(Model-Free) Data-Driven Computational Mechanics

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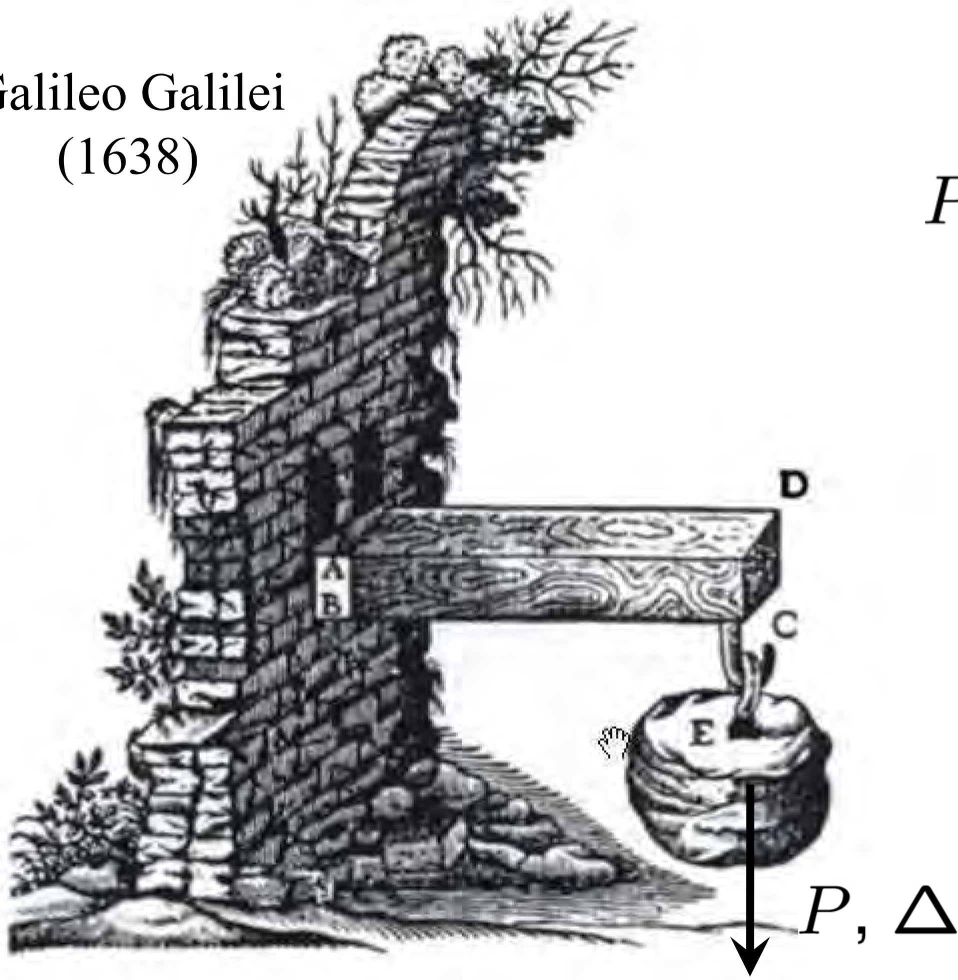
R. Eggersmann, S. Reese (RWTH Aachen)

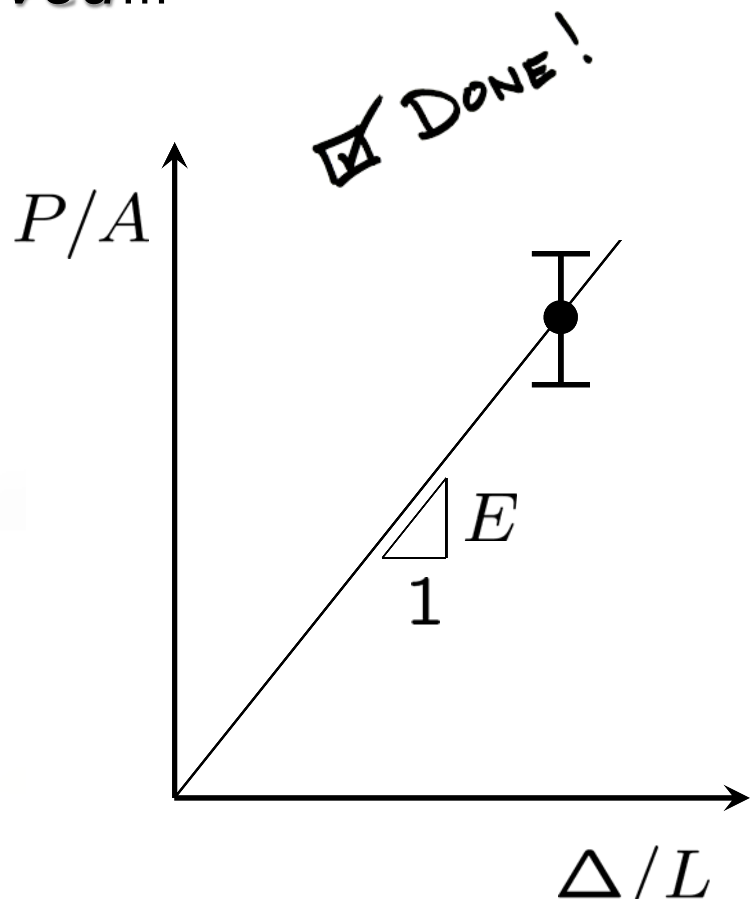
GALCIT Colloquium – April 17, 2020
(Advanced seminar course Ae 208 abc)

Materials data through the ages…

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

Galileo Galilei
(1638)





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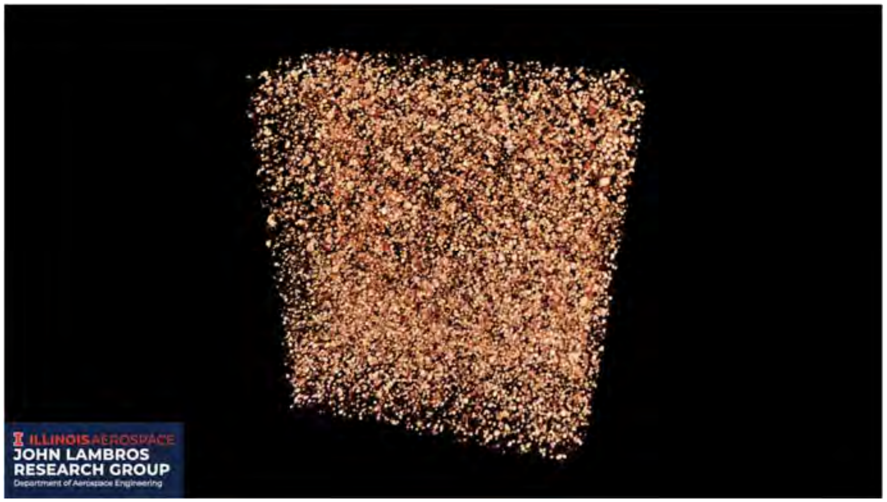
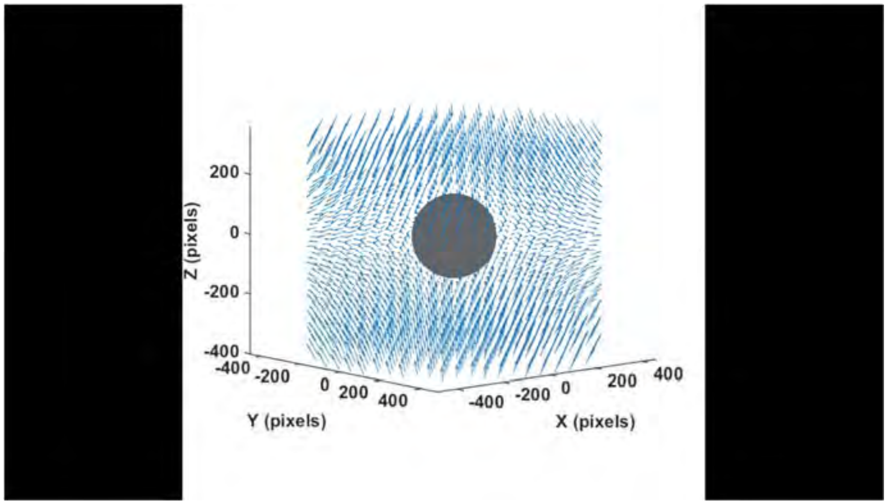
The new data-rich world…

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



3D tomographic reconstruction of particles in battery electrode



3D DIC-measured full-field internal displacements in compressed PDMS sample

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

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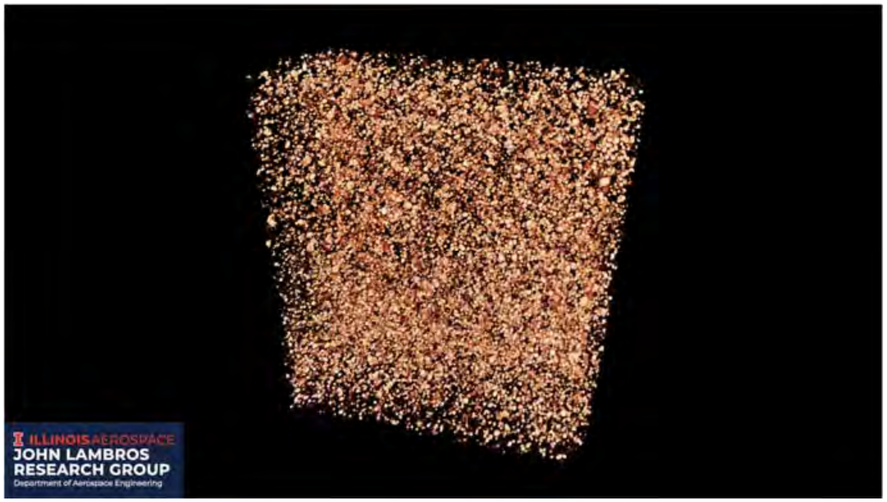

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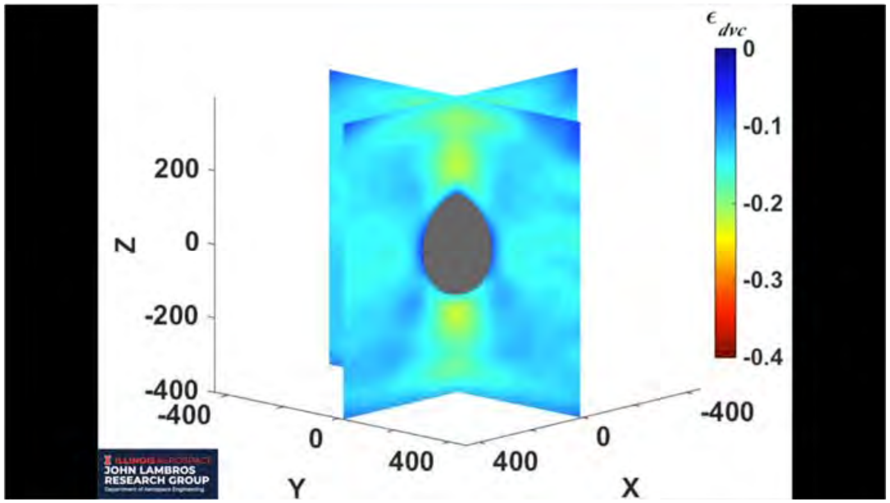

3D DIC-measured internal-strain full-field compressed PDMS sample

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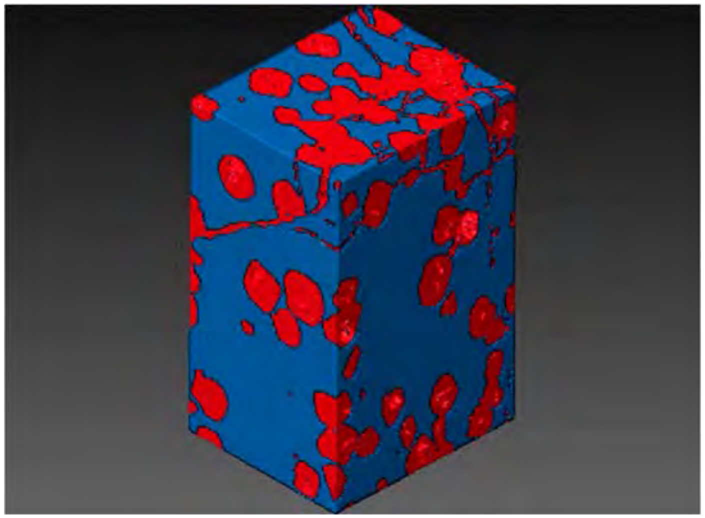
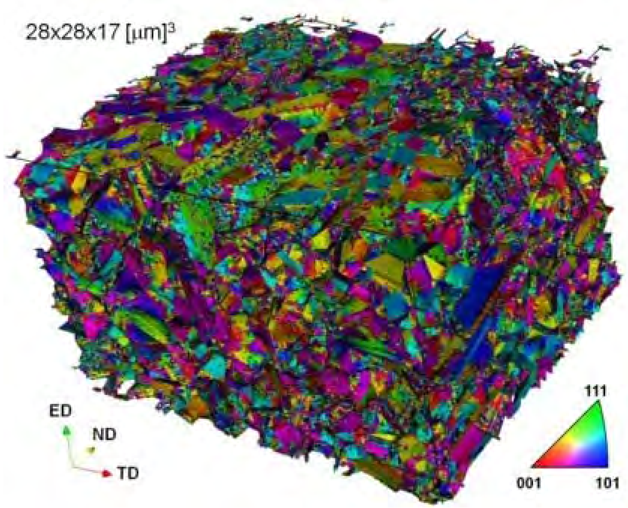


Two-phase μCT analysis of Ti2AlC/Al composite[1]



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.

Data Science, Big Data…

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

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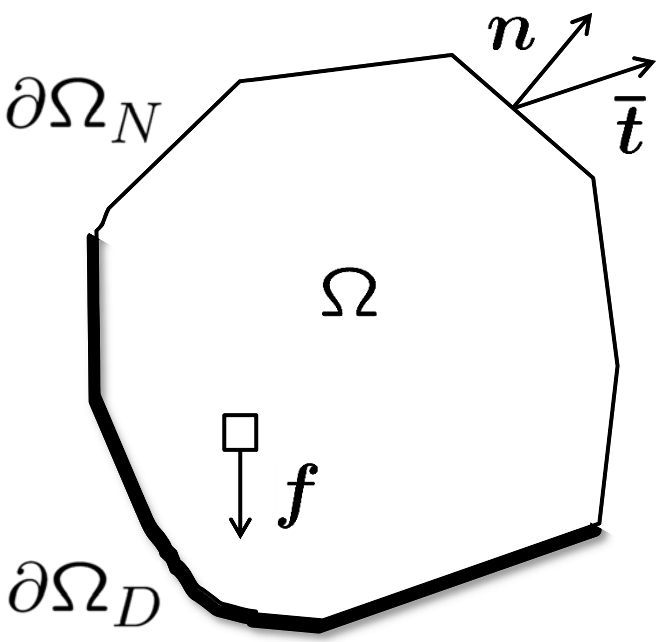
Data Science, Big Data…

- *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... The field theories of science have distinct math structure which must be accounted for...*

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

Differential structure of field equations

- 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: $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}\Big(\epsilon(\boldsymbol{x})\Big)$

Differential structure of field equations

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

Universal laws!
Material independent!
Exactly known!
Uncertainty-free!
Similarly:
Maxwell, Einstein, Schrödinger...

i) Kinematics + Dirichlet:

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

∂!

ii) Equilibrium + Neumann:

$$\text{div}\, \boldsymbol{\sigma} + \boldsymbol{f} = \boldsymbol{0}$$
$$\boldsymbol{\sigma}\boldsymbol{n} = \bar{\boldsymbol{t}}, \quad \text{on } \partial\Omega_N$$

δ!

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

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Differential structure of field equations

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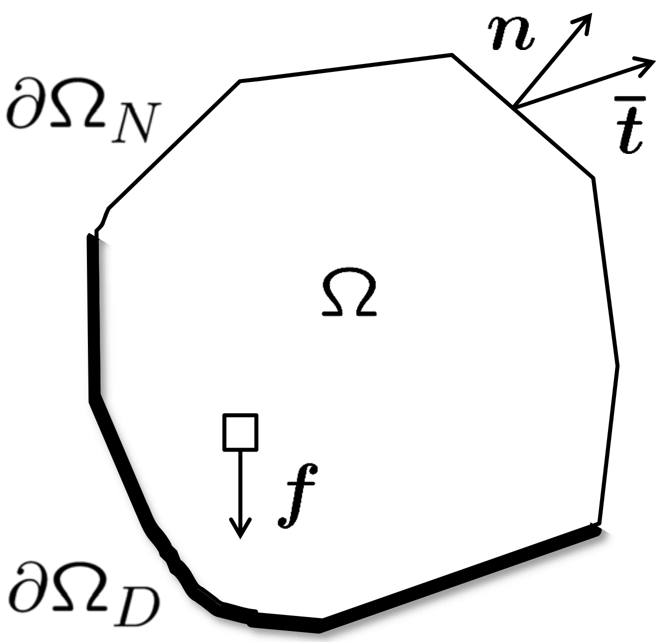

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iii) Material law: $\underbrace{\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}\Big(\epsilon(\boldsymbol{x})\Big)}$

Unknown! Epistemic uncertainty!

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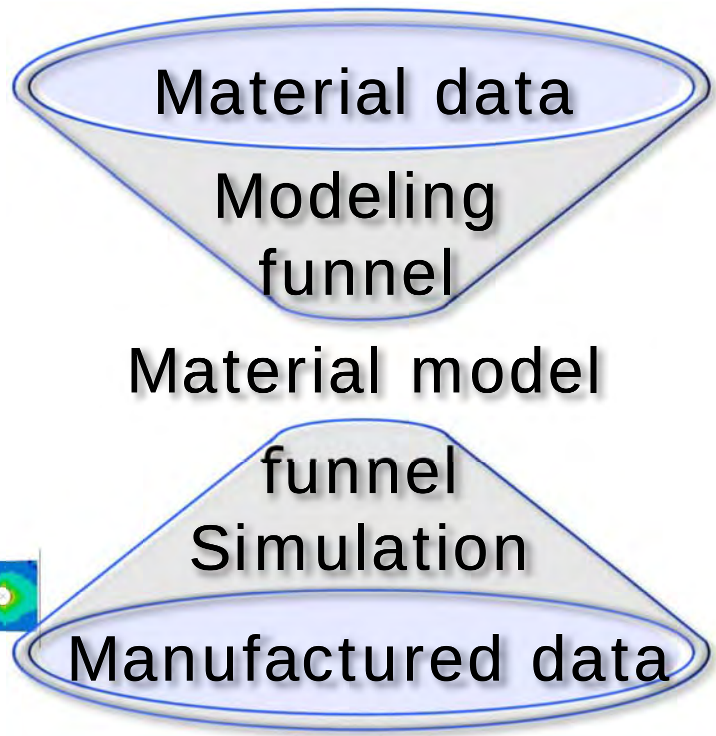
Adapting to a new data-rich world...

Classical Model-Based Computational Science...

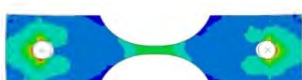
Alternative: Model-Free Data-Driven Computing!

Modern microscopy generates massive data sets

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



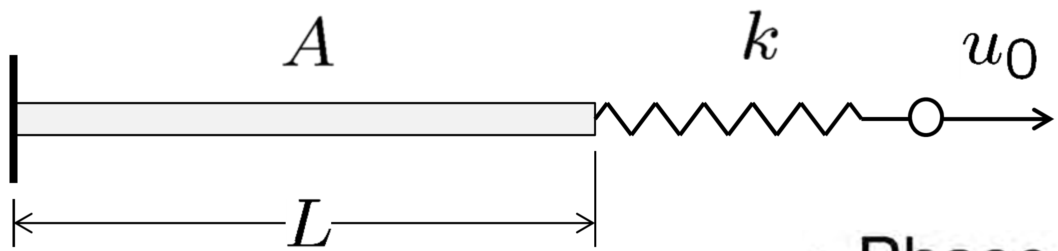
Modelling entails massive loss of information!

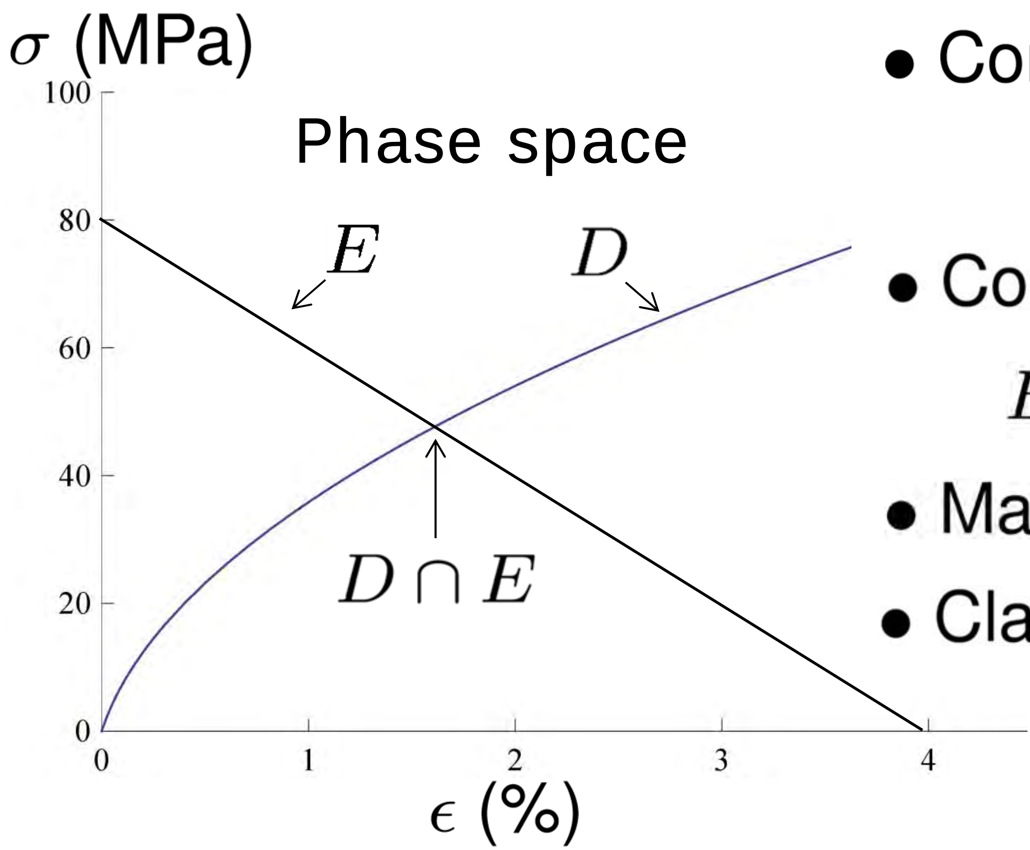


Set/solve problems directly from data!

Eliminate modeling bottleneck!

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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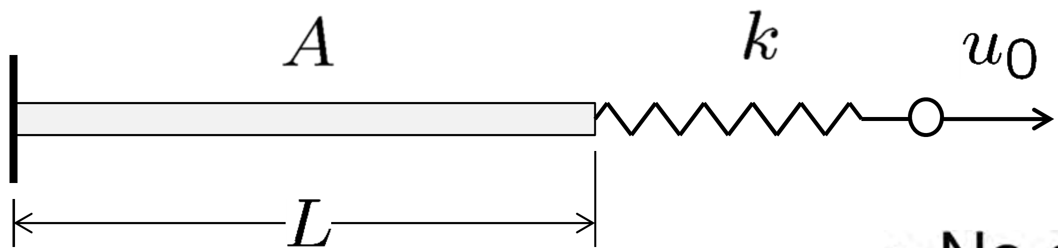
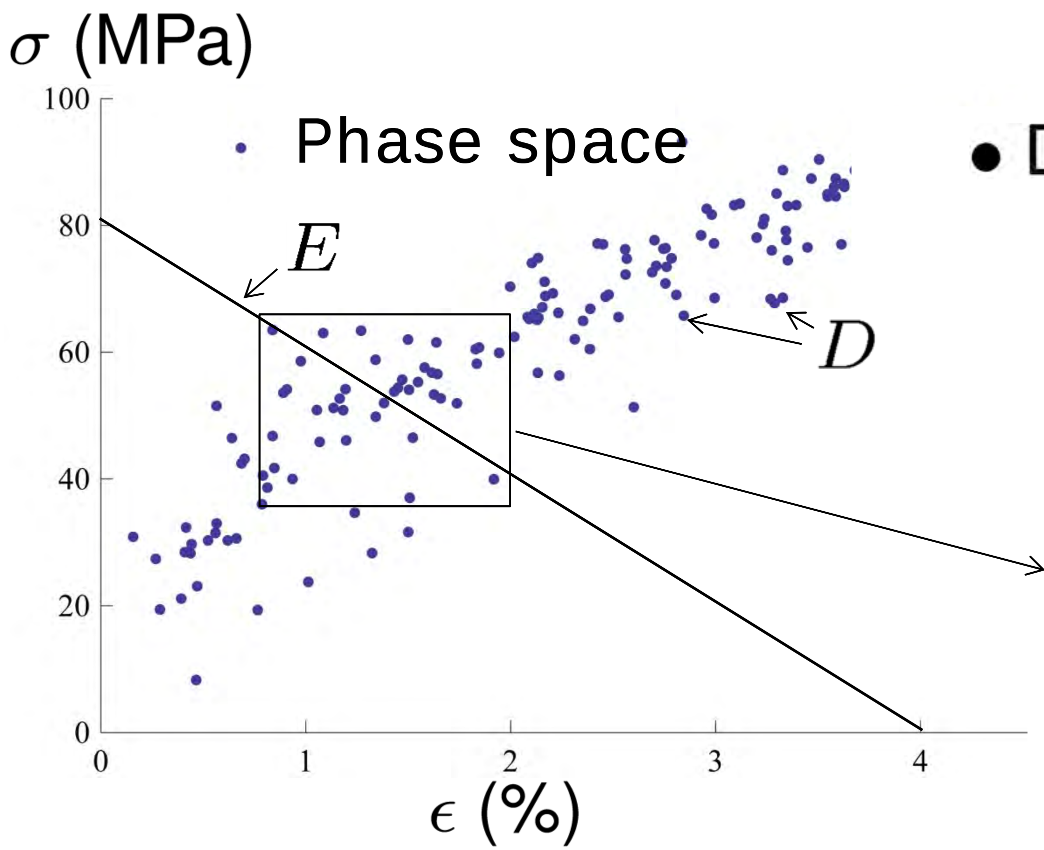
Elementary example: Bar and spring



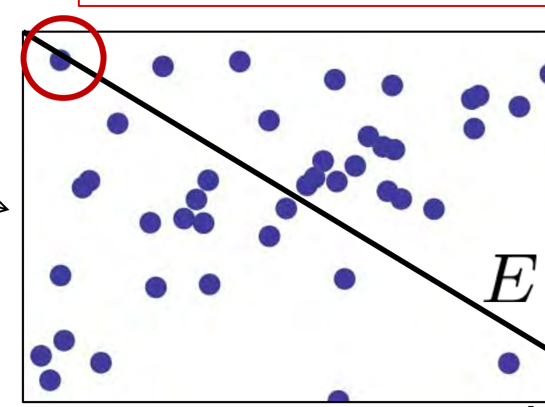


- No classical solutions!

$$D \cap E = \emptyset$$

- Data-driven solution:

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



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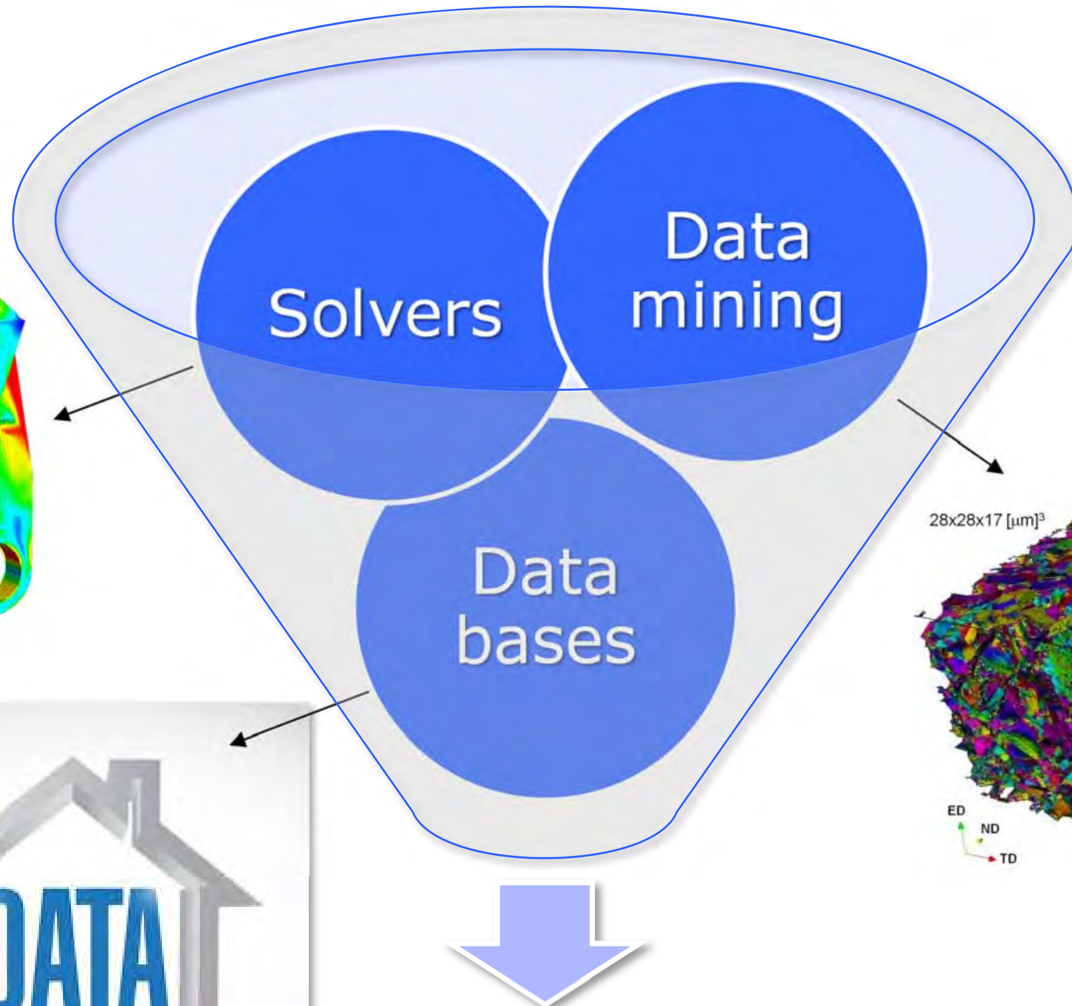
The general Data-Driven (DD) problem

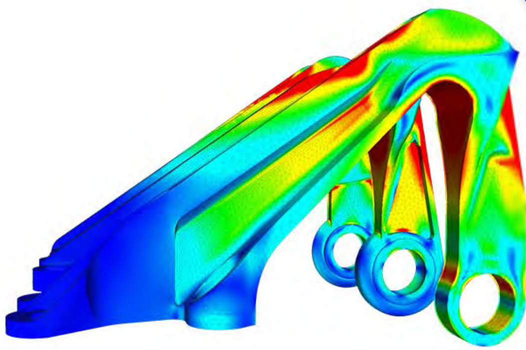
- The Data-Driven paradigm[1]: Given,
  - *D = {fundamental material data},*
  - *E = {compatibility + equilibrium},*

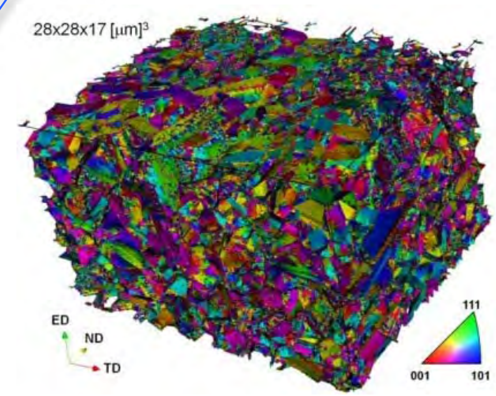
  Find: argmin$\{d(z, D),\ z \in E\}$
- ***The aim of Data-Driven analysis is to find the compatible strain field and the equilibrated stress field closest to the material data set***
- Raw *fundamental* (stress & strain) material data is used (unprocessed) in calculations
- No material modeling, no loss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

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

The (model-free) DD ecosystem…







DD

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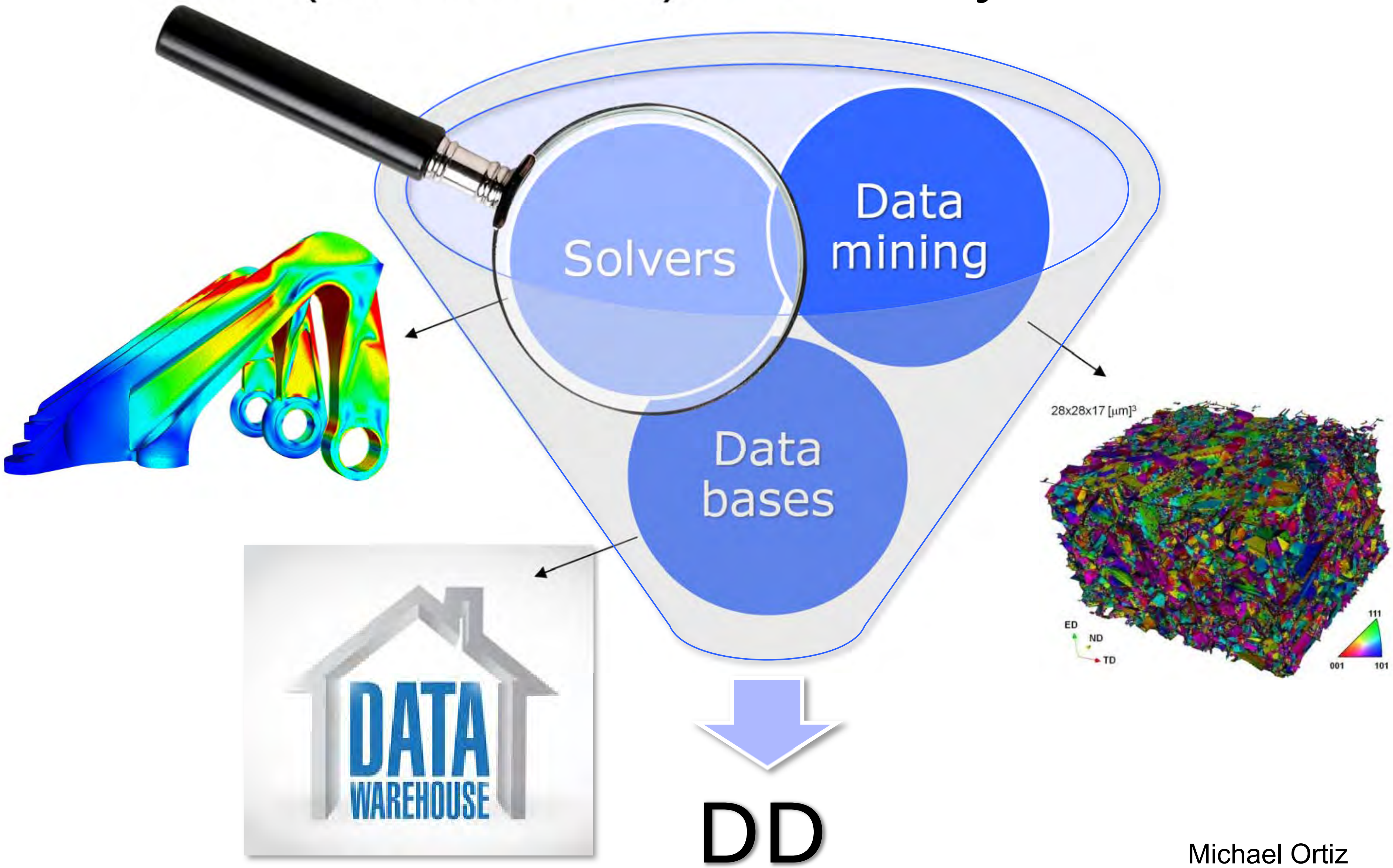
The (model-free) DD ecosystem…



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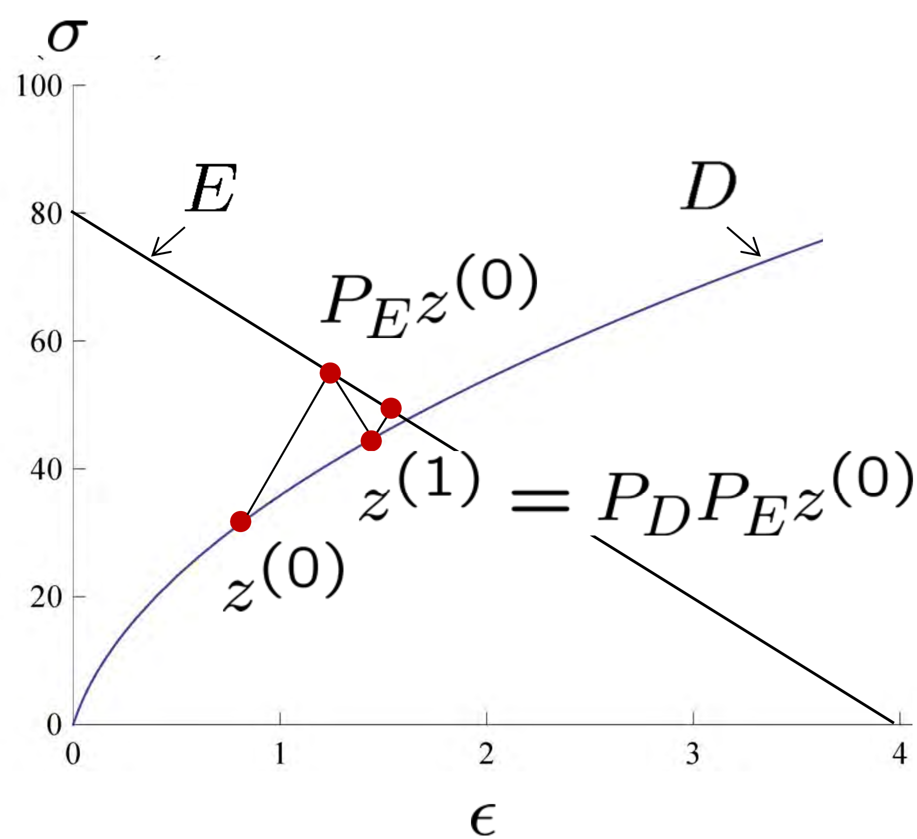
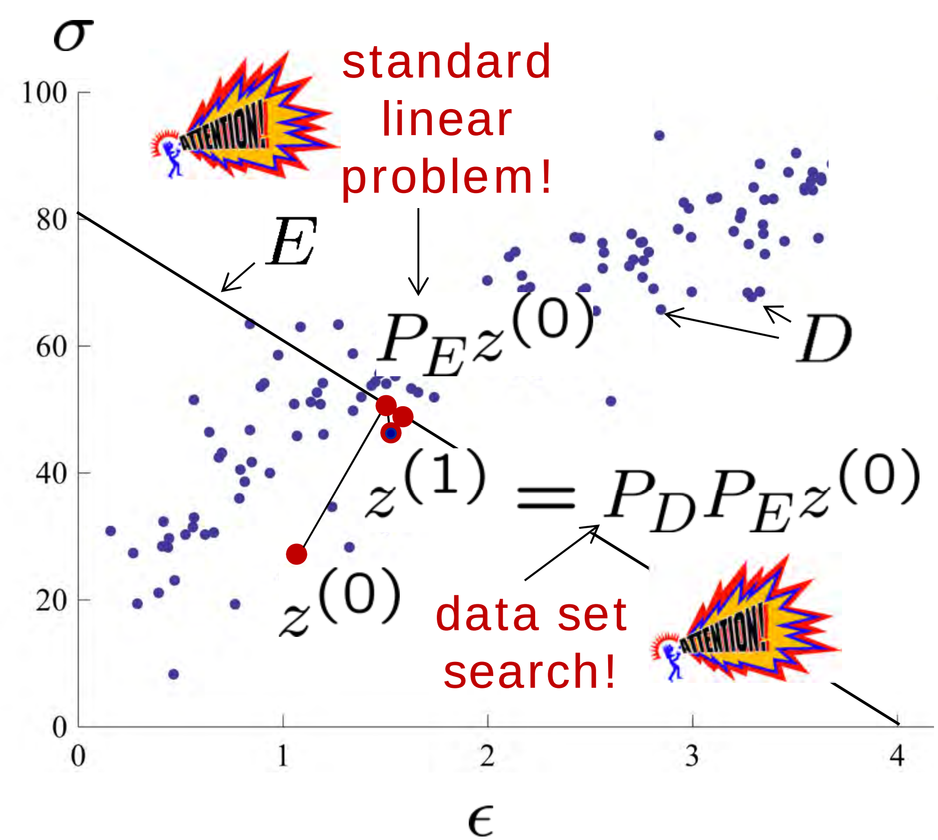
DD solvers: Fixed-point iteration

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

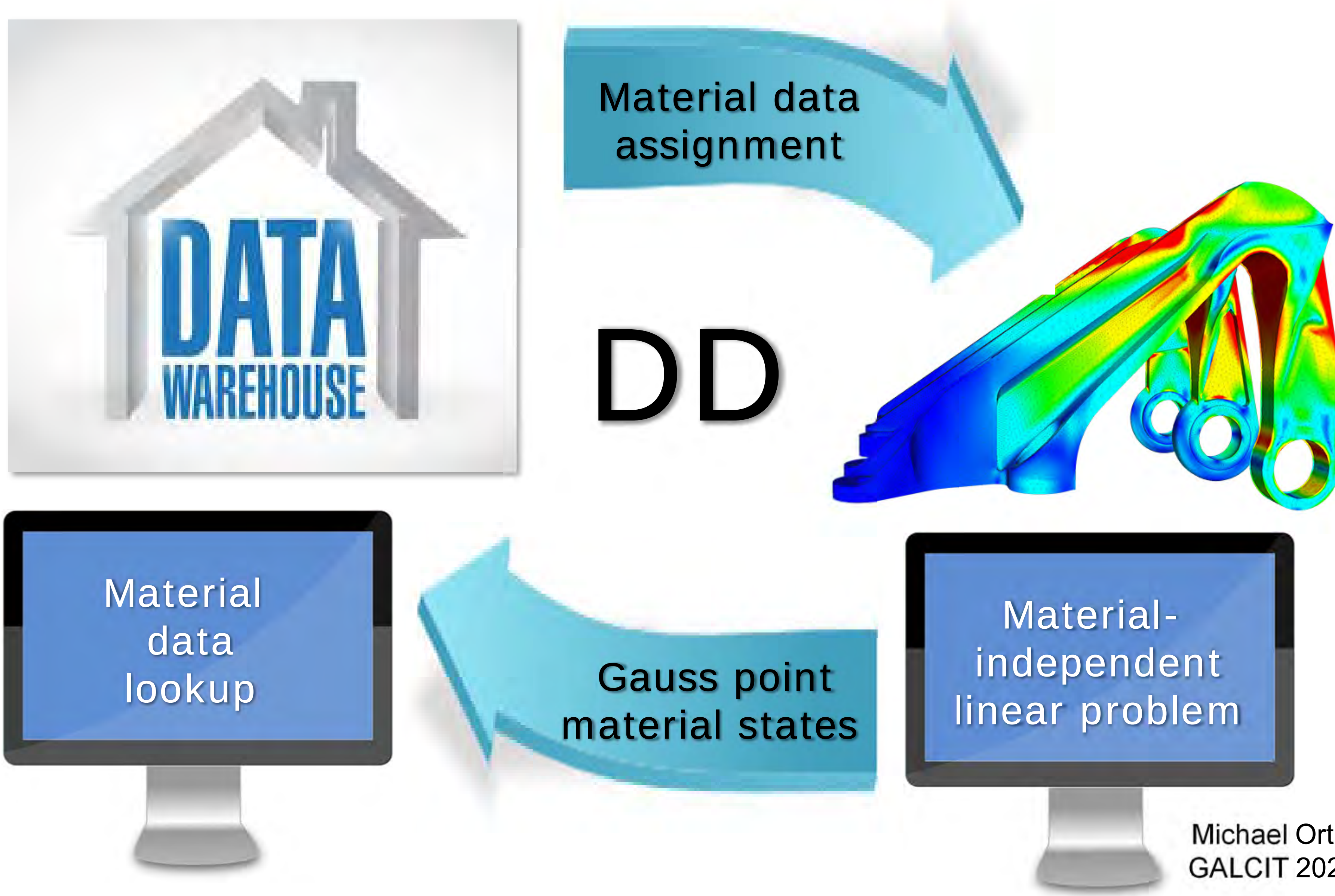




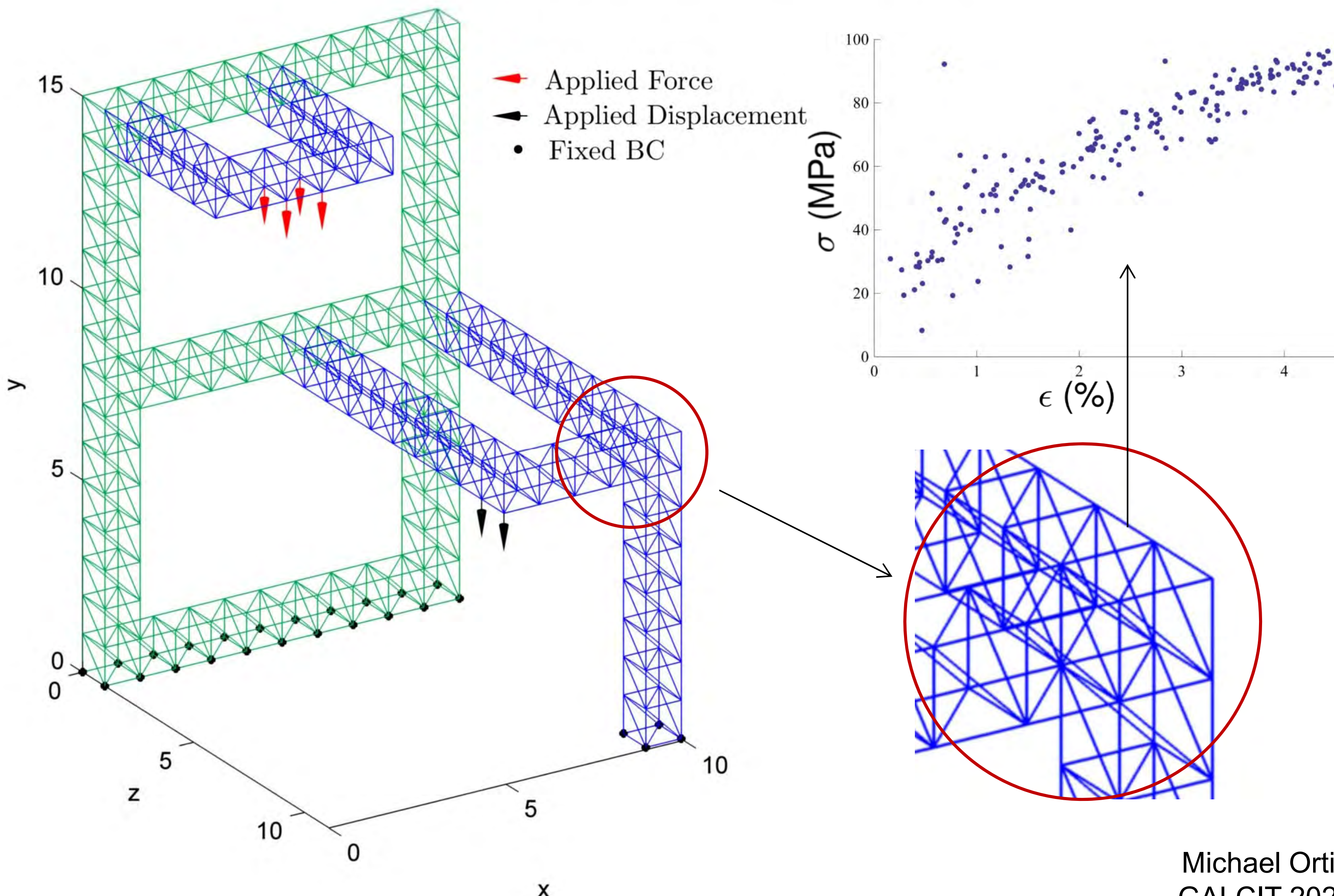
[1]T. Kirchdoerfer and M. Ortiz (2015) arXiv:1510.04232.

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

The DD information flow



Test case: 3D Truss



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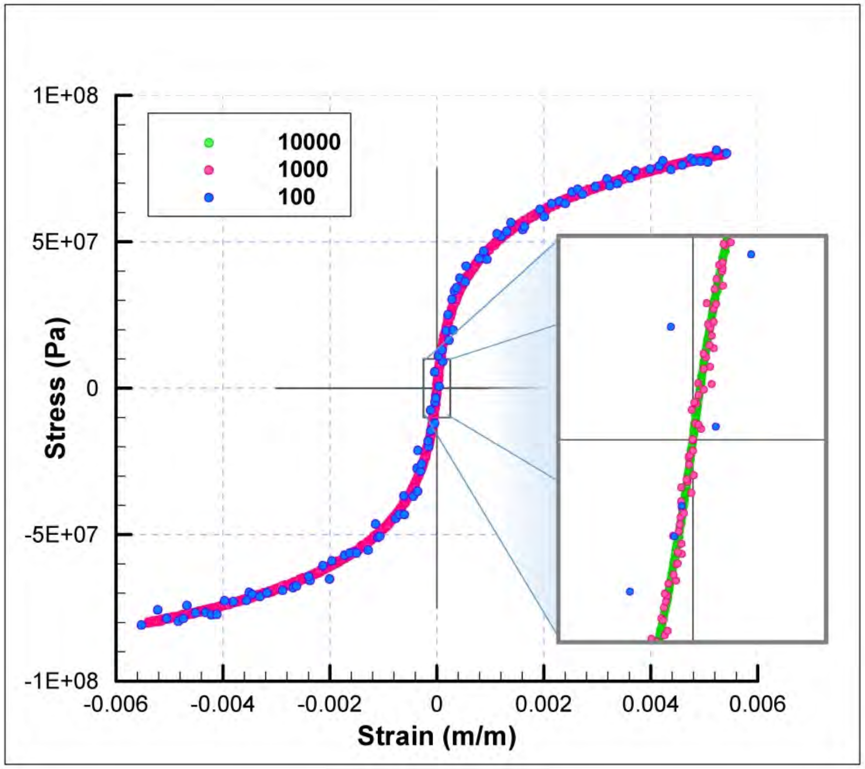
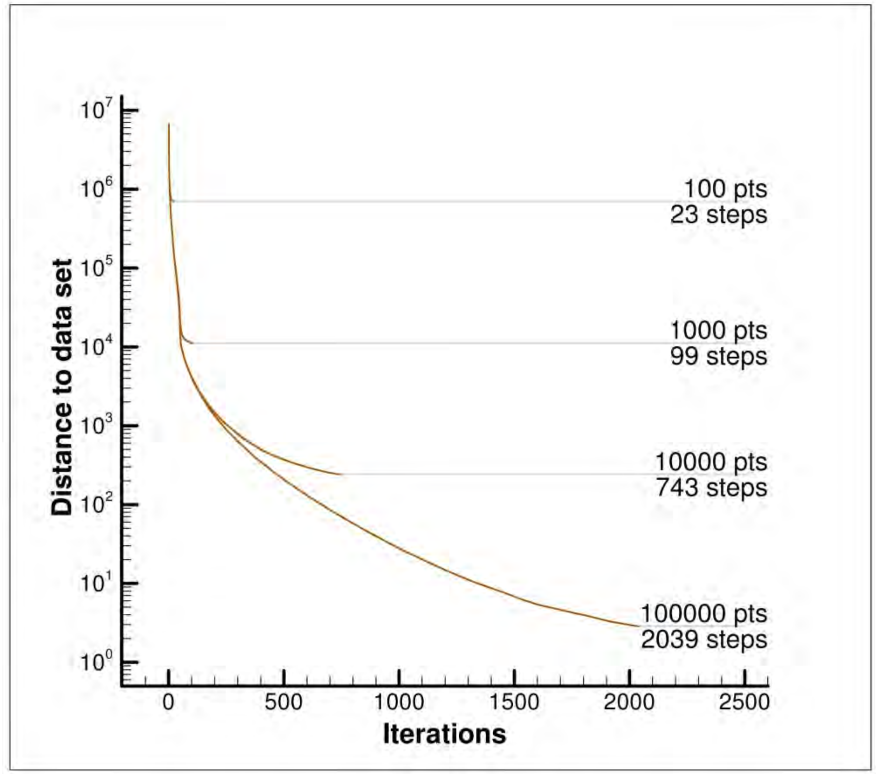
Convergence of fixed-point solver



Radomized 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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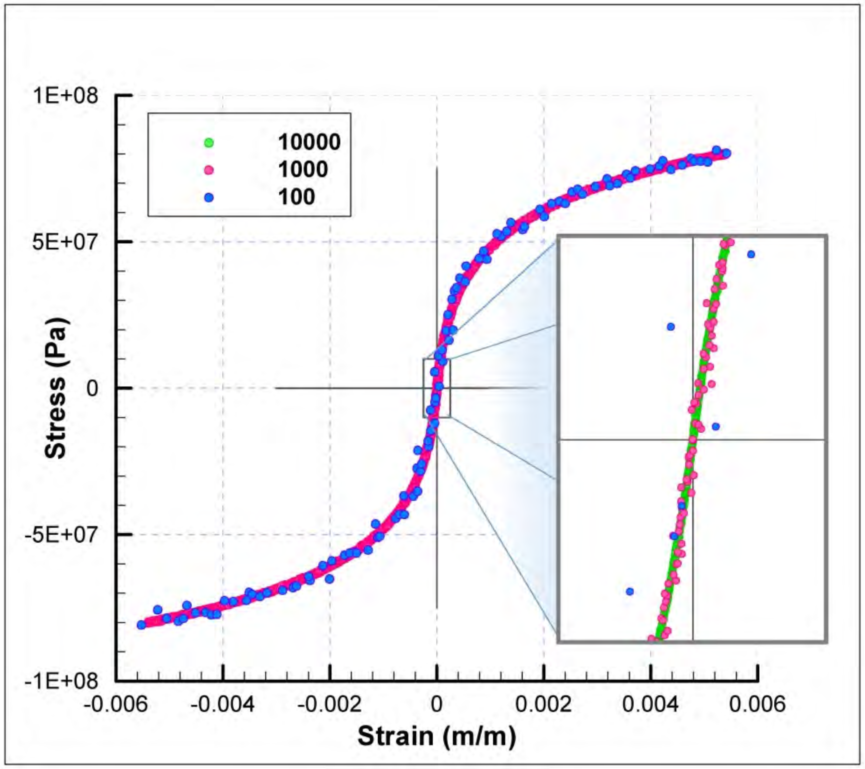
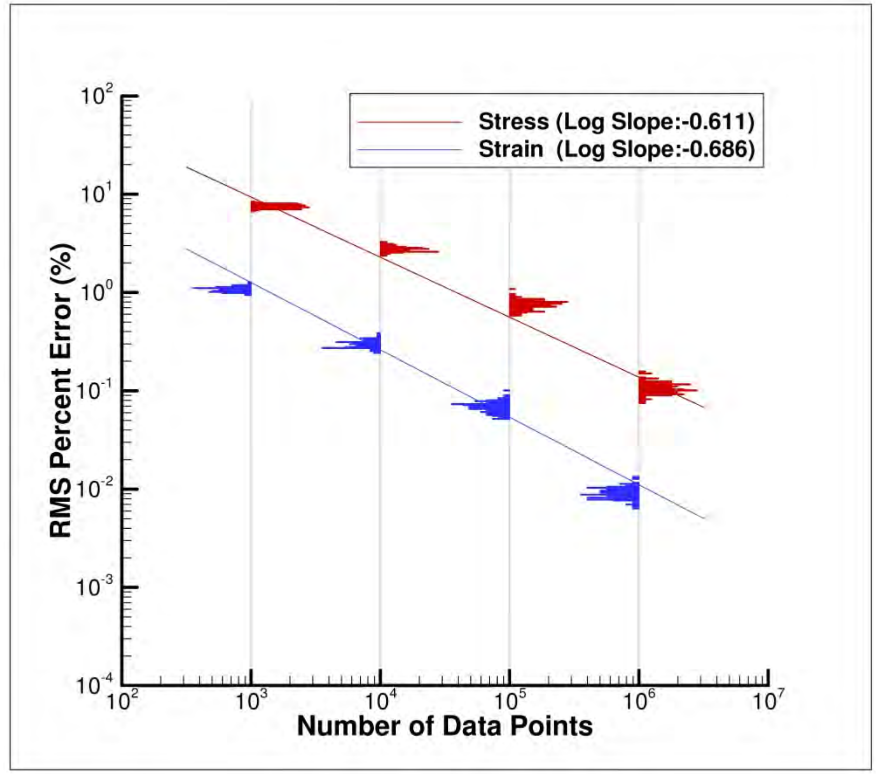
Convergence of fixed-point solver



Radomized material-data sets of increasing size and decreasing scatter



Convergence with respect to data set

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

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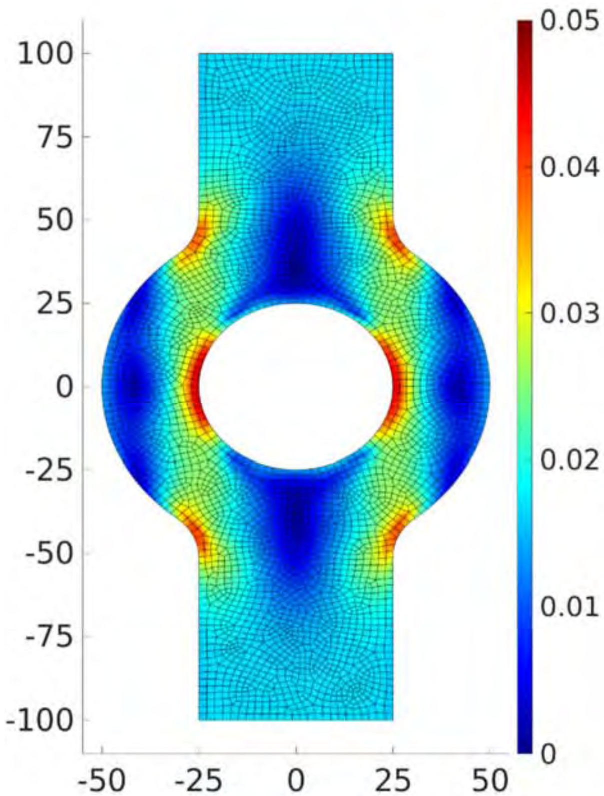
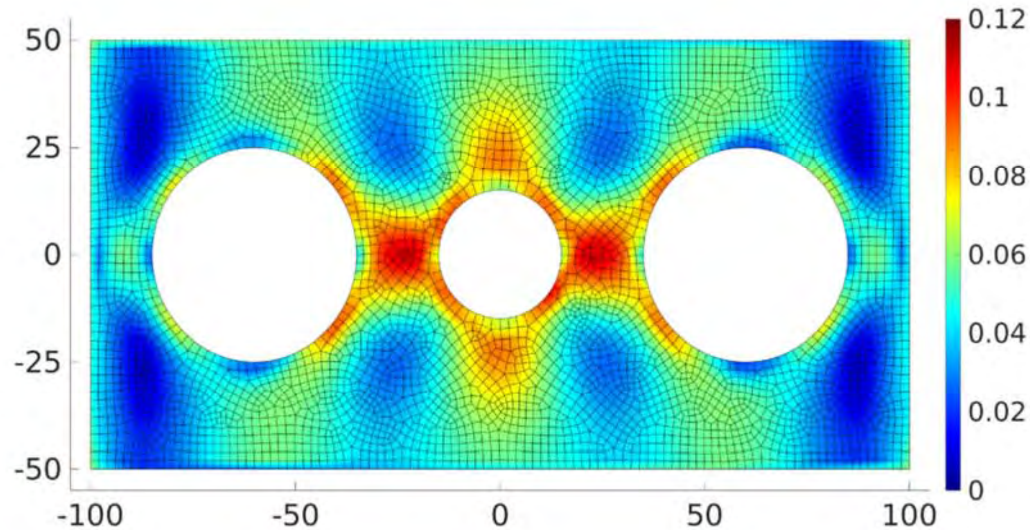
Data-Driven solvers and FE analysis

- (Model-free) Data-Driven solvers can be easily implemented within a finite-element framework





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(R. Eggersmann & S. Reese, 2019)

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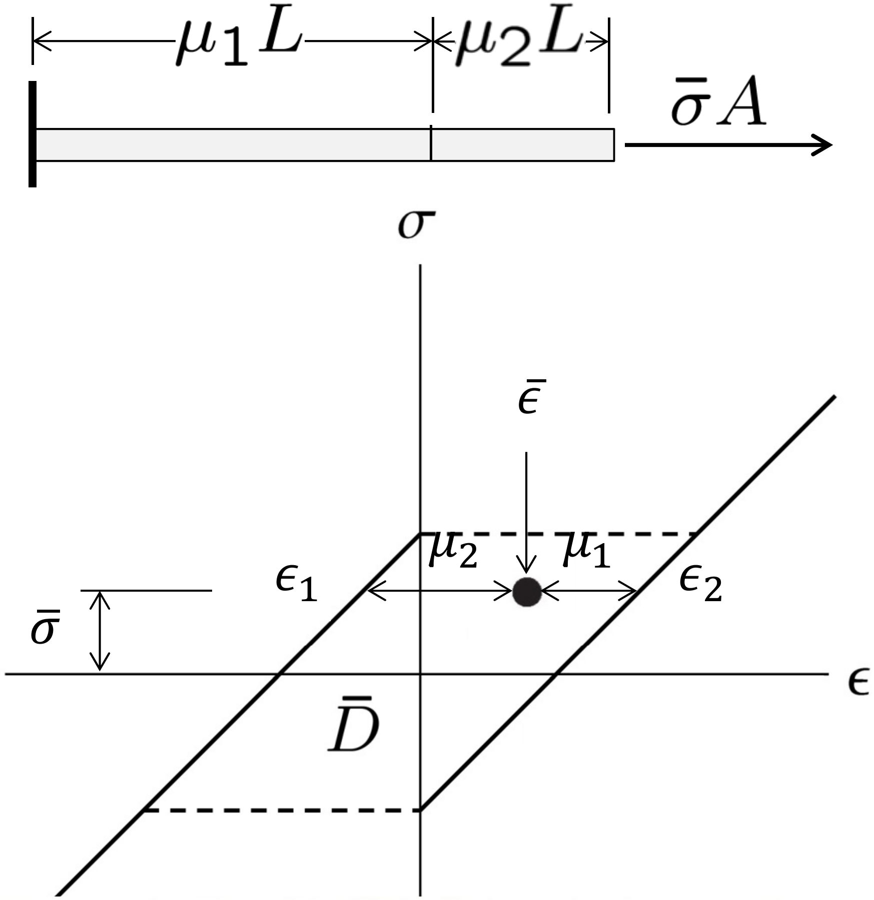
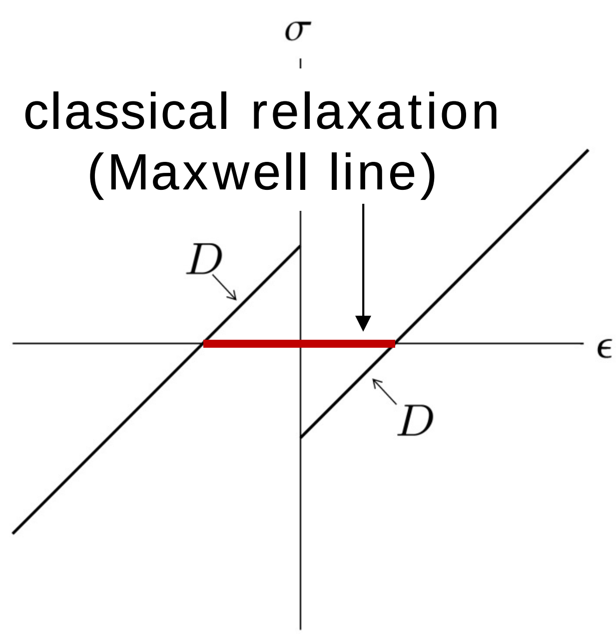
Data-Driven elasticity - Relaxation



- Constraint set:
  - i) $\sigma(x) = \bar{\sigma} A.$
  - ii) $\bar{\epsilon} = \fint \epsilon(x)\, dx.$
- Data set (double well):

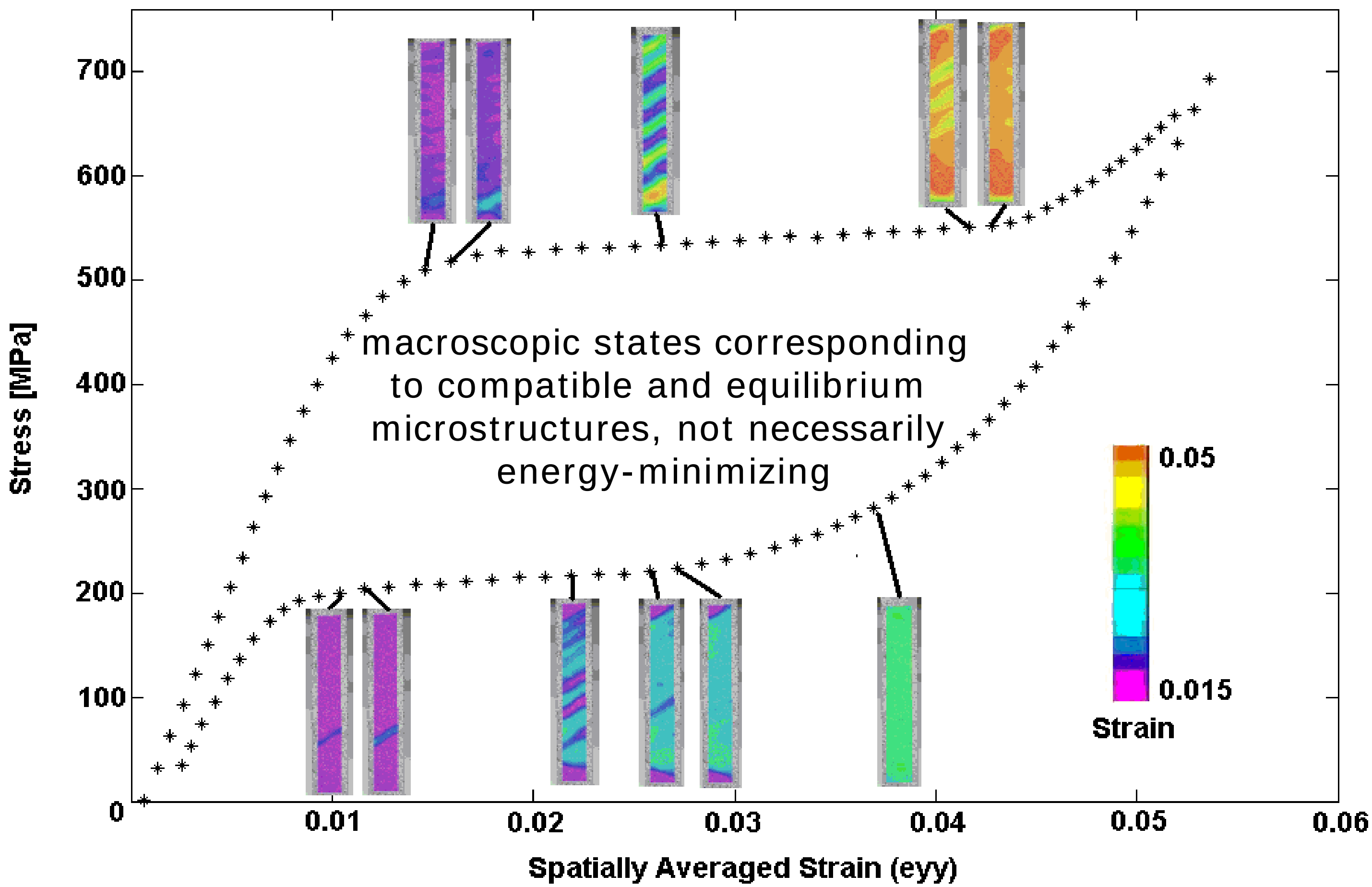


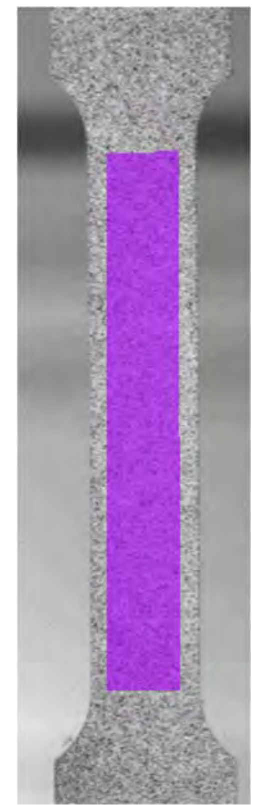
Theorem (DD Relaxation)

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

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

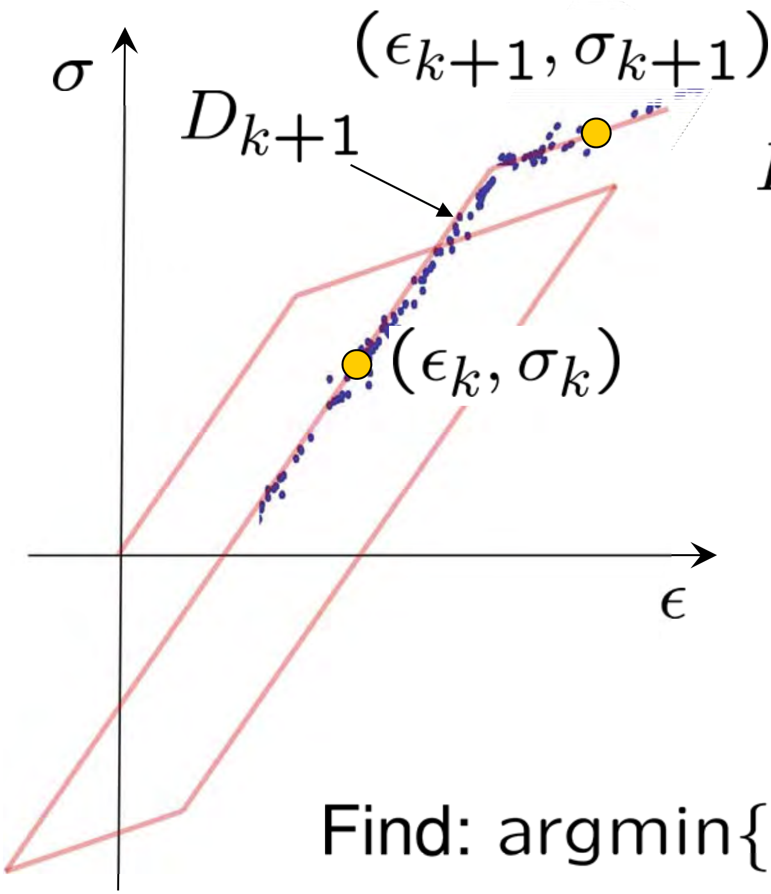
Phase transformation in nitinol (2D DIC)





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

Data-Driven inelasticity



- Material set representation:

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

- Need material history data! (from material testing along selected loading paths...)
- History data must provide adequate path coverage...
- Data-driven problem:

$$\text{Find: argmin}\{d(z, D_{k+1}),\ z \in E_{k+1}\}$$

time dependent!

R. Eggersmann, T. Kirchdoerfer, L. Stainier, S. Reese and M. Ortiz, *CMAME*, **350** (2019) 81-99.

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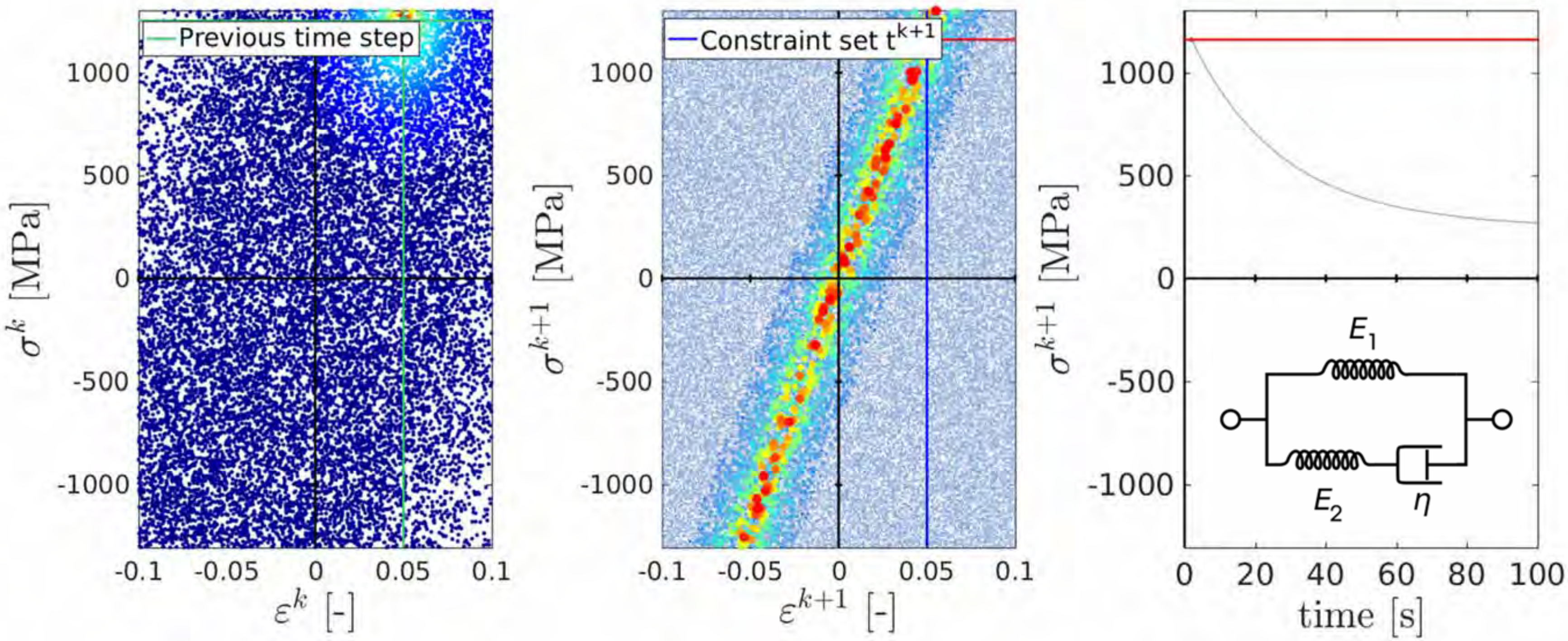
Data-Driven Inelasticity

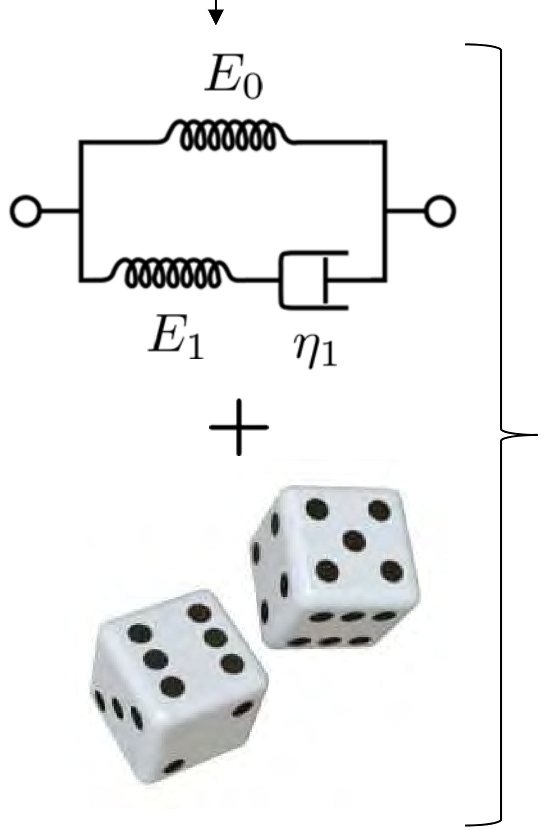
- Example: Data-Drive linear viscoelasticity
  - *(Randomized) Standard Linear Solid*
  - *Relaxation test (constant strain)*

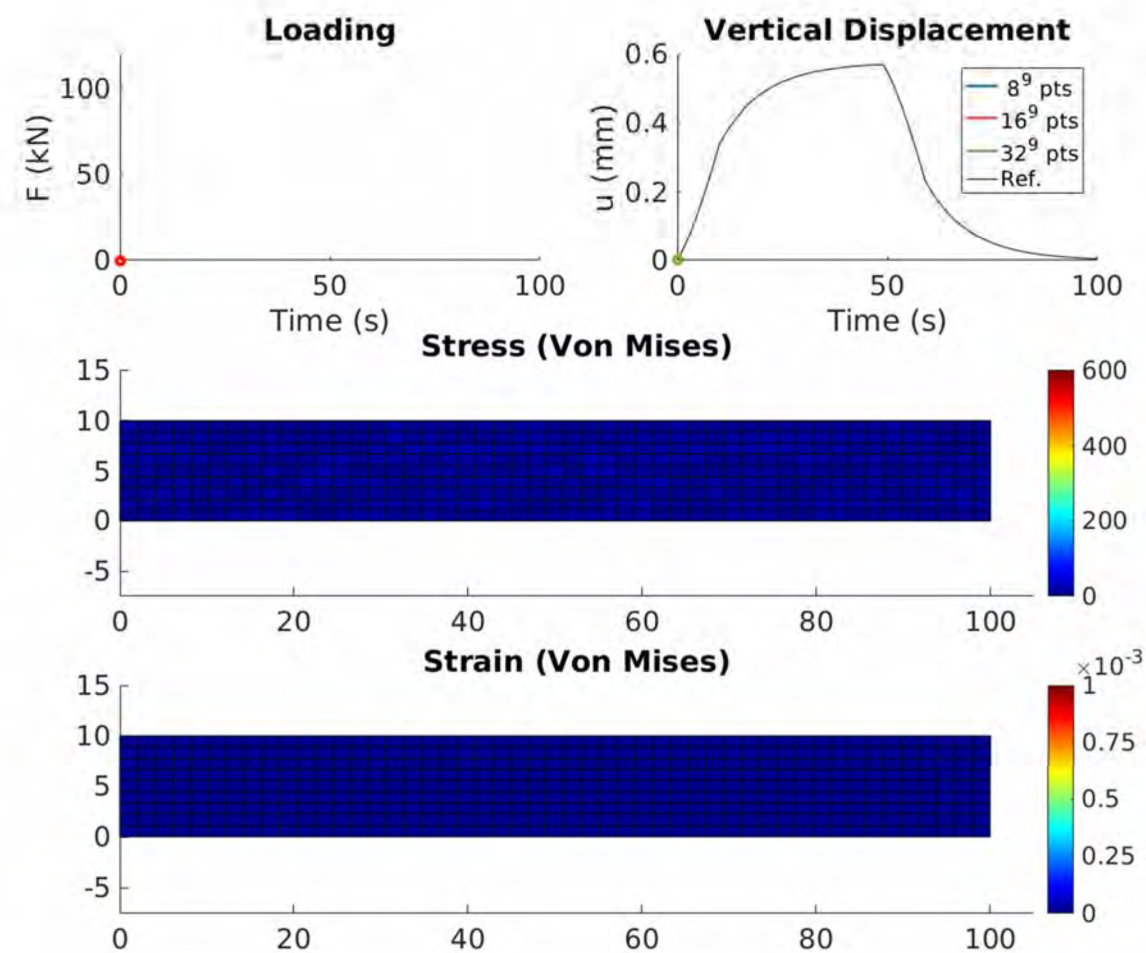


R. Eggersmann, T. Kirchdoerfer, L. Stainier,
S. Reese and M. Ortiz, *CMAME*, **350** (2019) 81-99.

Data-Driven viscoelasticity

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





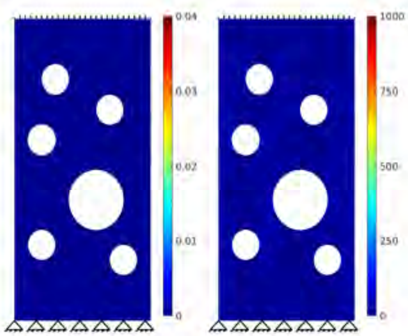
R. Eggersmann *et al.*, *CMAME*, **350** (2019) 81-99.

Data-Driven plasticity

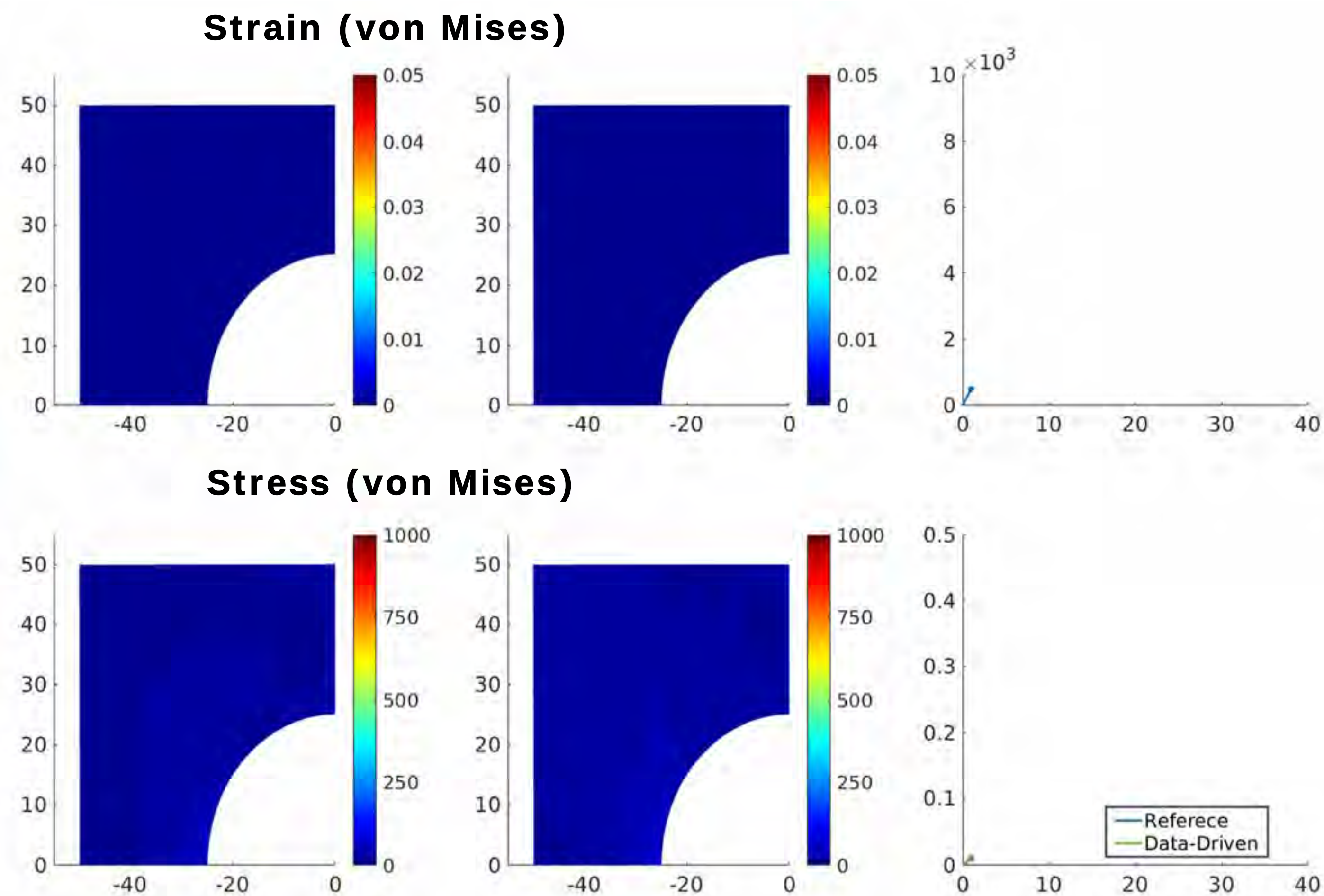
- Material set: $D_{k+1} = \left\{ (\epsilon_{k+1}, \sigma_{k+1}) \, : \, (\epsilon_k, \sigma_k) \right\}$

J2 plasticity kinematic hardening

+



Virtual test



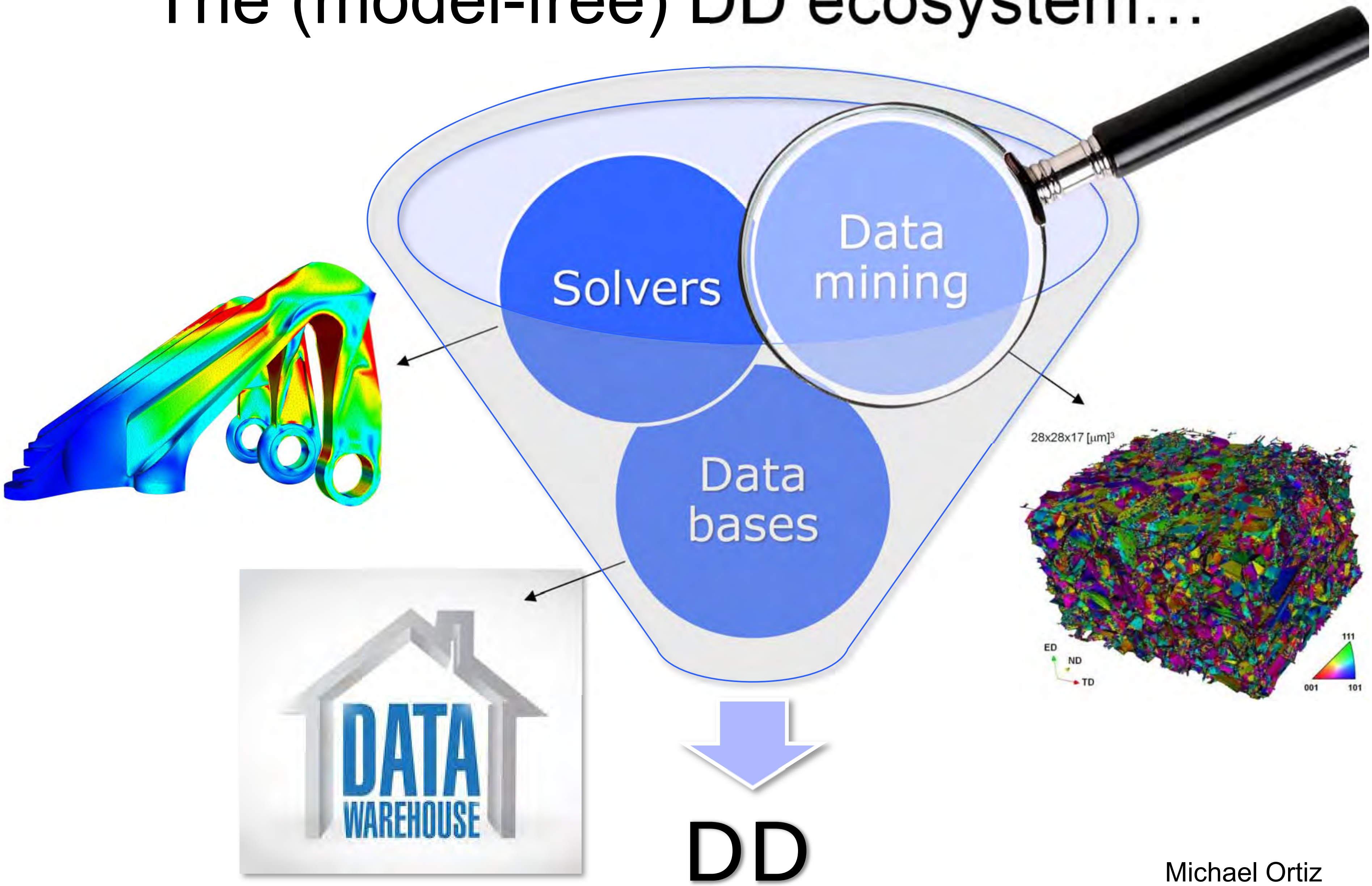
(R. Eggersmann & S. Reese, 2019)

(Model-Free) Data-Driven solvers

- Finite elasticity, finite kinematics[1,2]
- Dynamics, time discretization[3]
- Random data, clustering (k-means), outliers[4,5]
- Probabilistic extension, model-free, prior-free Data-Driven inference (work in progress...)
- Fast Data searching, k-d trees, scalable Nearest-Neighbor algorithms (in progress...)

[1]L.T.K. Nguyen and M.A. Keip, *Comput. Struct.*, **194** (2018) 97–115
[2]S. Conti, S. Müller and M. Ortiz, ARMA, (2020) in press.
[3]T. Kirchdoerfer and M. Ortiz, IJNME, **113**(11) (2018) 1697-1710.
[4]T. Kirchdoerfer and M. Ortiz, *CMAME*, **326** (2017) 622-41.
[5]T.F. Korzeniowski and K. Weinberg, CMAME, **350** (2019) 554-570.

The (model-free) DD ecosystem…



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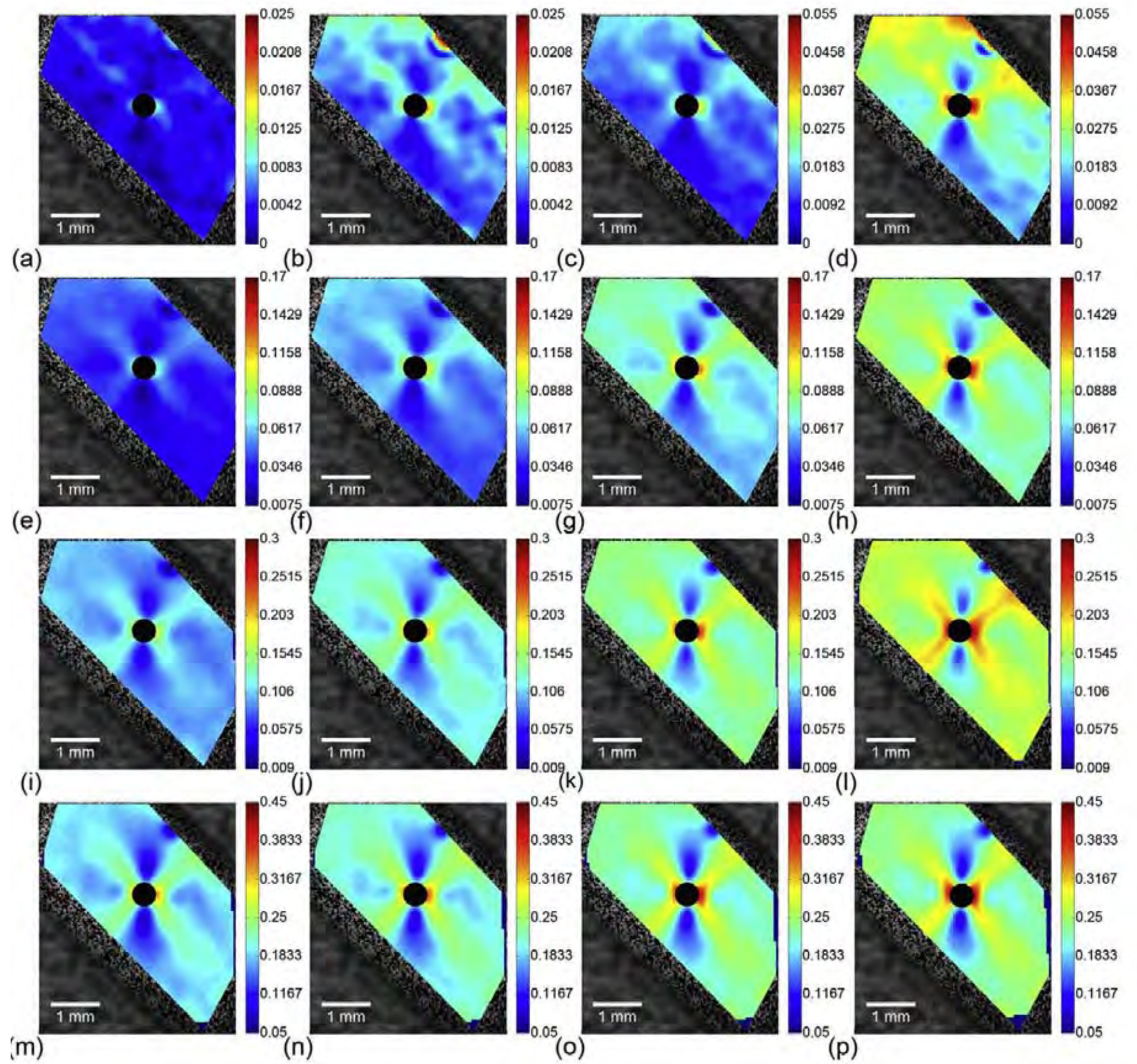
Full-field (DIC) microscopy data

Perforated shear-compression specimen (SCS) (Hopkinson bar)



Bodelot, L., *et al*., *International Journal of Plasticity*, **74** (2015) 58-74.

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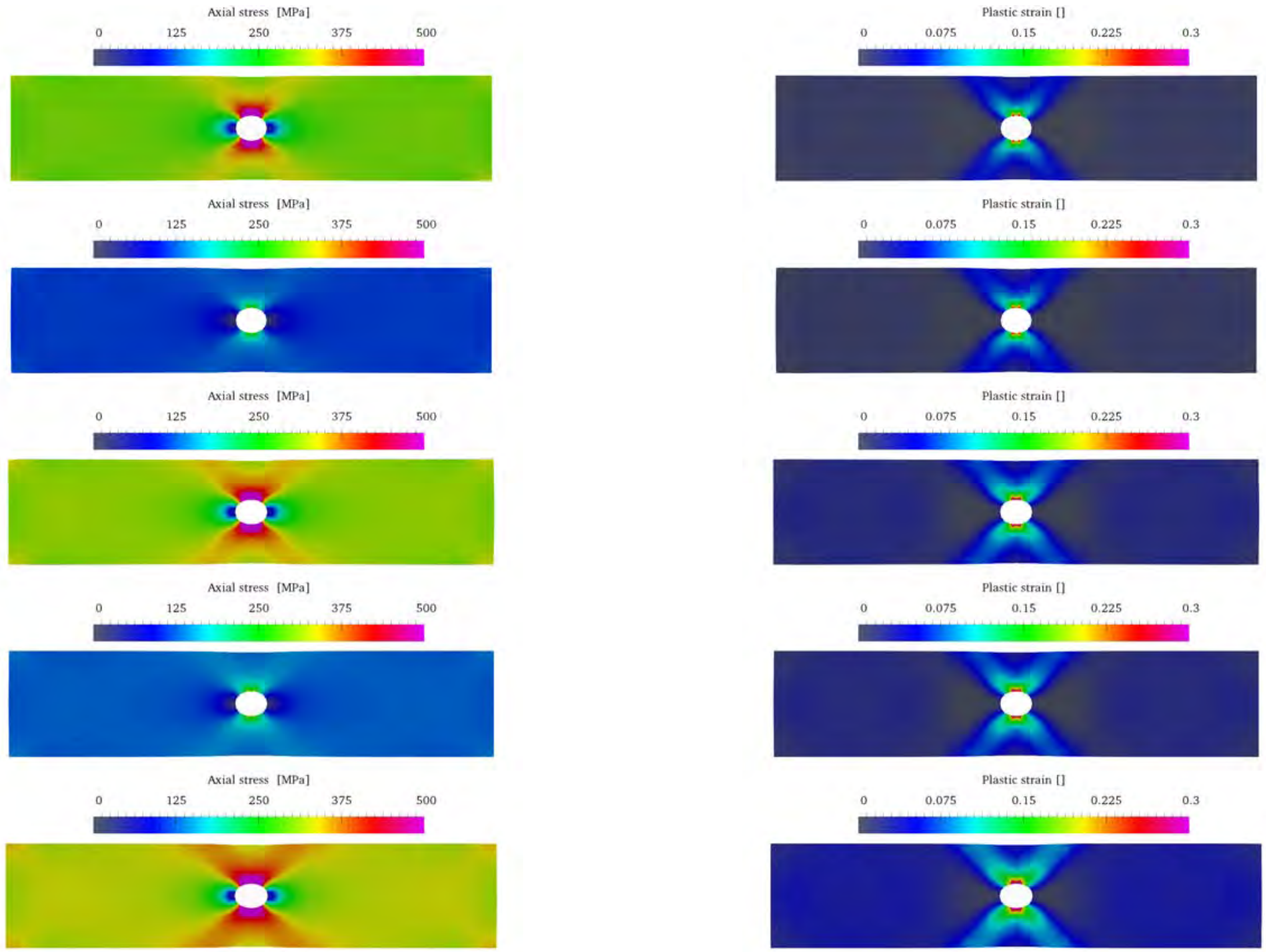
Full-field (DIC) microscopy data



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

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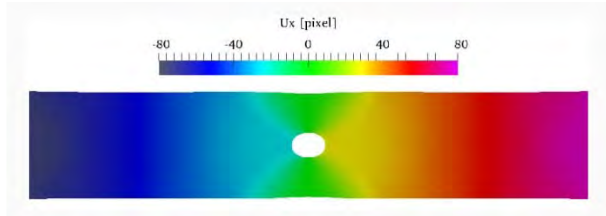
DD material identification (DDMI)



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

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

- Stresses σ_e^α cannot be measured directly!
- Material-data set:

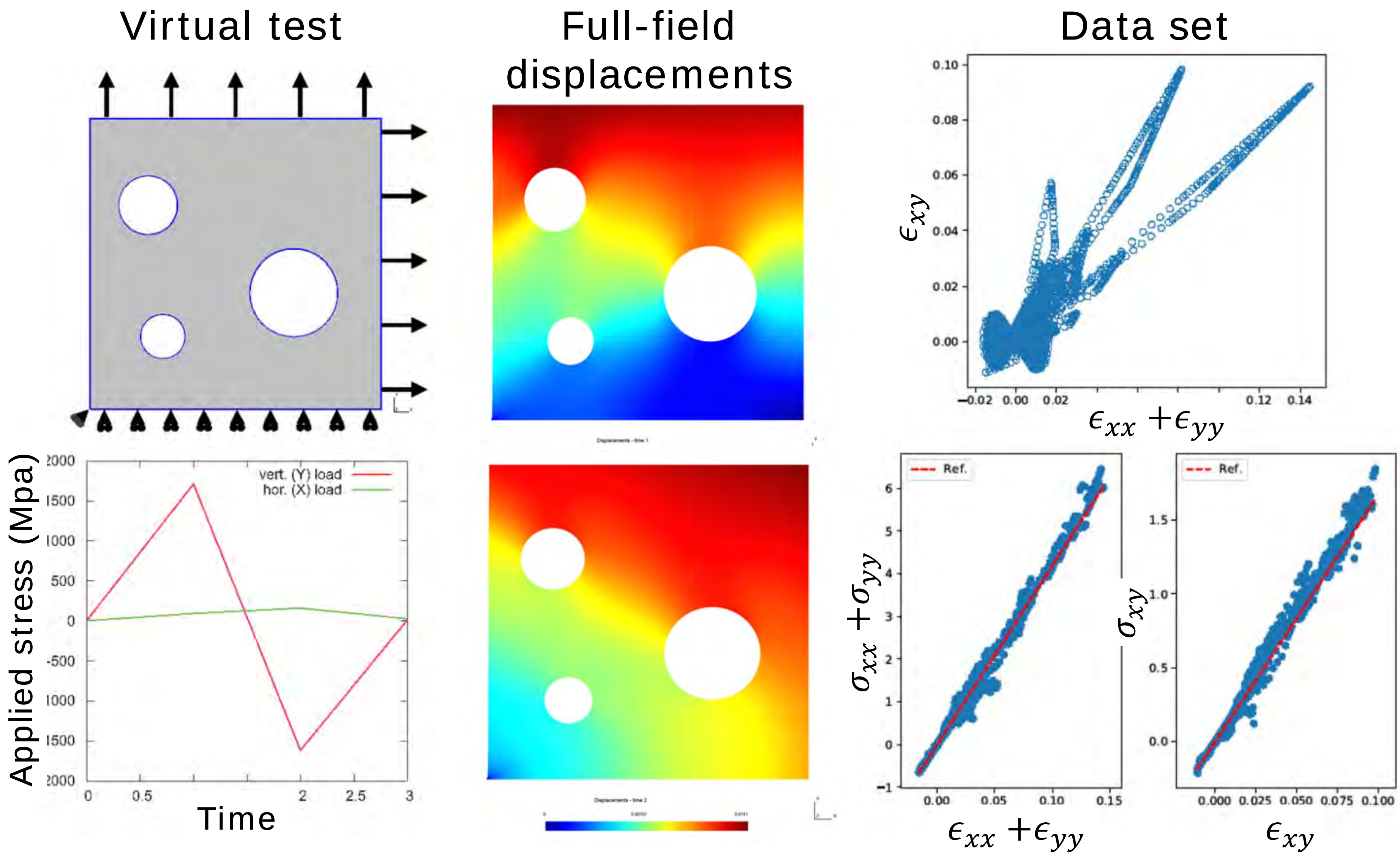
$$D = \cup_{\alpha=1}^{M} \{\epsilon_e = B_e u^\alpha, \textstyle\sum_{e=1}^{m} w_e B_e^T \sigma_e = f^\alpha\}$$

- DD self-consistent material-data identification:

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

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

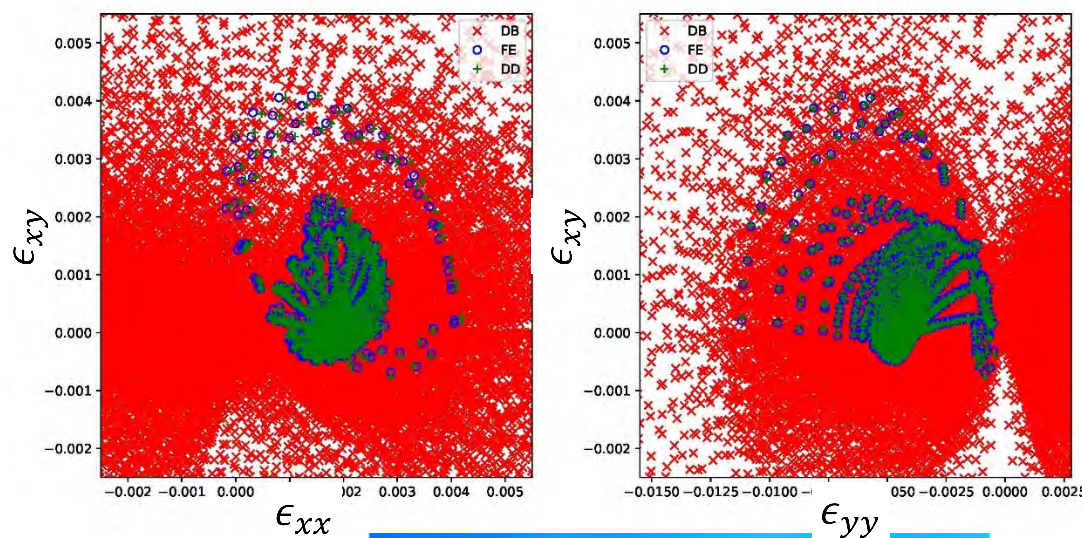
DD material identification (DDMI)

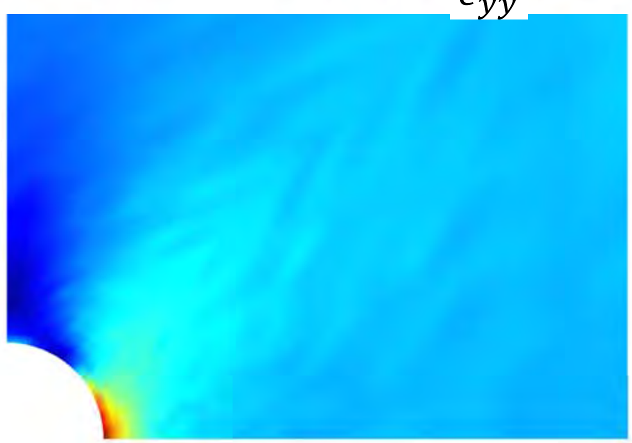


L. Stainier, A. Leygue and M. Ortiz, *Comp. Mech.*, **64** (2019)(2) .

DD material identification (DDMI)

strain coverage

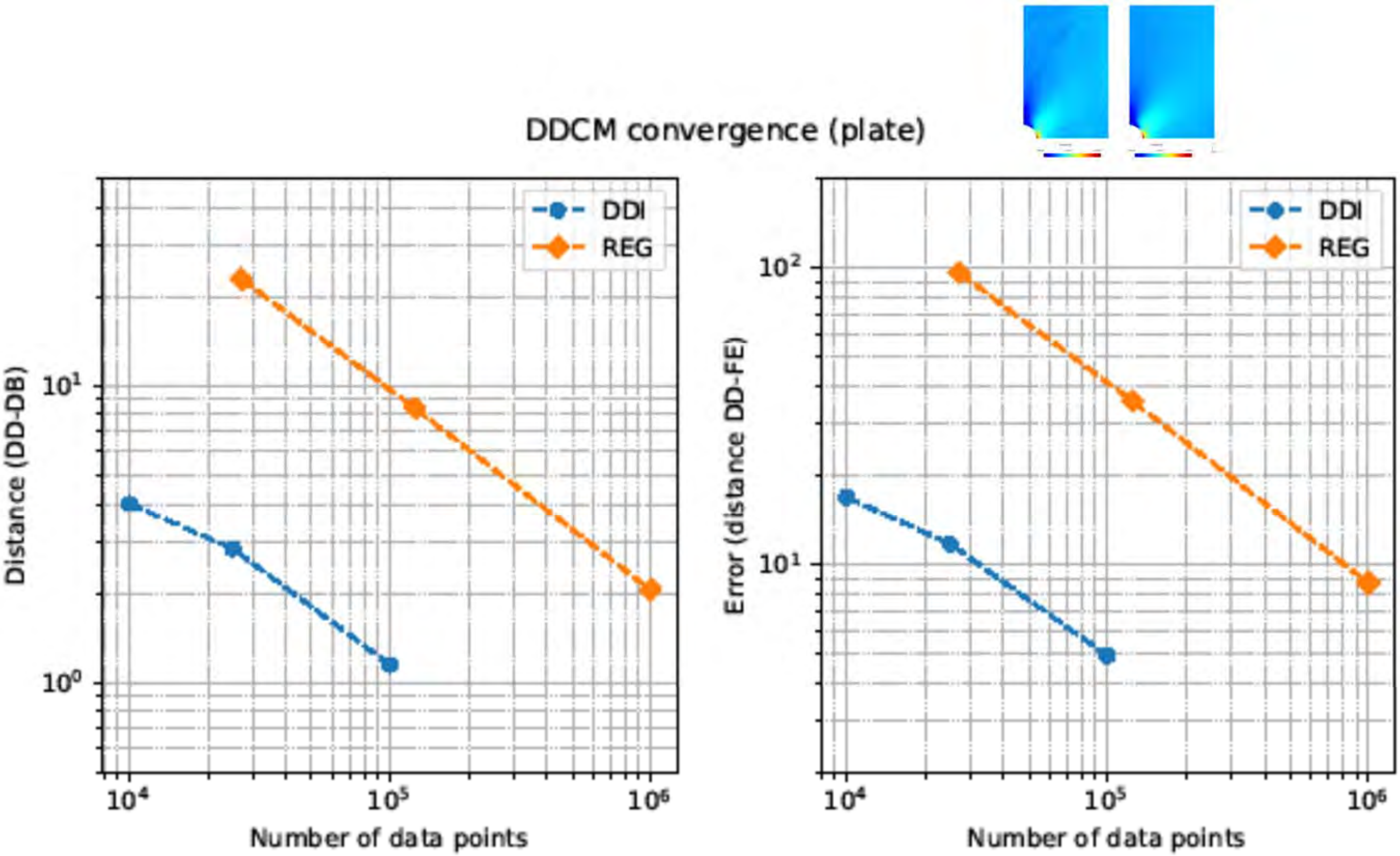




Stress (DD)

Stress (FE)

DD material identification (DDMI)



L. Stainier, A. Leygue and M. Ortiz, *Comp. Mech.*, **64** (2019)(2) .

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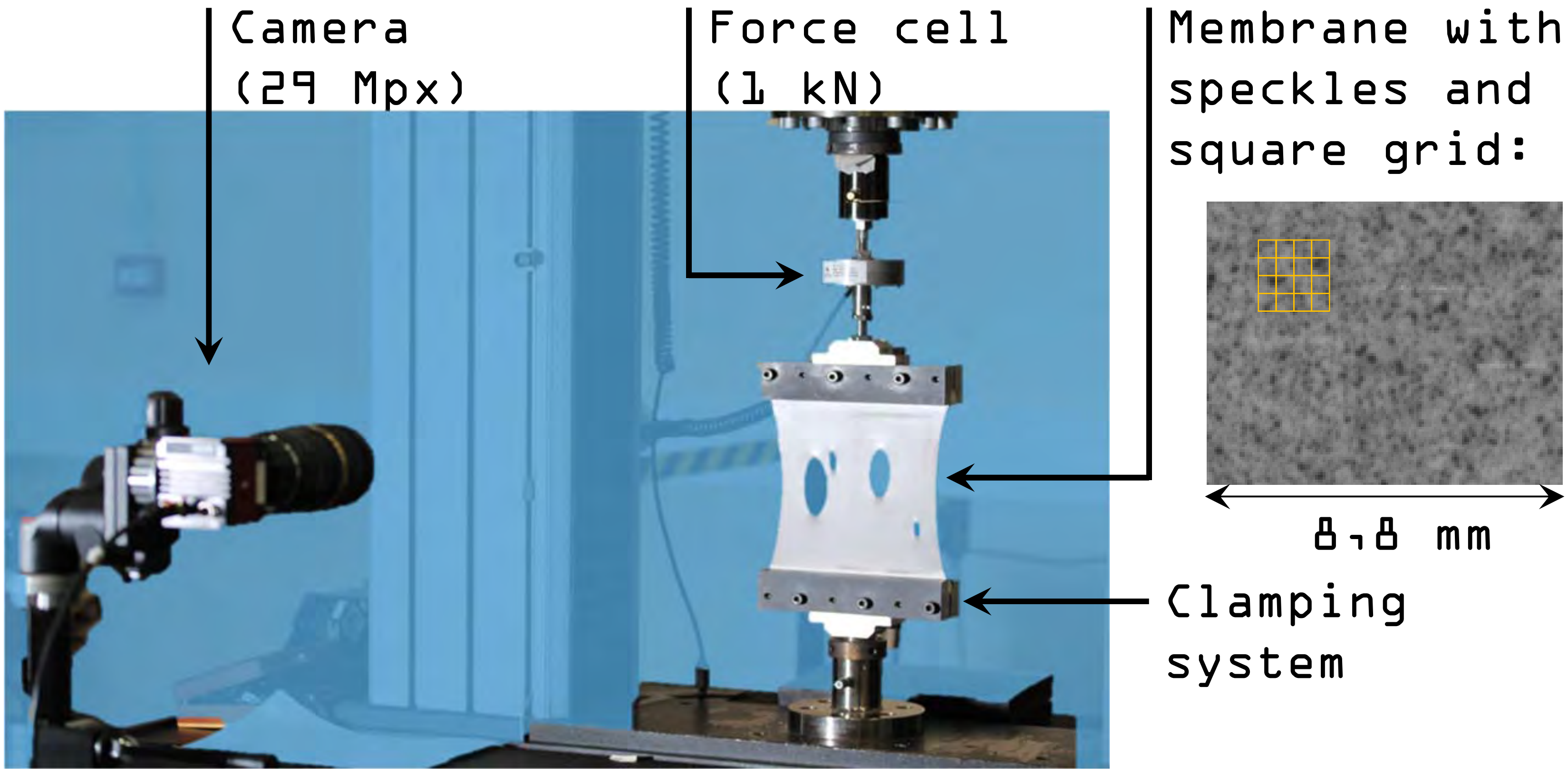
DDMI at Central Nantes

- Tests on perforated silicone sheets



(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

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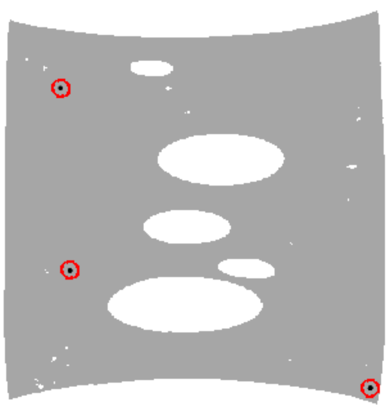
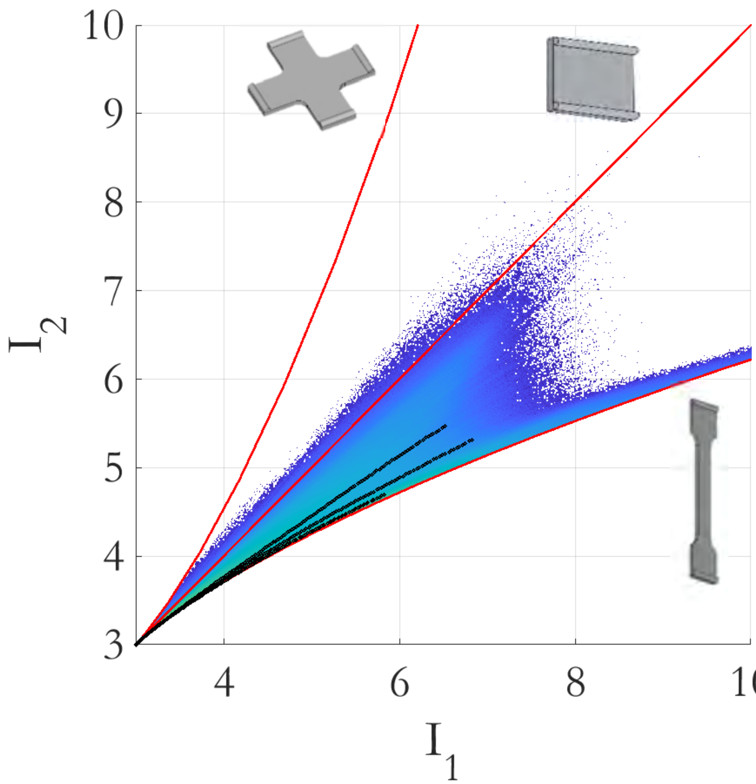
DDMI at Central Nantes

Displacement field (DIC)

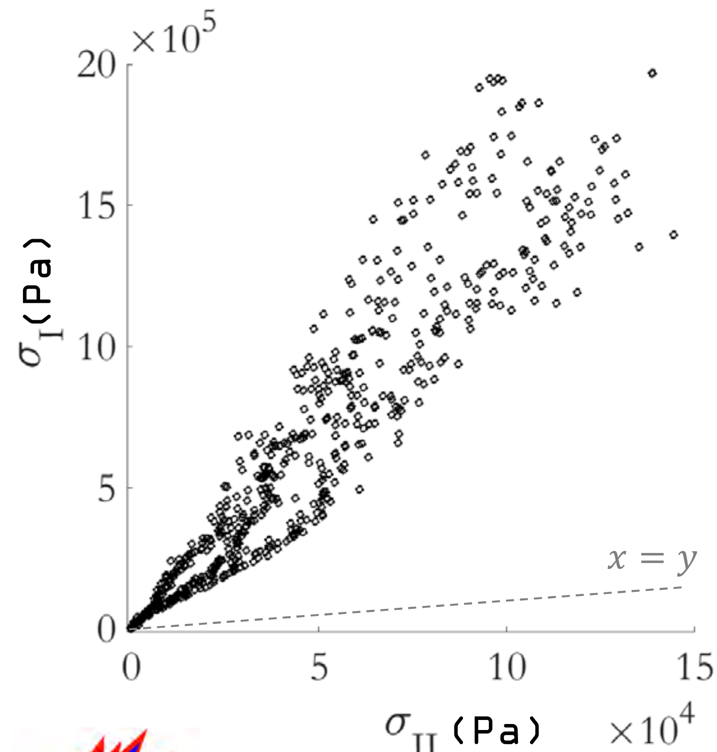
(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

DDMI at Central Nantes





Strain data



Stress data

(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

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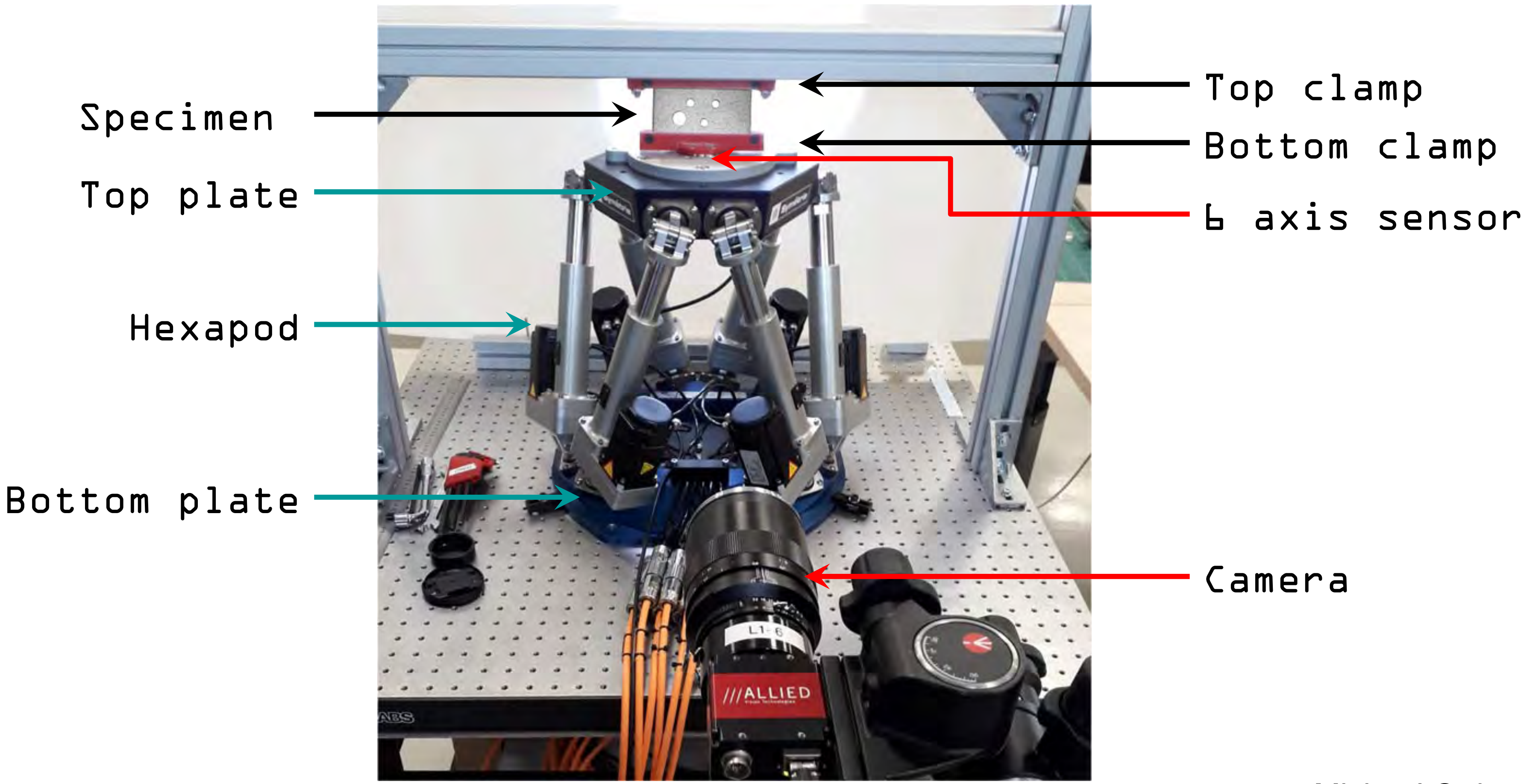
DDMI at Central Nantes

- Hexapod testing machine



(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

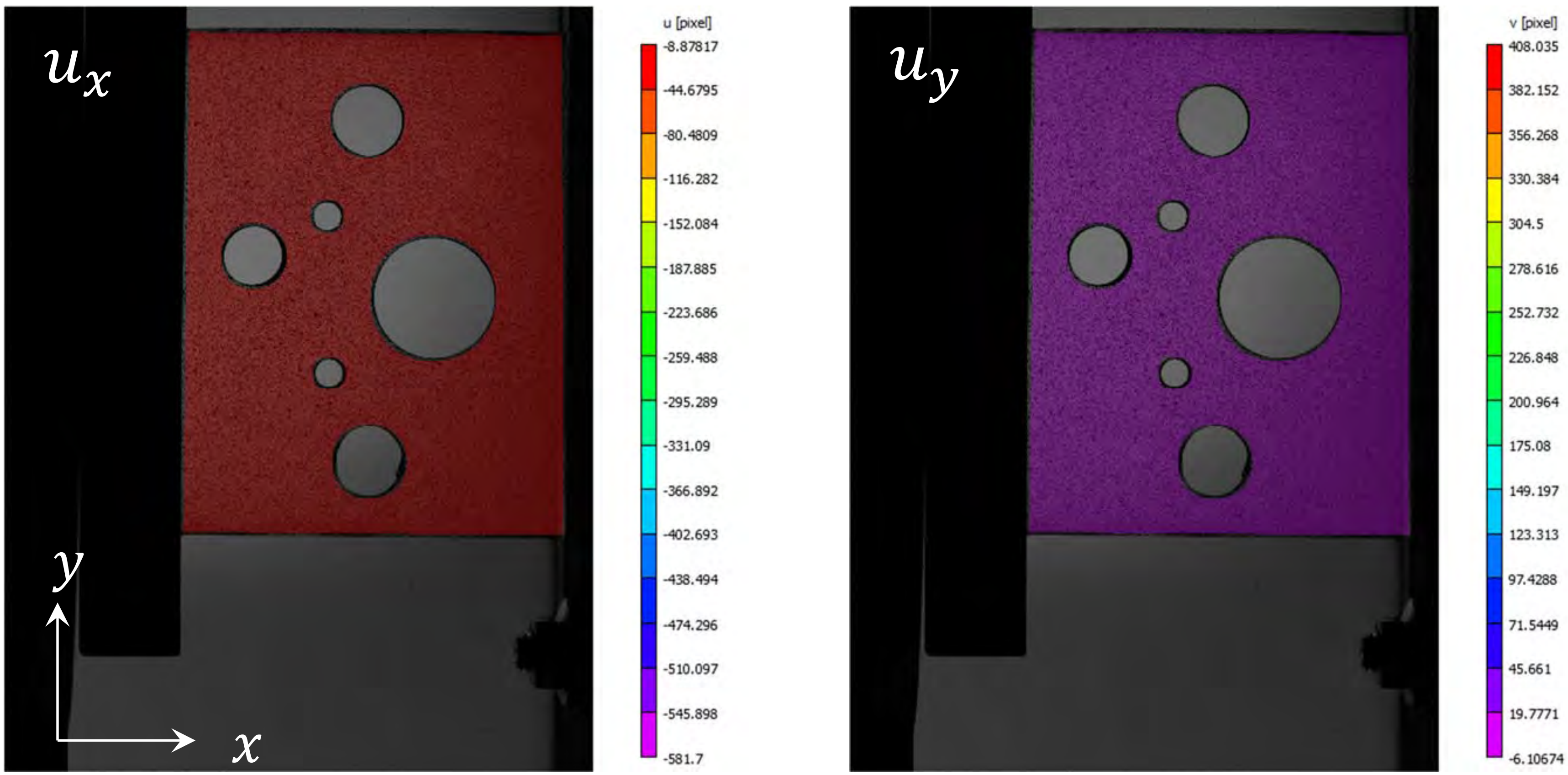
DDMI at Central Nantes

Hexapod in operation

(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

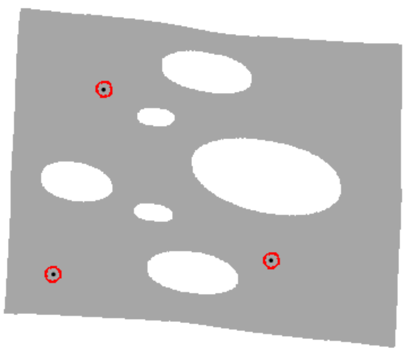
DDMI at Central Nantes

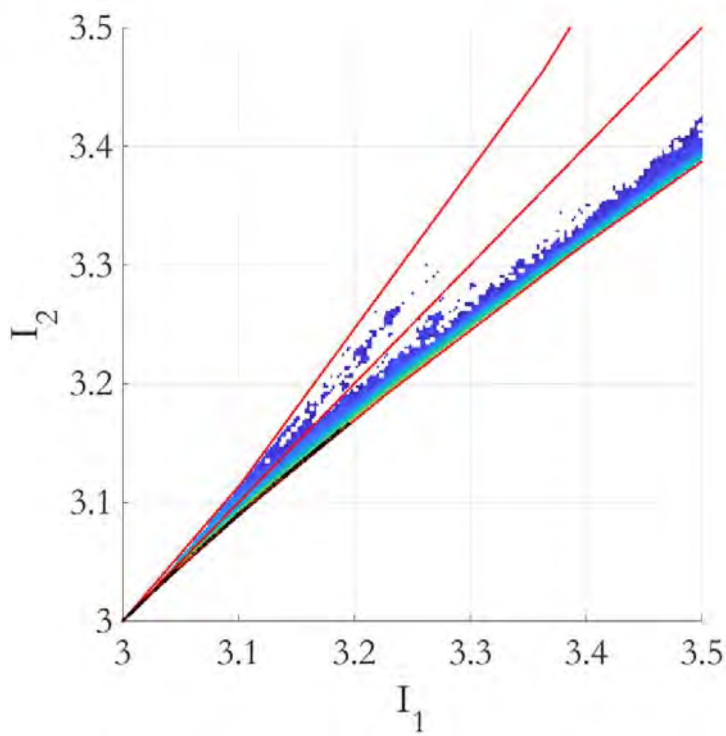
Displacement field (DIC)



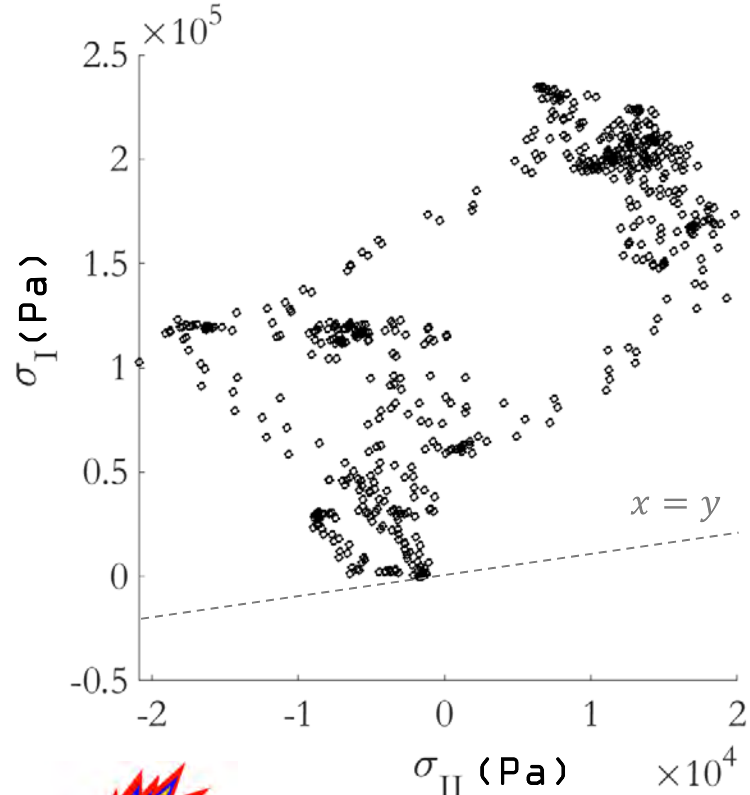
(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

DDMI at Central Nantes





Strain data

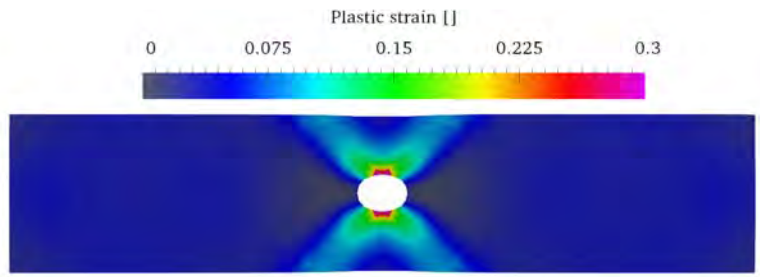


Stress data

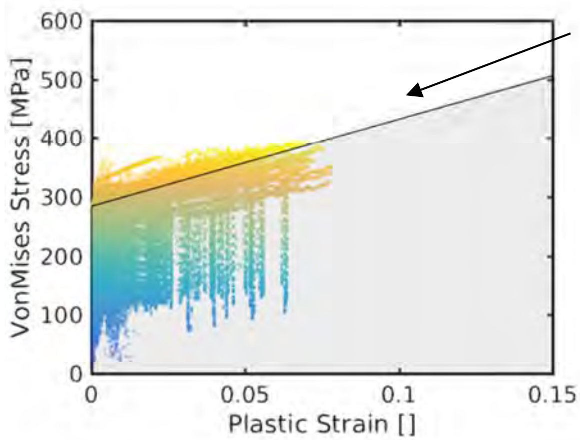
(M. Dalémat, M. Coret, A. Leygue and E. Verron, 2019)

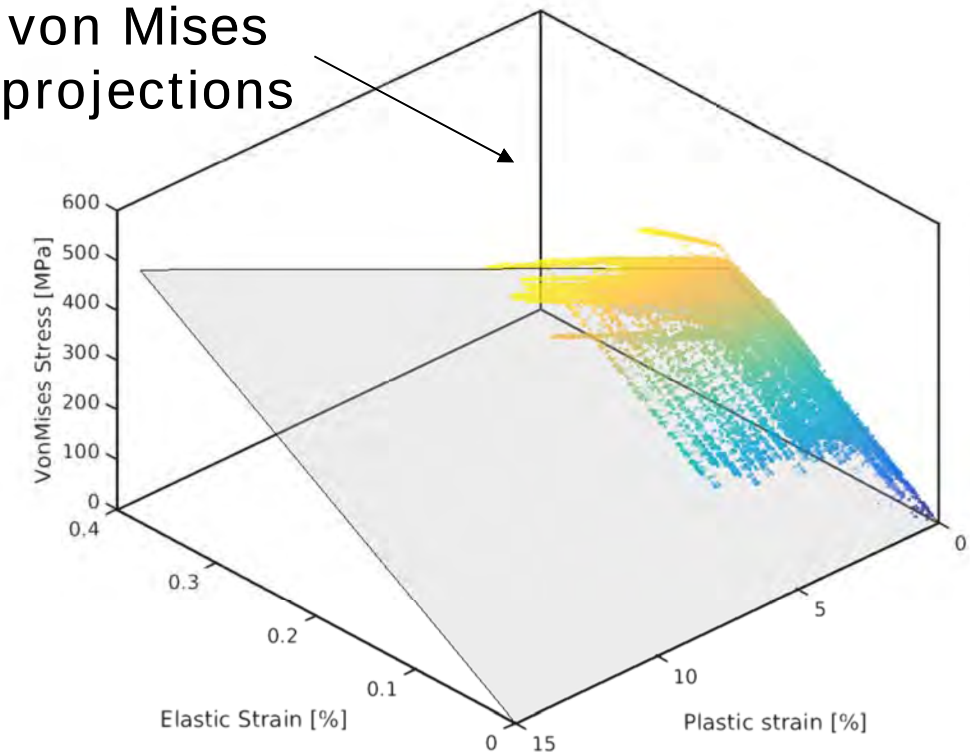
DD material identification (DDMI)

304L stainless steel
perforated specimen



von Mises
projections





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

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

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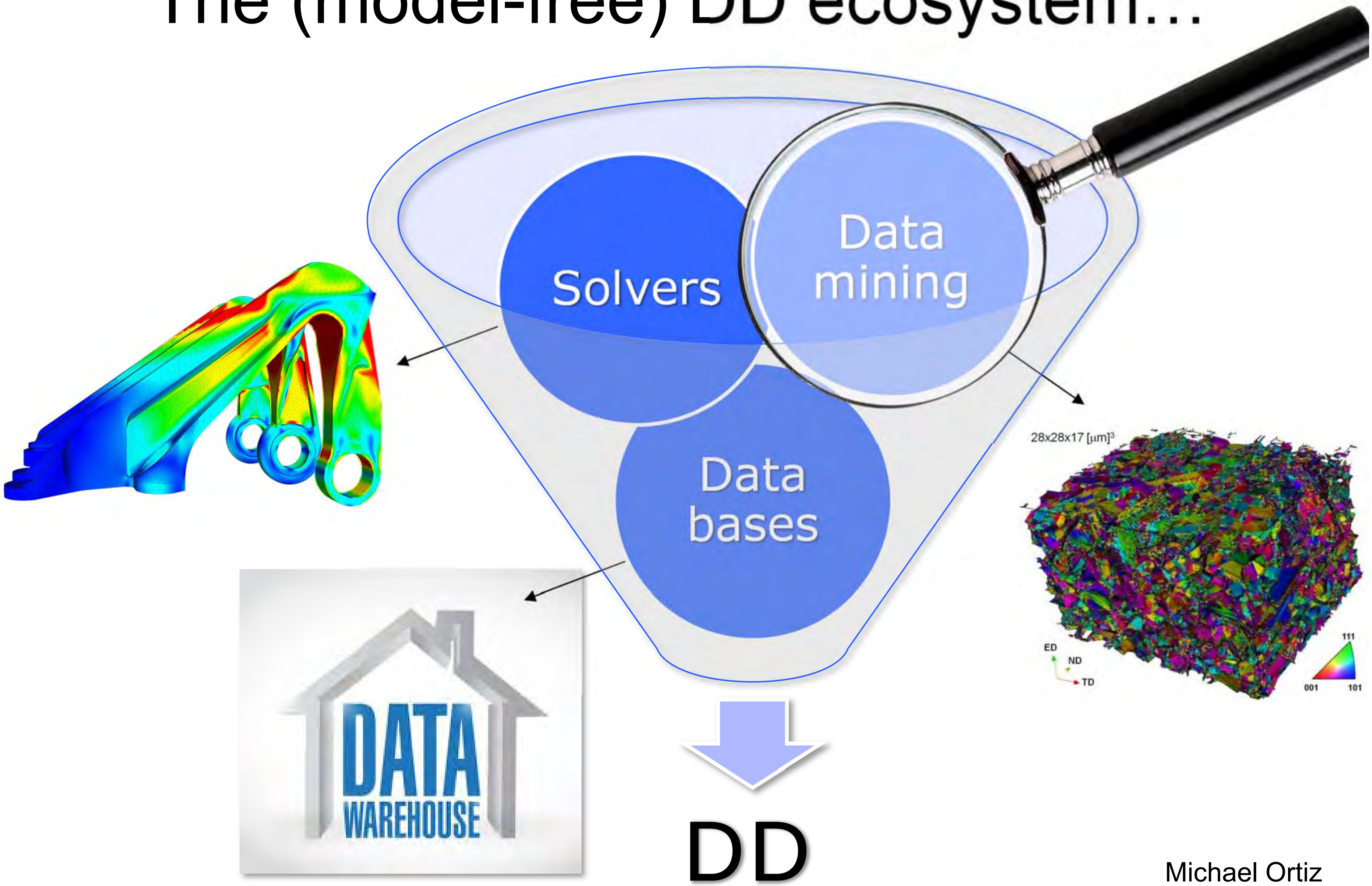
The (model-free) DD ecosystem…



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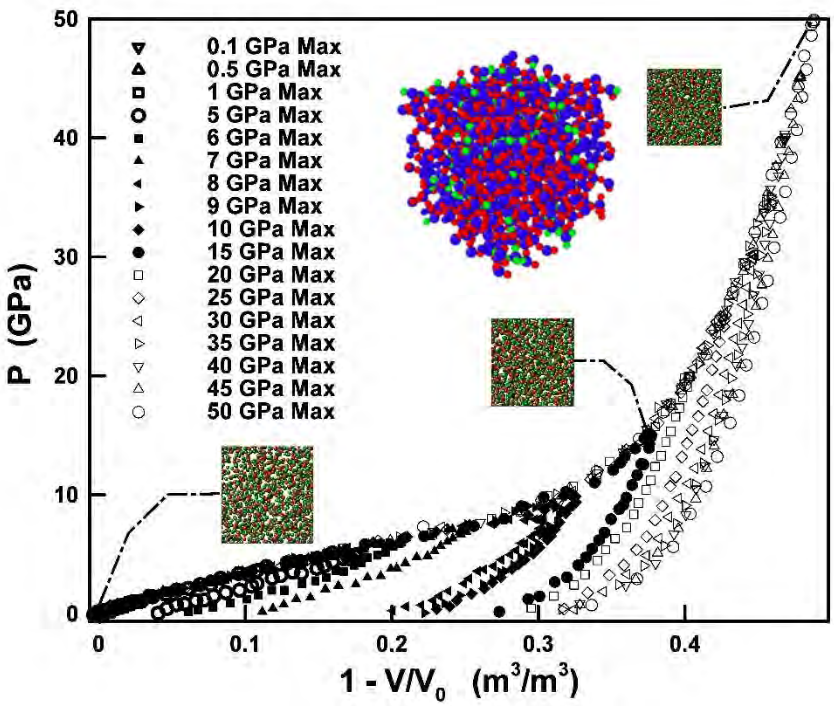
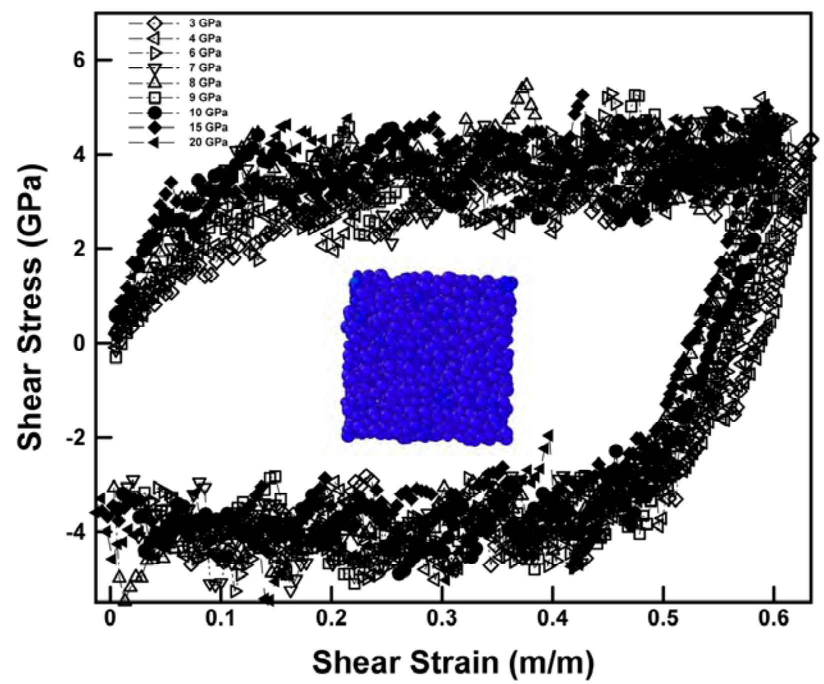
Multiscale data mining – SiO2 glass

- Fused Silica (SiO_2), molecular dynamics (LAMMPS)



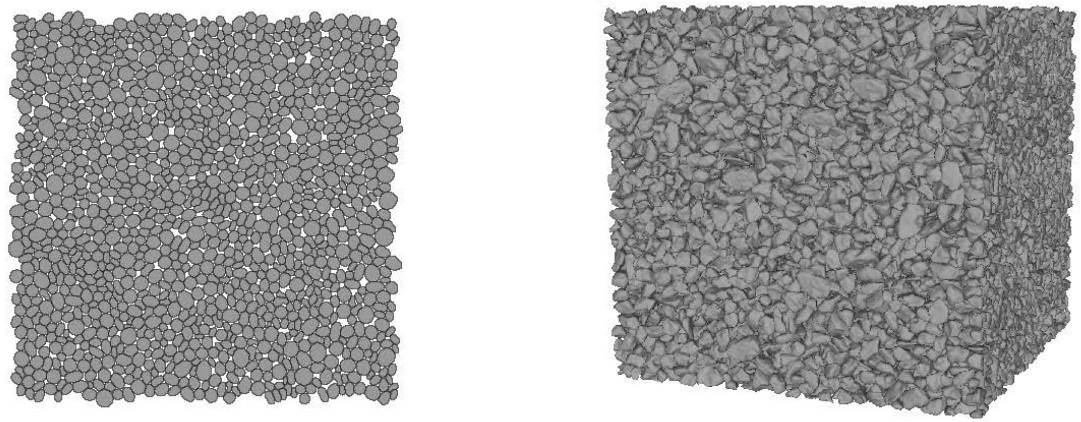
Pressure-volume
MD data



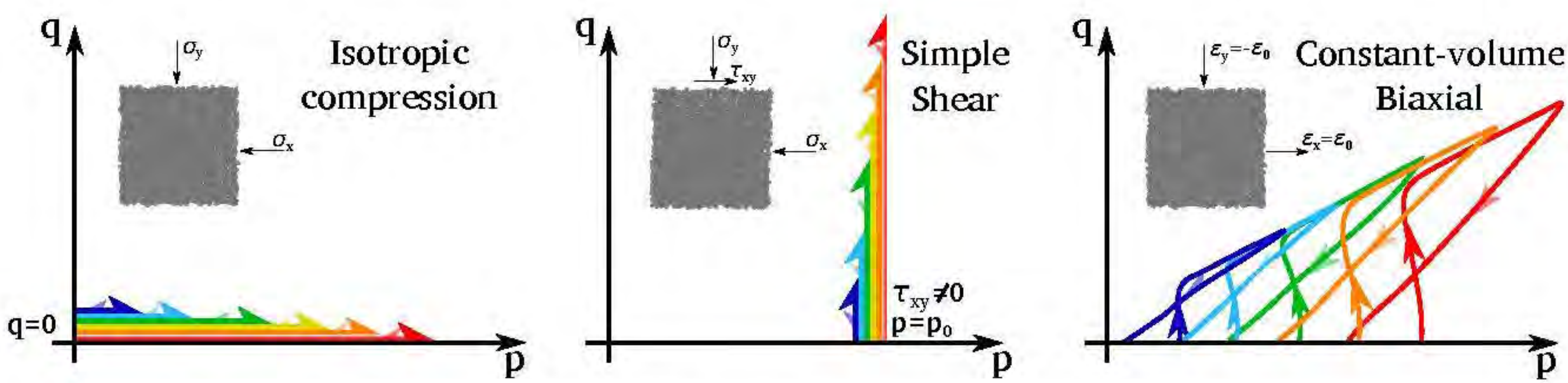
Pressure-shear
MD data

Schill W, Heyden S, Conti S, Ortiz M., *JMPS*, 2018;**113**:105-25

Multiscale data mining − Sand



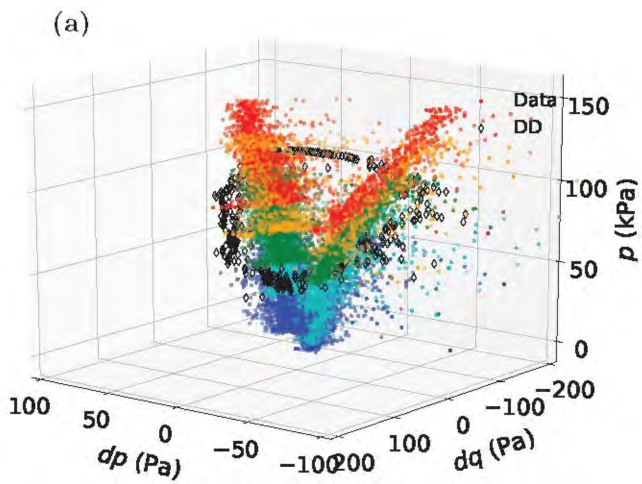
2D and 3D RVE and granular assemblies for LS-DEM analysis



Stress paths for material point simulations and data mining

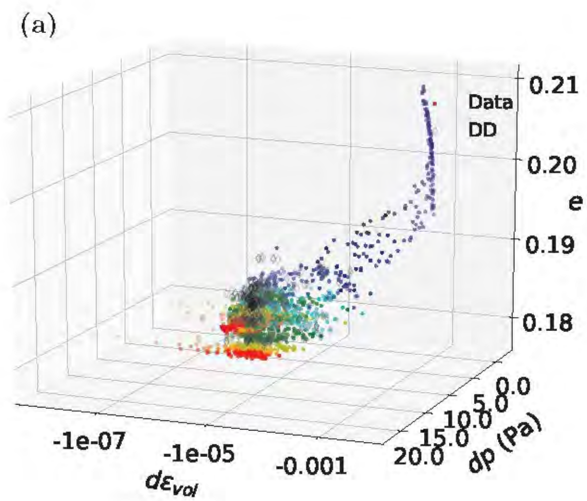
(K. Karapiperis etal., 2020)

Multiscale data mining − Sand

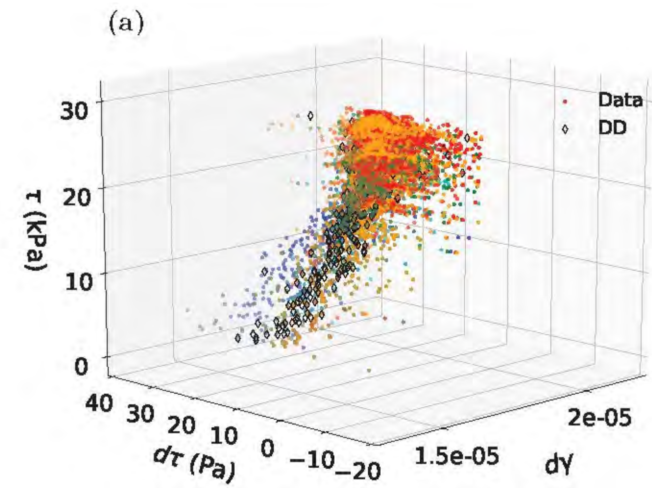


Isotropic compression

Simple shear



Biaxial compression



Data computed from
RVE LS-DEM calculations

(K. Karapiperis etal., 2020)

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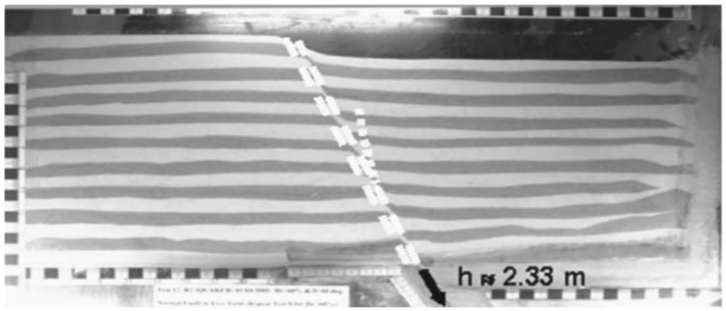
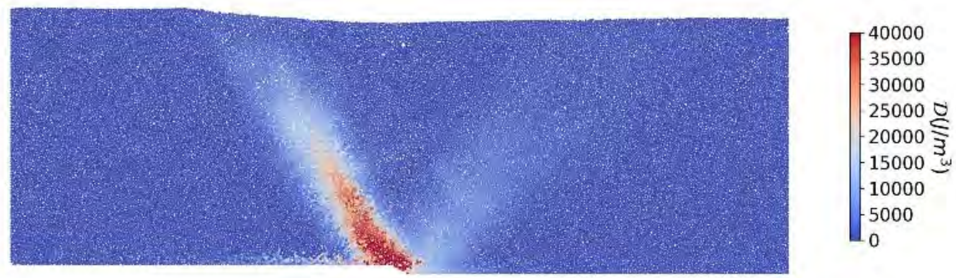
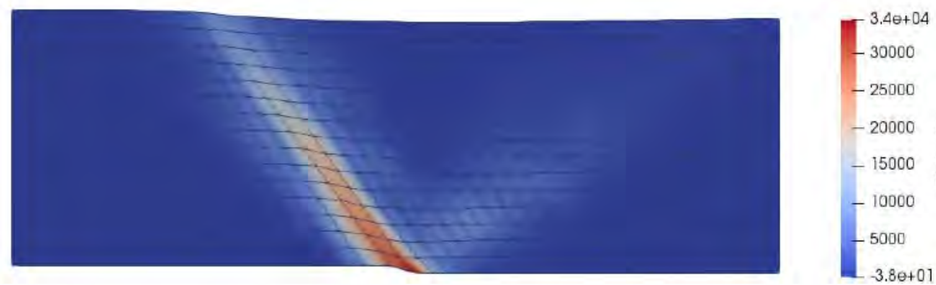
(Model-free) Data-Driven simulations

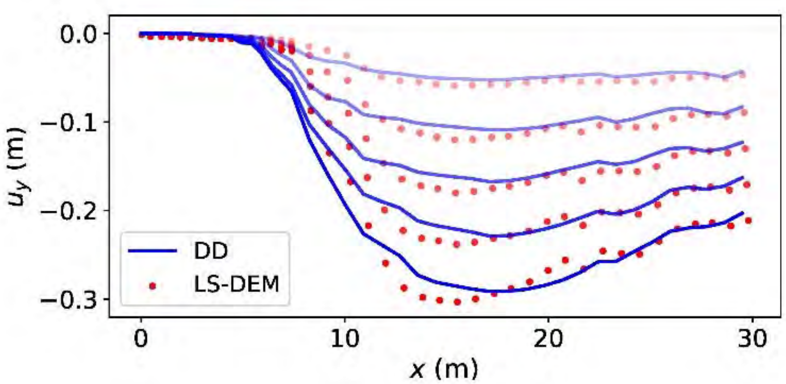


Experimental fault
rupture experiment
(Anastapoulos etal.. 2007)





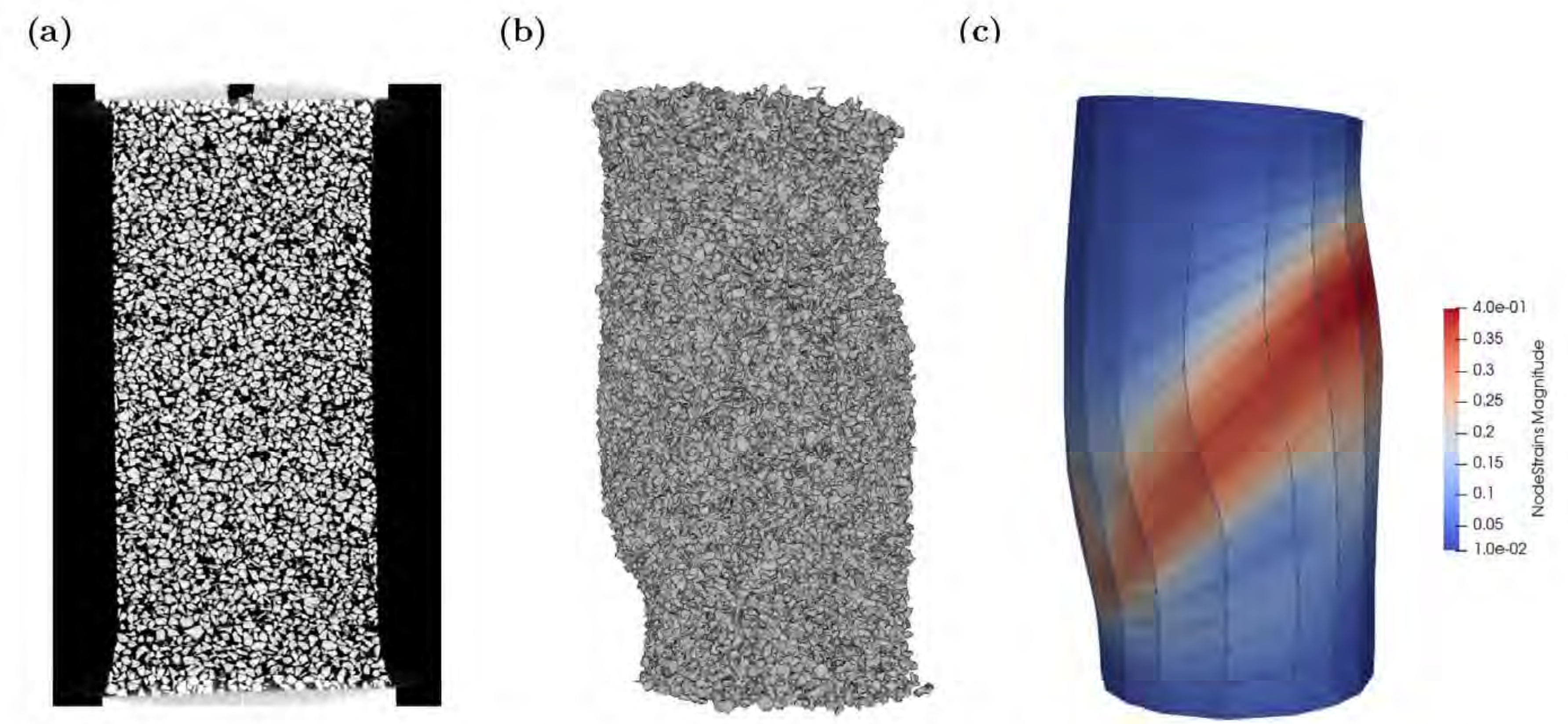
Top: LS-DEM simulation
Bottom: DD simulation



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

(K. Karapiperis etal., 2020)

(Model-free) Data-Driven simulations



a) XRCT of Hostun sand specimen at the end of isotropic compression.
b) LS-DEM simulation of triaxial compression of the sand specimen.
c) Data-Driven simulation and predicted shear band.

(K. Karapiperis etal., 2020)

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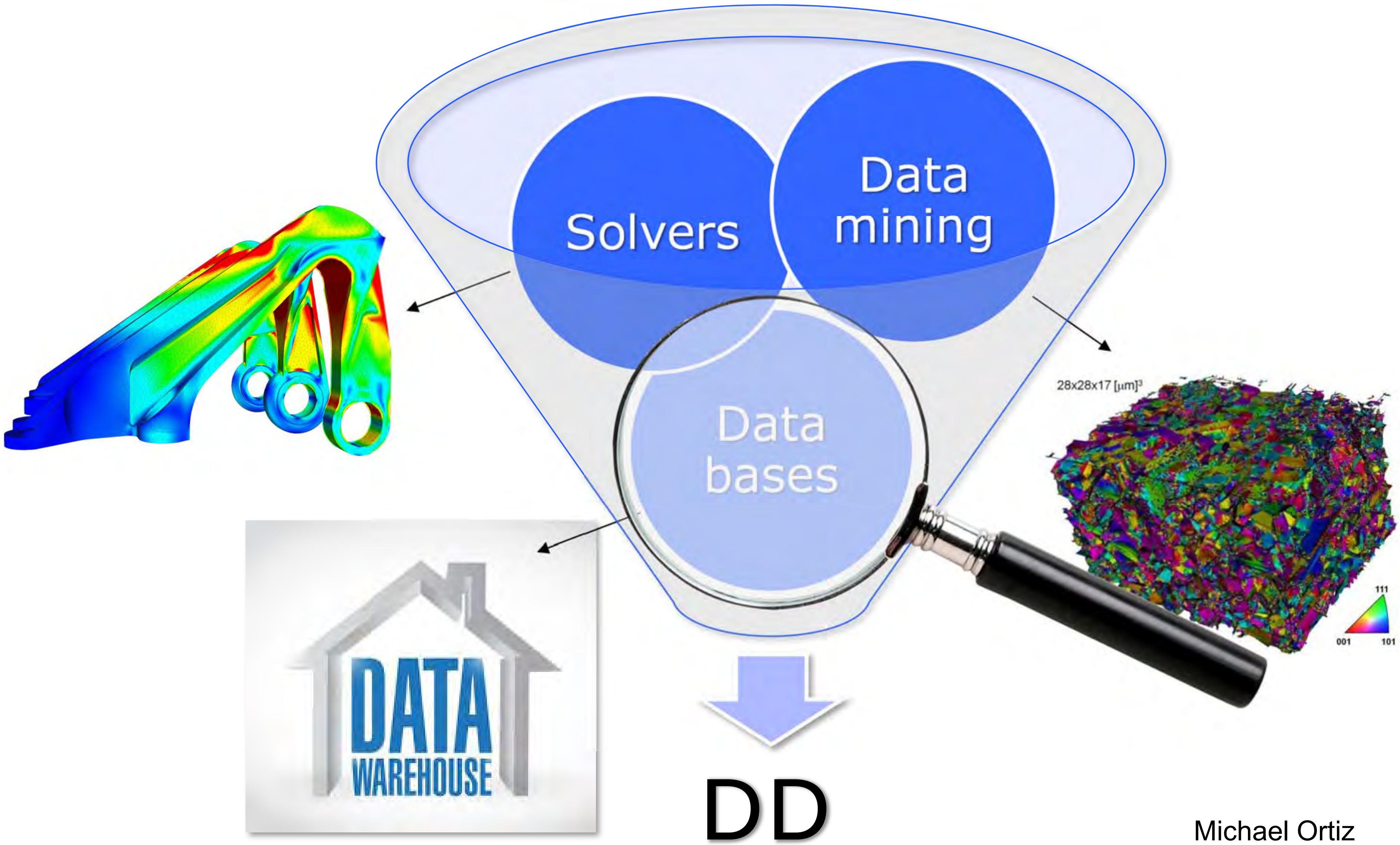
Data mining, generation, upscaling

- DD can extract data from *full-field experimental microscopy* (TEM, SEM, DIC, EBSD...)
- DD generates *fundamental data without prior assumptions* on the form of constitutive response
- Data can be *mined* from lower-scale calculations, used in upper-scale calculations (*DD upscaling*)
- DD sets forth new opportunities for *synergism* between experimental science and scientific computing, new multiscale analysis paradigms

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

The (model-free) DD ecosystem…



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Publically-editable data repositories

- Reliance on *fundamental data* (stress and strain only, no model-dependent data) makes *material data fungible*, mergeable, interchangeable…
- *Publically editable repositories* have proven tremendous capacity for organic growth…
- *Objective: Publicly-editable material data repository (Wikimat?):*
  - *Fundamental data and nothing but fundamental data:*
    - *stress-strain, strain rate*
    - *temperature-entropy, time-energy*
    - *temperature gradient-heat flux*
  - *Scripts for interfacing with commercial FE packages*

Concluding remarks

- *The MFDD ecosystem*:
  - Solver standardization (material independent)
  - Data identification from full-field microscopy
  - Multiscale analysis and upscaling
  - Data repositories (publically editable)
- *Data-driven computing* is likely to be a *growth area* in an increasingly *data-rich world!*

Thank you!