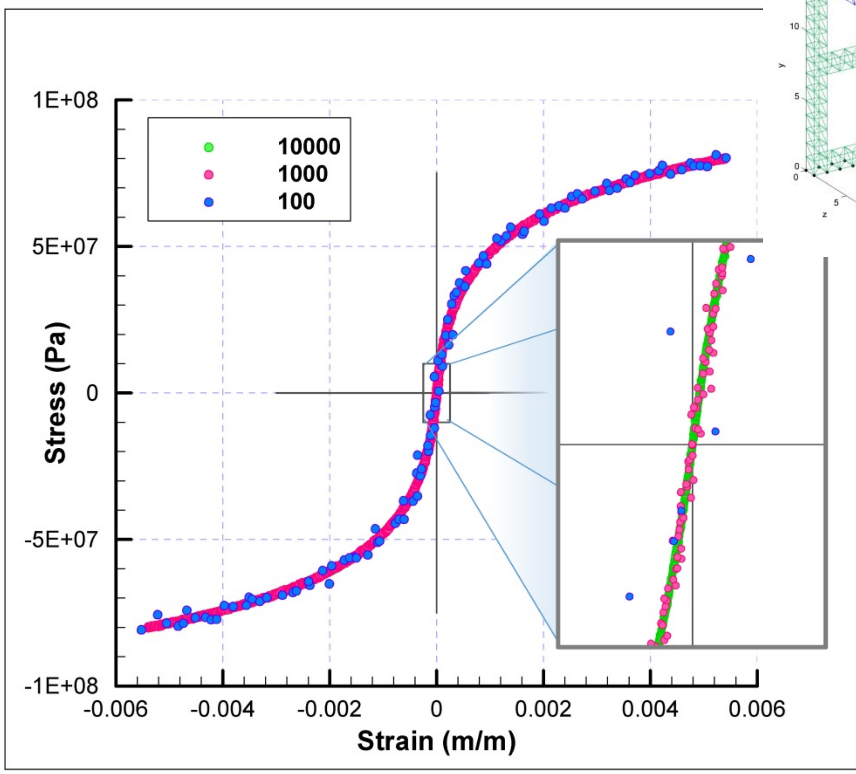


Material-data sets
of increasing size
and decreasing scatter

Convergence,
local data assignment
iteration

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

Truss test: Convergence wrt data



Material-data sets
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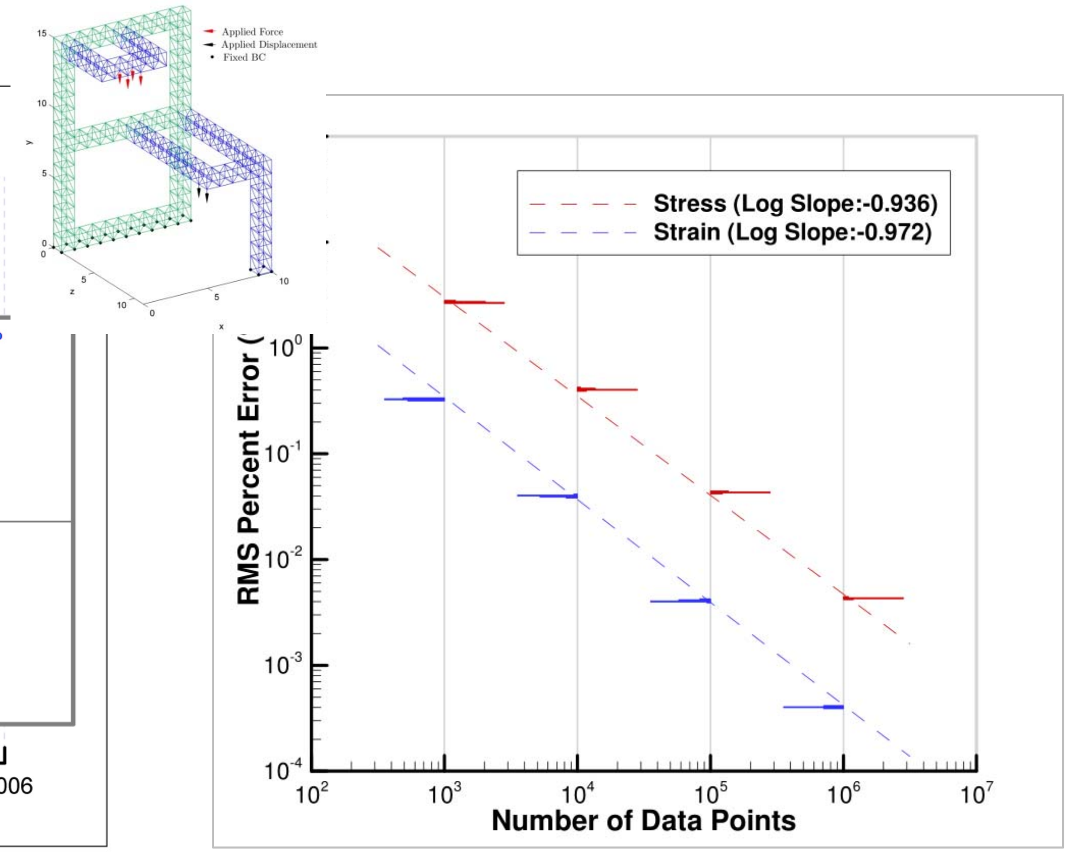

Convergence
with respect to sample size
(with initial Gaussian noise)

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

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Time-dependent problems: Dynamics

- Time discretization: $t_0, \ldots, t_{k+1} = t_k + \Delta t, \ldots$
- Constraint set (time dependent): $E_{k+1} =$

$$\Big\{ \underbrace{\epsilon_{e,k+1} = B_e u_{k+1},}_{\text{compatibility}} \quad \underbrace{\sum_{e=1}^{m} w_e B_e^T \sigma_{e,k+1} = f_{k+1}^{\text{ext}} - M a_{k+1}}_{\text{dynamic equilibrium}} \Big\}$$

- Newmark algorithm (3-point multistep scheme):

$$u_{k+1} = u_k + \Delta t \, v_k + \Delta t^2 \Big((1/2 - \beta) a_k + \beta a_{k+1} \Big)$$
$$v_{k+1} = v_k + \Delta t \, \Big((1 - \gamma) a_k + \gamma a_{k+1} \Big)$$

T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

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- Constraint set representation (3-point scheme):

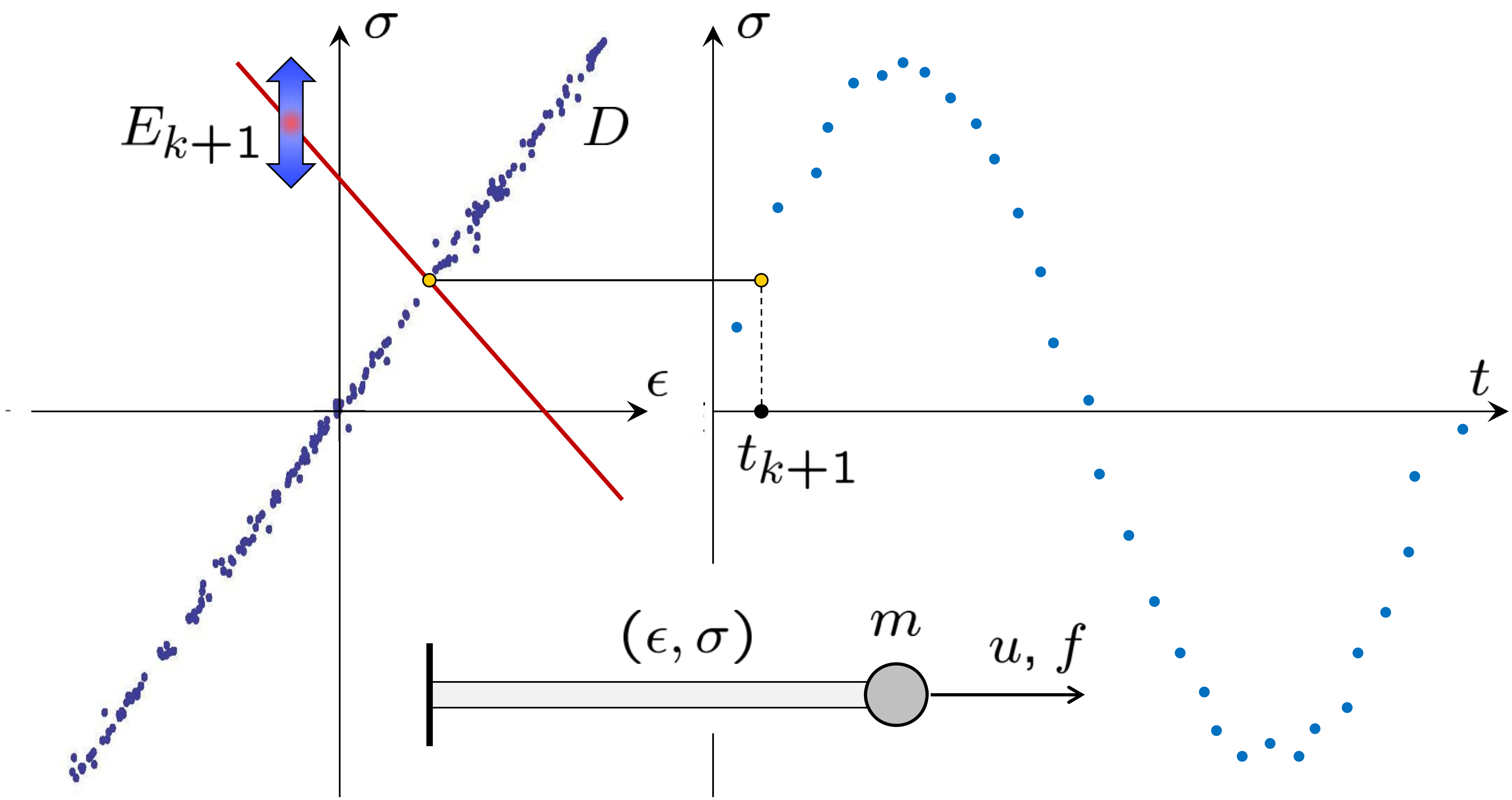
$$E_{k+1} = \{(\epsilon_{k+1}, \sigma_{k+1}) \; : \; \underbrace{(u_k, f_k), \; (u_{k-1}, f_{k-1})}_{\text{causality}}\}$$

- Data-driven problem:

$$\min_{(\epsilon^*,\sigma^*)\in D} \left(\min_{(\epsilon_{k+1},\sigma_{k+1})\in E_{k+1}} |(\epsilon_{k+1}-\epsilon^*, \sigma_{k+1}-\sigma^*)|^2 \right)$$

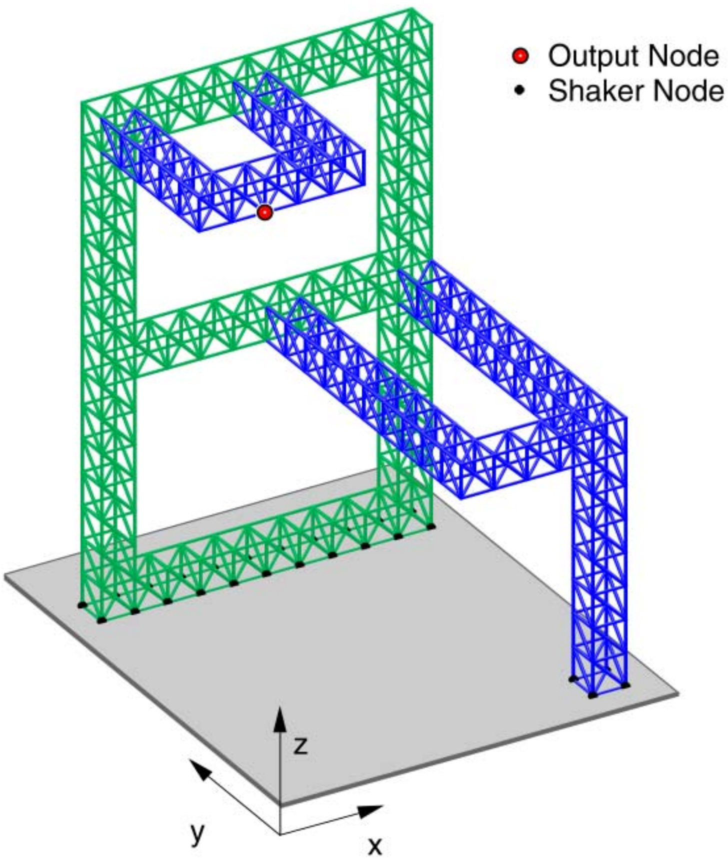
T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

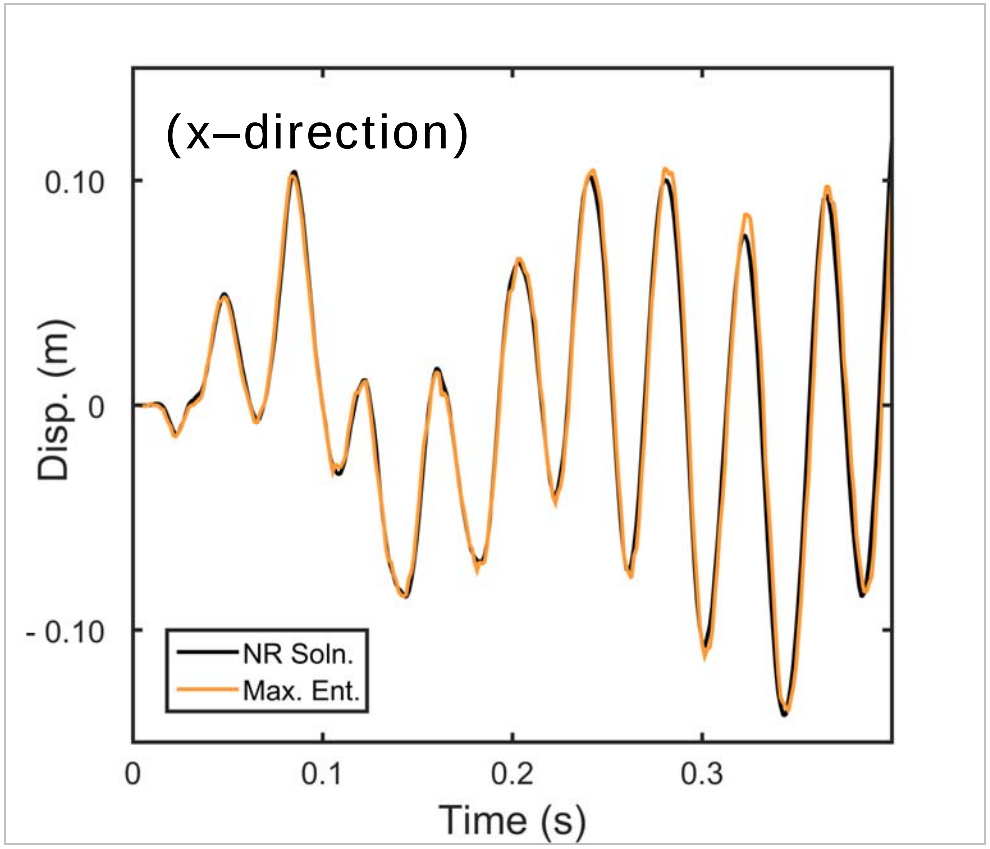
Time-dependent problems: Dynamics



T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

Test case: Truss dynamics





Data-Driven solution vs. direct Newmark solution

T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

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Data-driven inelasticity

- Constraint set (time dependent): $E_{k+1} =$

$$\left\{\epsilon_{e,k+1} = B_e u_{k+1}, \quad \sum_{e=1}^{m} w_e B_e^T \sigma_{e,k+1} = f_{k+1}^{\text{ext}}\right\}$$

- History-dependent (local) material data sets:

$$D_{e,k+1} = \left\{(\epsilon_{e,k+1}, \sigma_{e,k+1}) \ : \ \text{past material history}\right\}$$

- Data-driven problem:

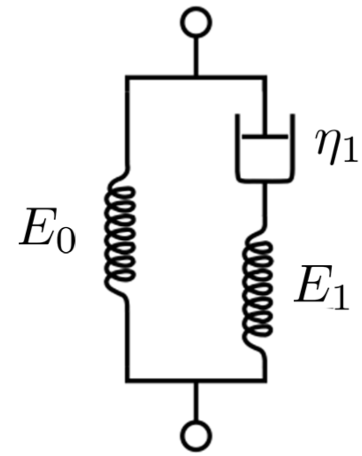
$$\min_{(\epsilon^*,\sigma^*)\in D_{k+1}} \left(\min_{(\epsilon_{k+1},\sigma_{k+1})\in E_{k+1}} |(\epsilon_{k+1}-\epsilon^*, \sigma_{k+1}-\sigma^*)|^2 \right)$$

- *Fundamental question: Data representability!*

R. Eggersmann, T. Kirchdoerfer, L. Stainier,
S. Reese and M. Ortiz, arXiv (2018).

Data-driven viscoelasticity

- Smooth kinetics (linear or nonlinear)
- Allows for differential representation
- Example: Standard Linear Solid,



$$\sigma + \tau_1 \dot{\sigma} - E_0 \epsilon - (E_0 + E_1) \tau_1 \dot{\epsilon} = 0$$

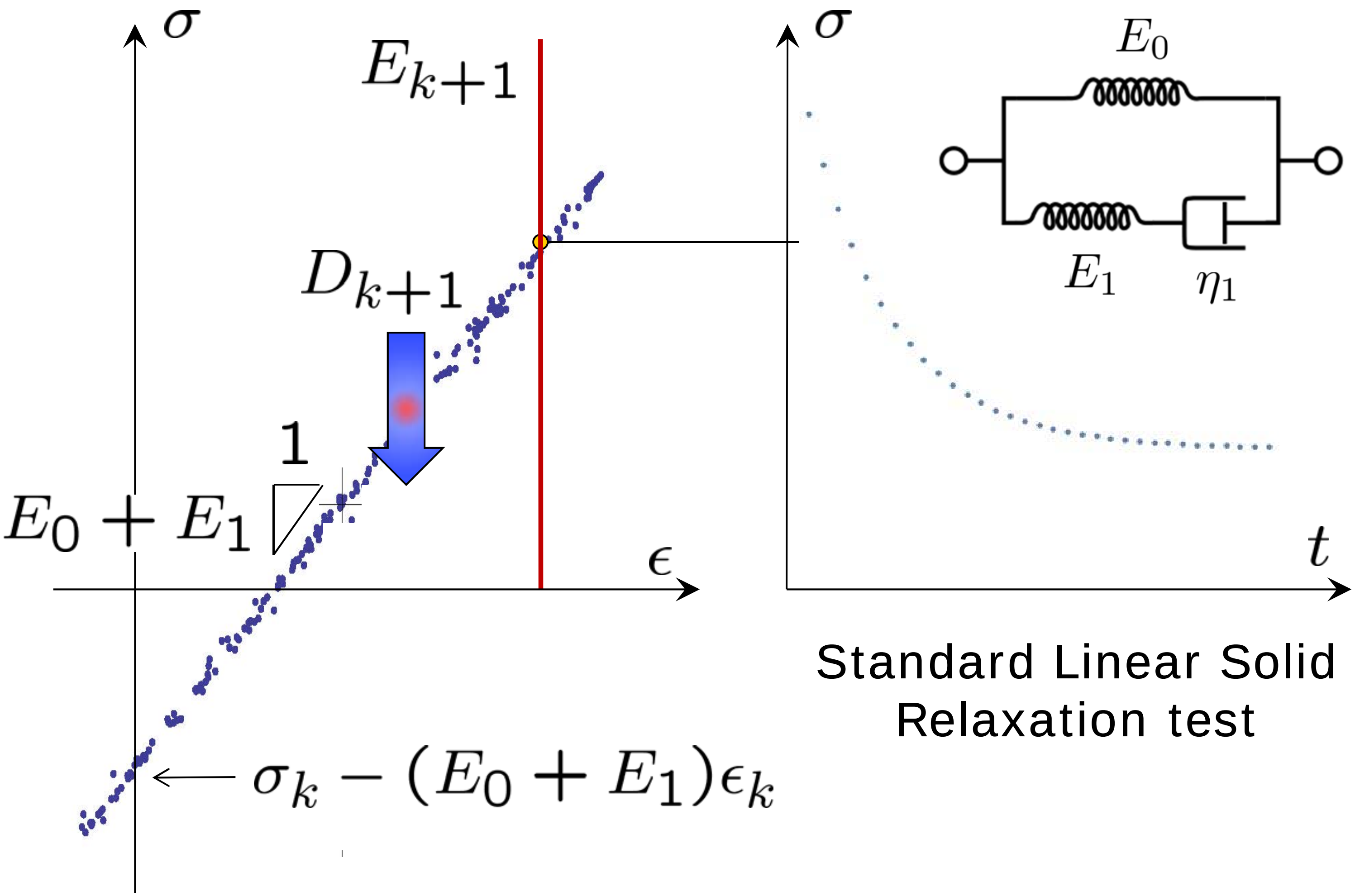
- Time discretization: $D_{k+1} =$

$$\left\{ \sigma_{k+1} + \tau_1 \frac{\sigma_{k+1} - \sigma_k}{t_{k+1} - t_k} - E_0 \epsilon_{k+1} - (E_0 + E_1) \tau_1 \frac{\epsilon_{k+1} - \epsilon_k}{t_{k+1} - t_k} = 0 \right\}$$

- General first-order differential materials:

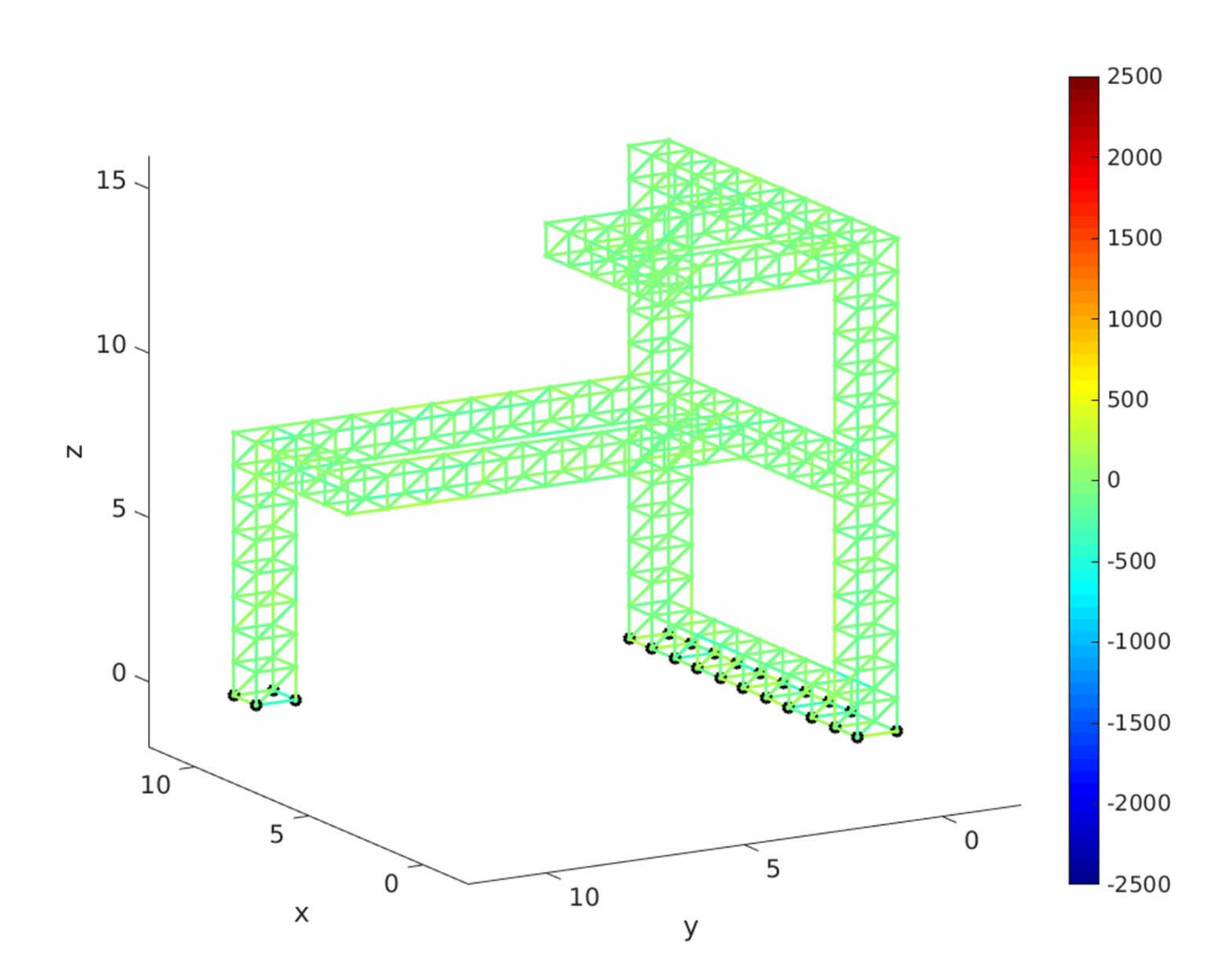
$$D_{k+1} = \left\{ (\epsilon_{k+1}, \sigma_{k+1}) \, : \, (\epsilon_k, \sigma_k) \right\}$$

Data-Driven viscoelasticity



Standard Linear Solid
Relaxation test

Data-Driven viscoelasticity



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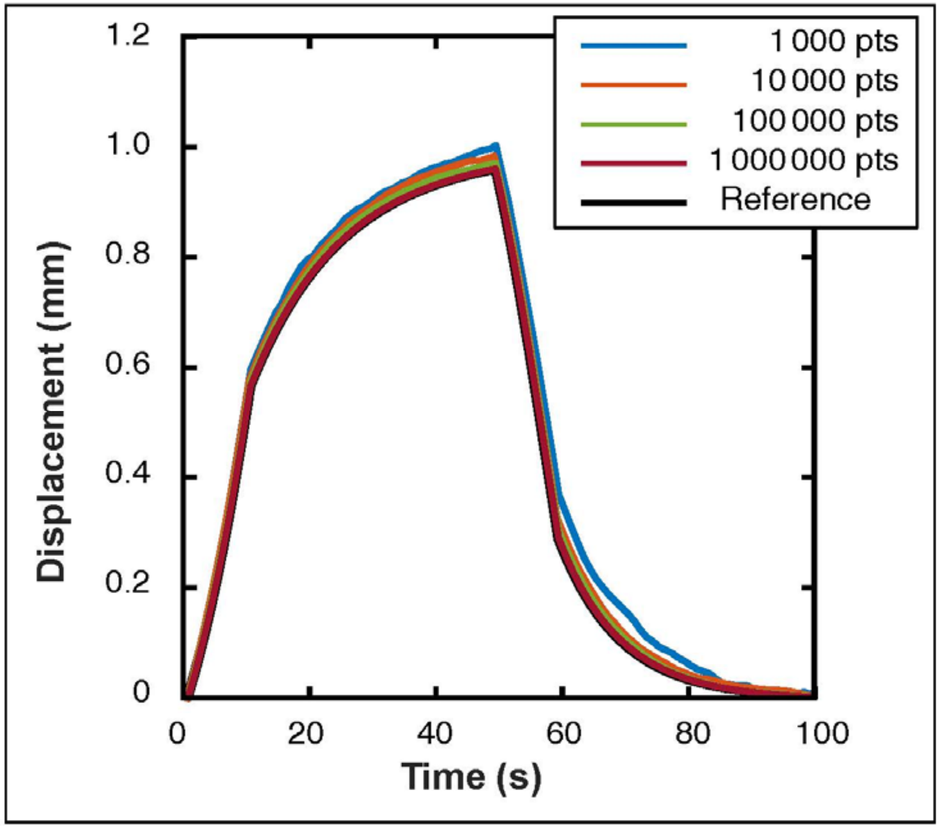
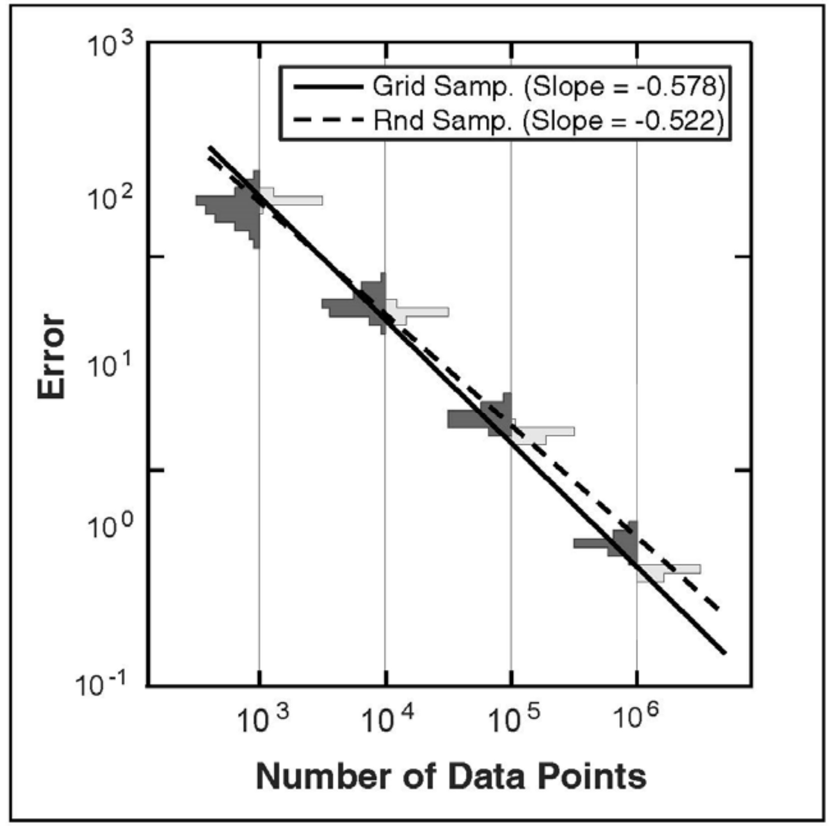


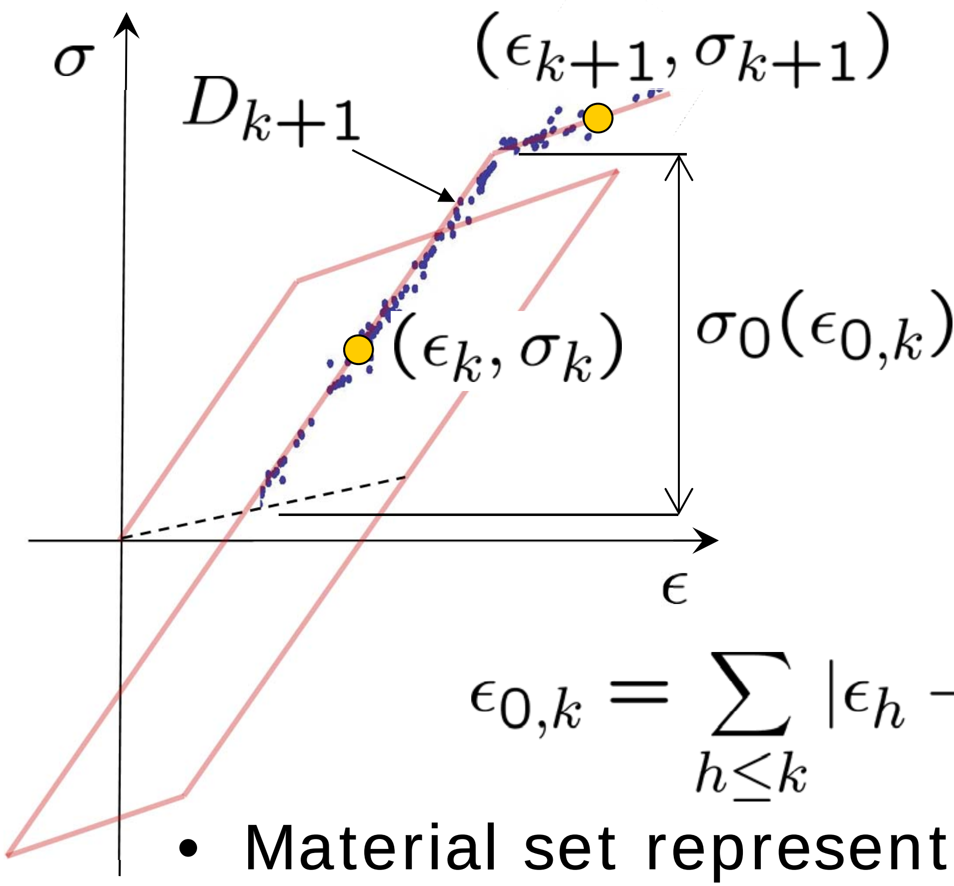


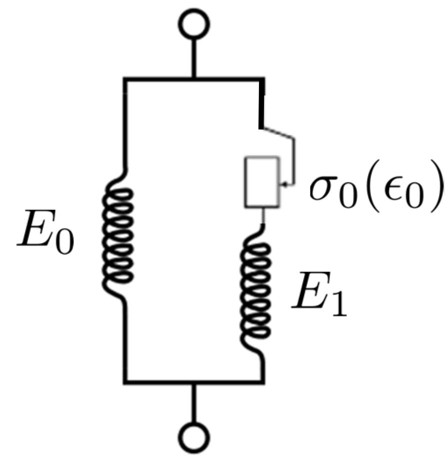
Convergence with respect to the data set

R. Eggersmann, T. Kirchdoerfer, L. Stainier, S. Reese and M. Ortiz, arXiv (2018).

Data-Driven plasticity

- Example: Isotropic/kinematic hardening





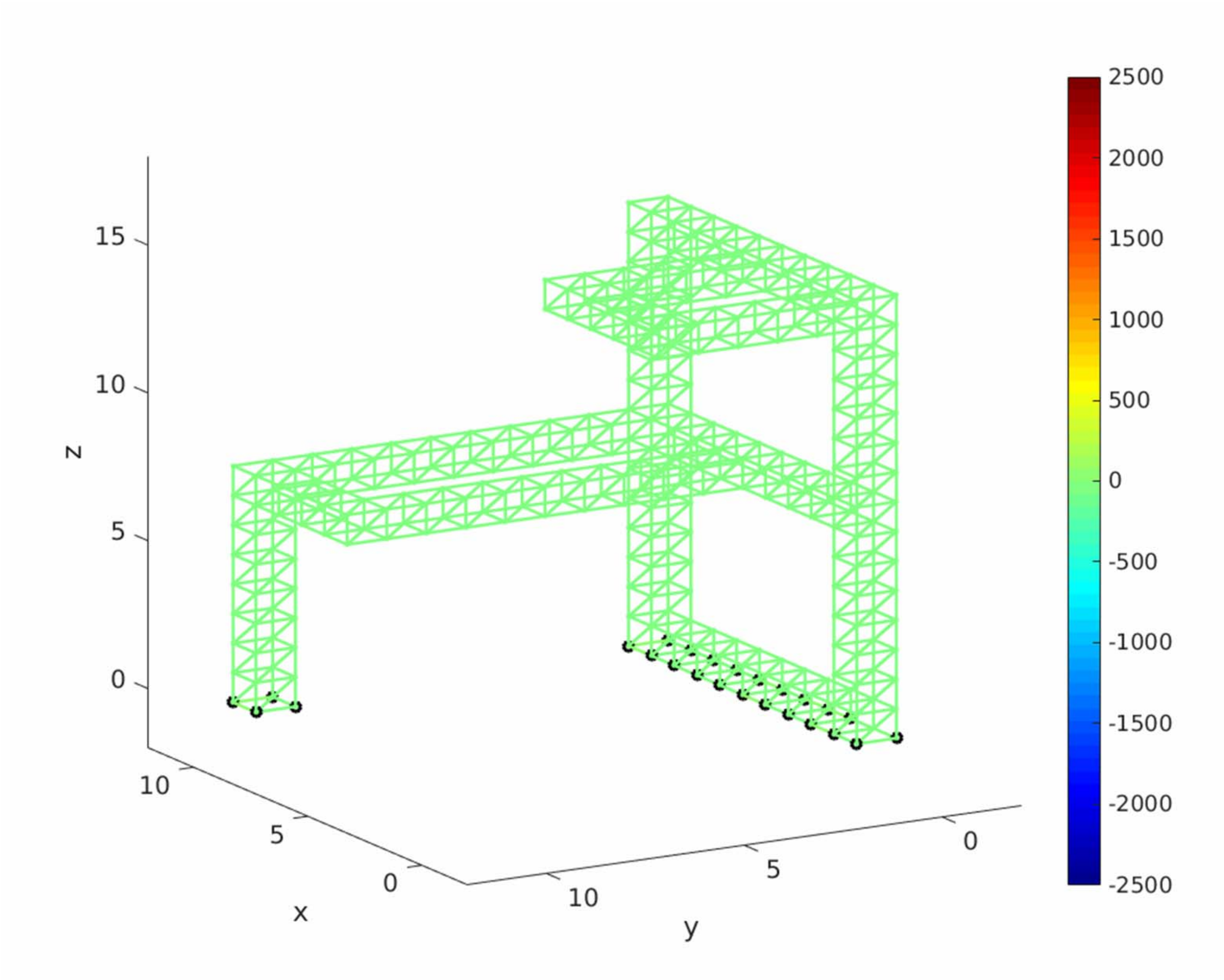
- History variable:

$$\epsilon_{0,k} = \sum_{h \leq k} |\epsilon_h - \epsilon_{h-1} - (\sigma_h - \sigma_{h-1})/E|$$

- Material set representation (diff + history):

$$D_{k+1} = \Big\{(\epsilon_{k+1}, \sigma_{k+1}) \ : \ (\epsilon_k, \sigma_k), \epsilon_{0,k}\Big\}$$

Data-Driven plasticity



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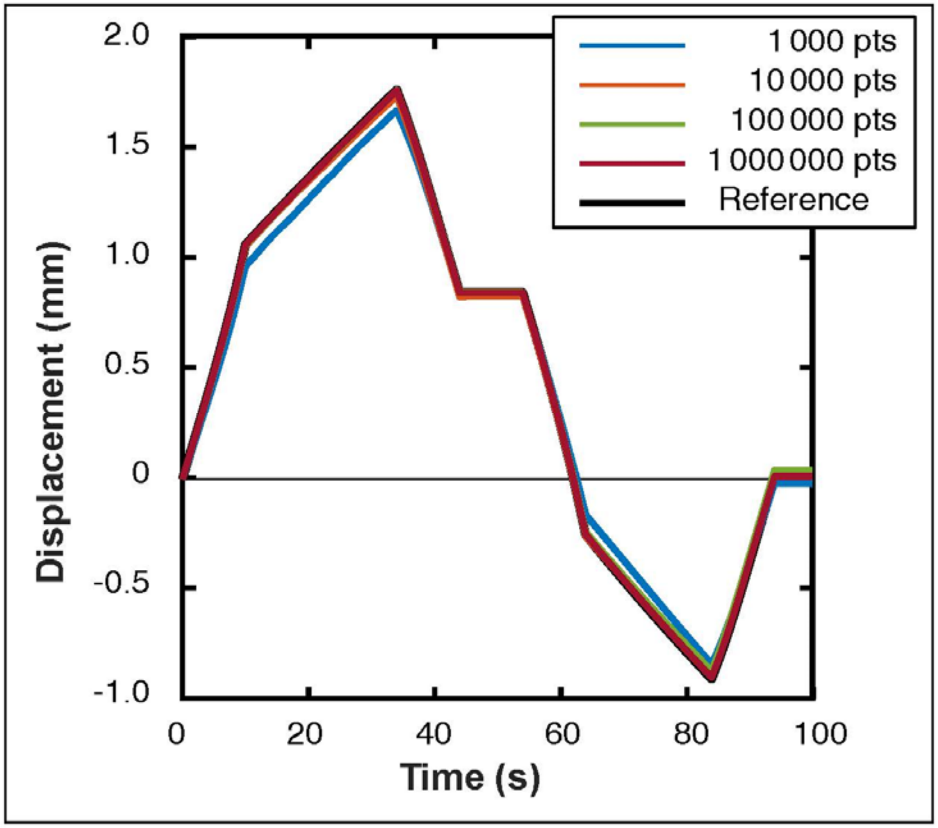

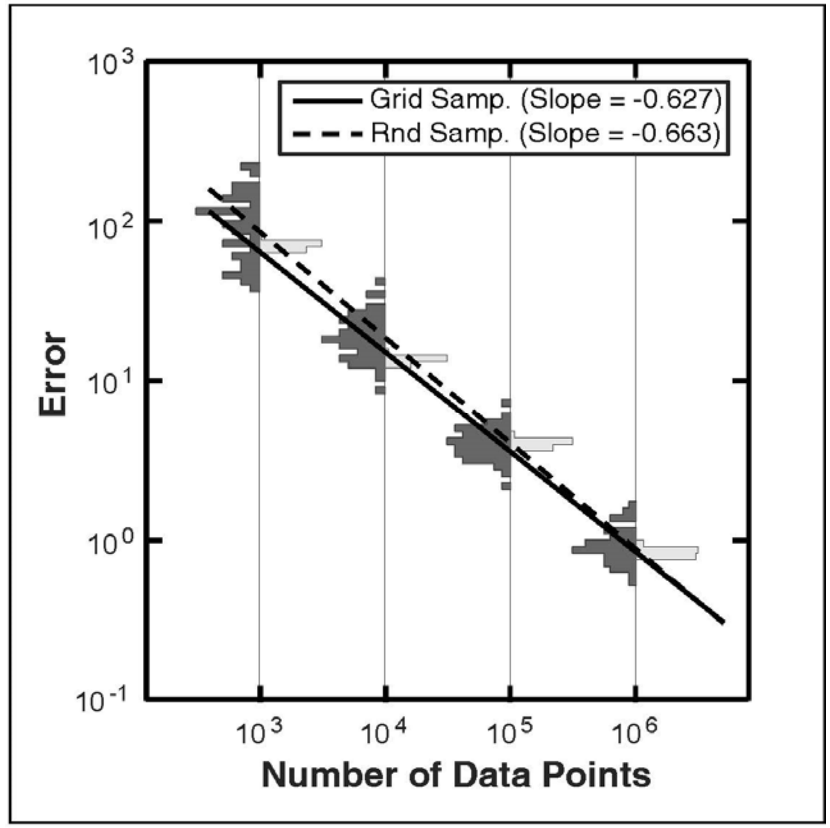

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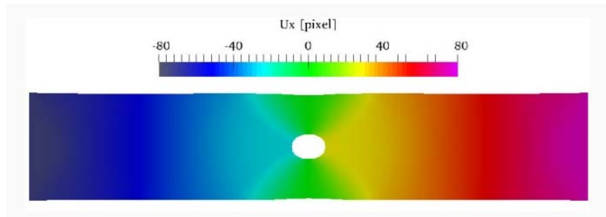
DD self-consistent material identification



- Full-field measurements (DIC), M loading cases:

$$D_{\text{exp}} = \{(\boldsymbol{u}^\alpha, \boldsymbol{f}^\alpha),\ \alpha = 1, \dots, M\}.$$

- Constraint set:

$$E = \cup_{\alpha=1}^{M} \{\epsilon_e = B_e u^\alpha, \textstyle\sum_{e=1}^{m} w_e B_e^T \sigma_e = f^\alpha\}$$

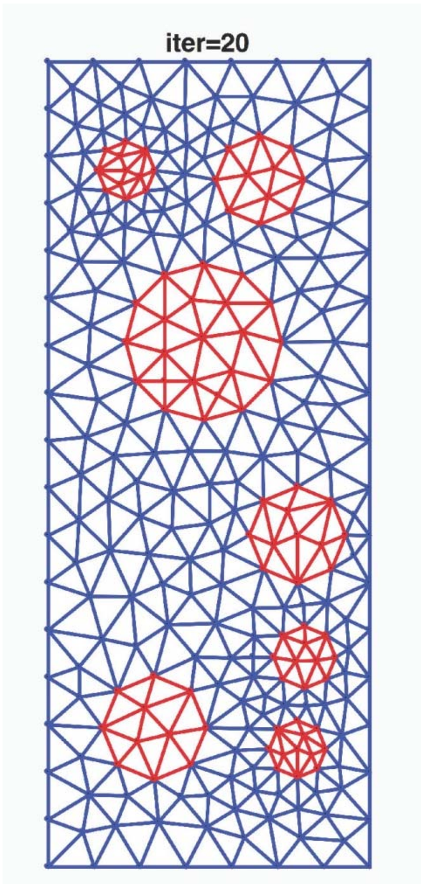
- Stresses σ_e^α cannot be measured directly!

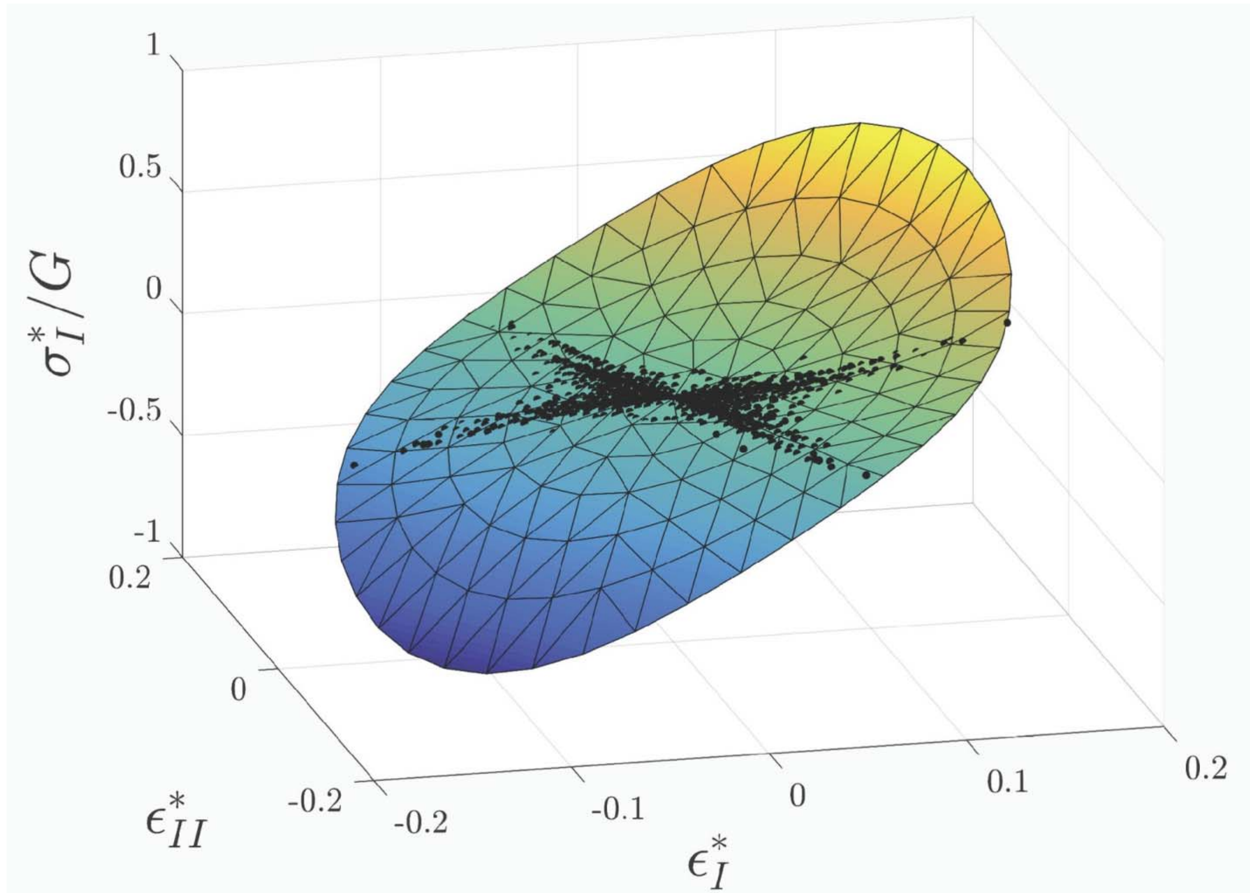
- DD self-consistent material-data identification:

$$\text{Given } D_{\text{exp}}: \quad \min_{(\boldsymbol{\epsilon}^*, \boldsymbol{\sigma}^*) \in \mathbb{R}^{12N}} \left(\min_{(\boldsymbol{\epsilon}, \boldsymbol{\sigma}) \in E} |(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^*, \boldsymbol{\sigma} - \boldsymbol{\sigma}^*)|^2 \right)$$

J. Rethore, HAL Id: hal-01454432, Feb. 2017.
J. Rethore and A. Leygue, HAL Id: hal-01452494, Feb. 2017.

DD self-consistent material identification

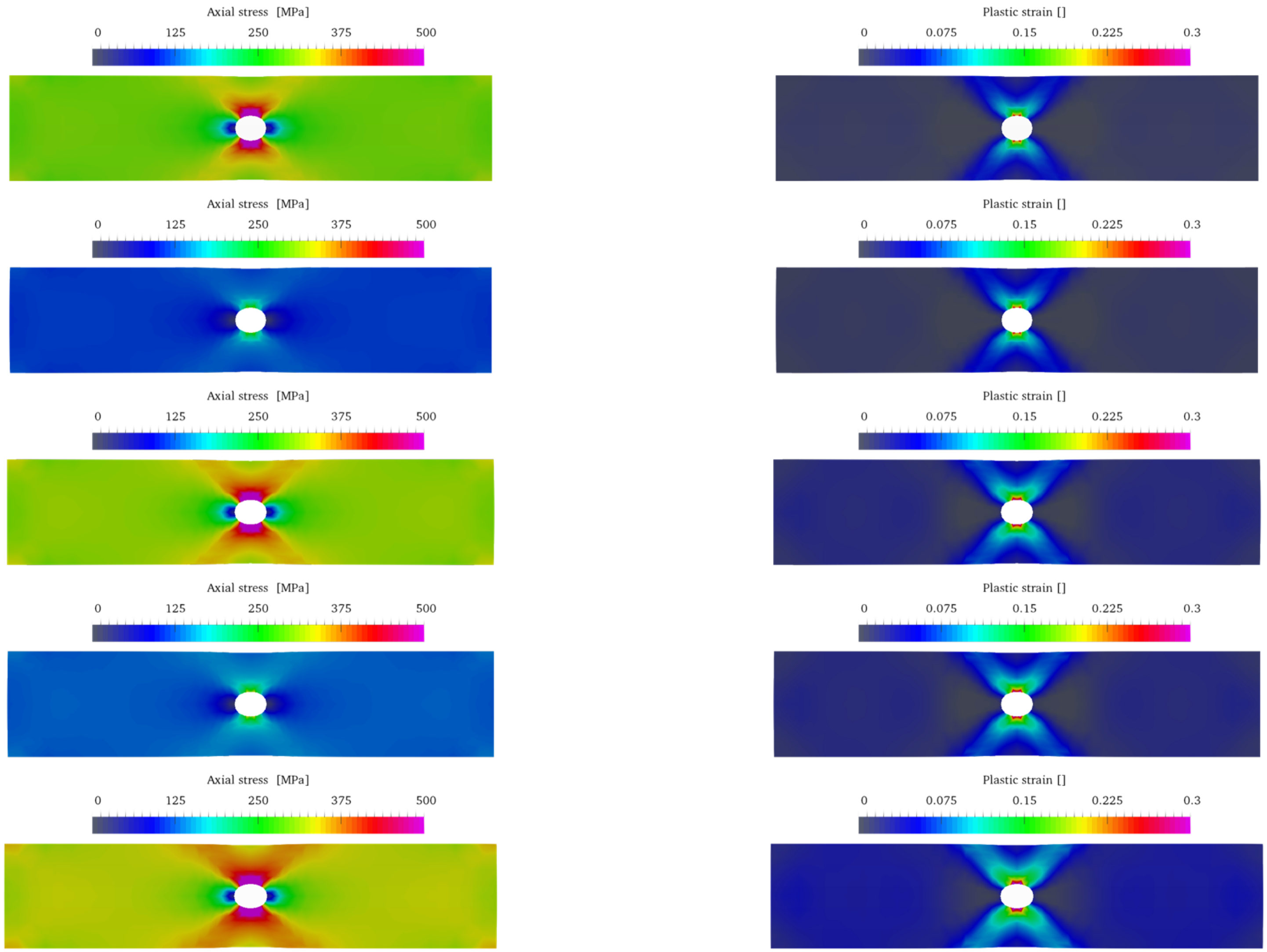




Nonlinear-elastic composite material with cubic symmetry

J. Rethore, HAL Id: hal-01454432, Feb. 2017.
J. Rethore and A. Leygue, HAL Id: hal-01452494, Feb. 2017.

DD self-consistent material identification



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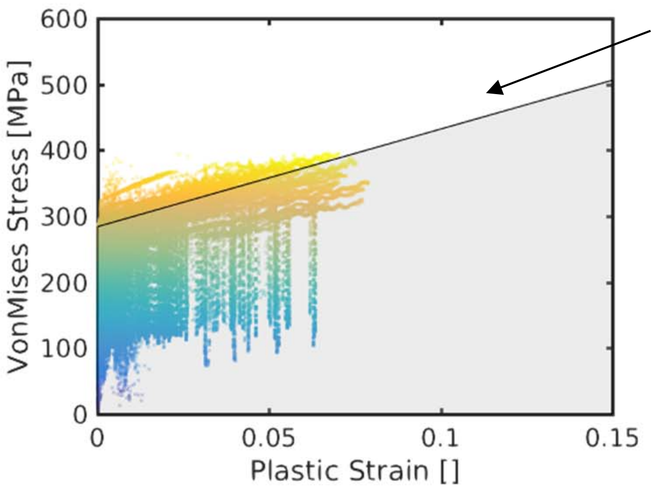
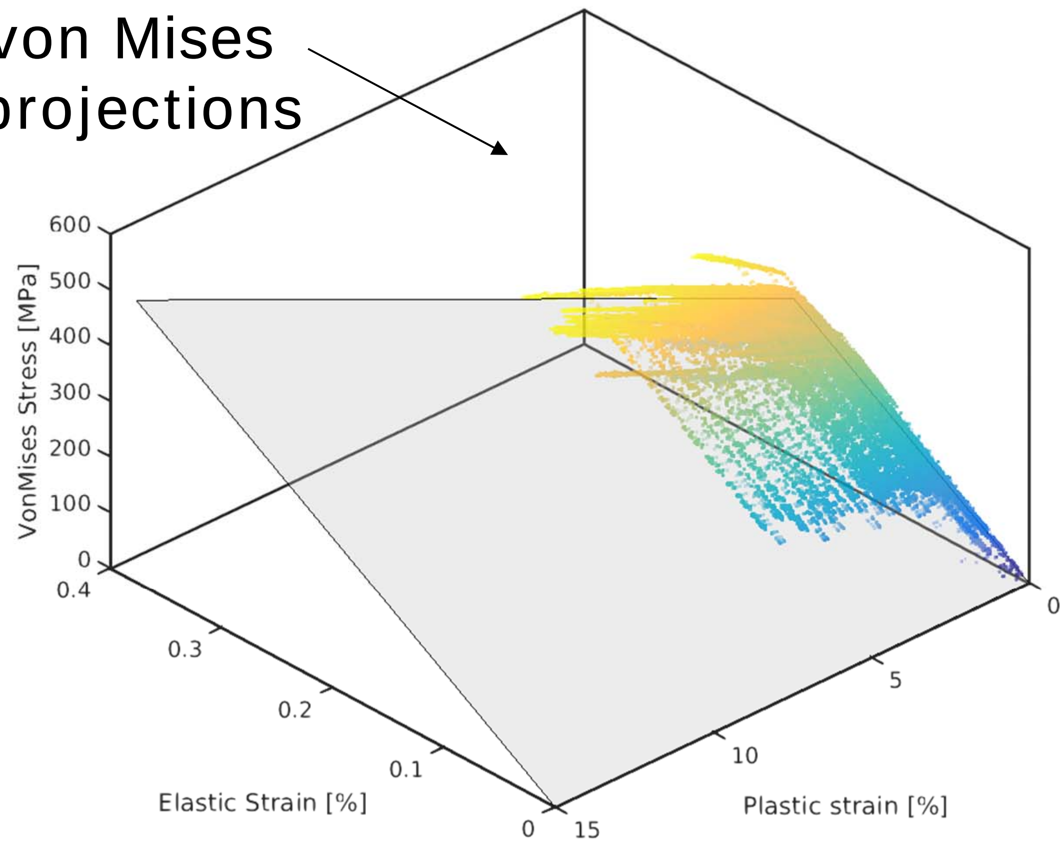
DD self-consistent material identification



von Mises projections



Elastic-plastic material data base, 600000 points in dimension 12

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Concluding remarks

- DD solvers provide a *new paradigm* in computational mechanics that builds directly on material data and bypasses the material modeling step entirely (*model-free!*)
- DD solvers lend themselves to *standardization*:
  - *Linear initial-strain problem (e.g., FE solver)*
  - *Linear initial-stress problem (e.g., FE solver)*
  - *Stress-strain look-up from material data repository*
- *Objective: Publicly-editable material data repository (Wikimat?):*
  - *Fundamental data (stress-strain, full-field, DIC)*
  - *Scripts for interfacing with commercial FE packages*

[1]T. Kirchdoerfer and M. Ortiz, *CMAME*, **326** (2017) 622-641.

Concluding remarks

- Reliance on *fundamental data* (stress and strain only, no model-dependent data) makes *material data fungible*, mergeable, interchangeable...
- Data can be *mined* from lower-scale calculations, used in upper-scale calculations (*DD upscaling*)
- Data can also be extracted from *full-field experimental data* (TEM, SEM, DIC, EBSD...)
- High-dimensional phase spaces: *Self-consistent DD material identification!*[1] (goal oriented)
- *Data-driven computing* is likely to be a *growth area* in an increasingly *data-rich world!*

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Concluding remarks

Thank you!