



(Model-Free) Data-Driven Computational Mechanics – Cutting out the Middlemen

Argyris Lecture

Michael Ortiz

California Institute of Technology

Rheinische Friedrich-Wilhelms Universität Bonn

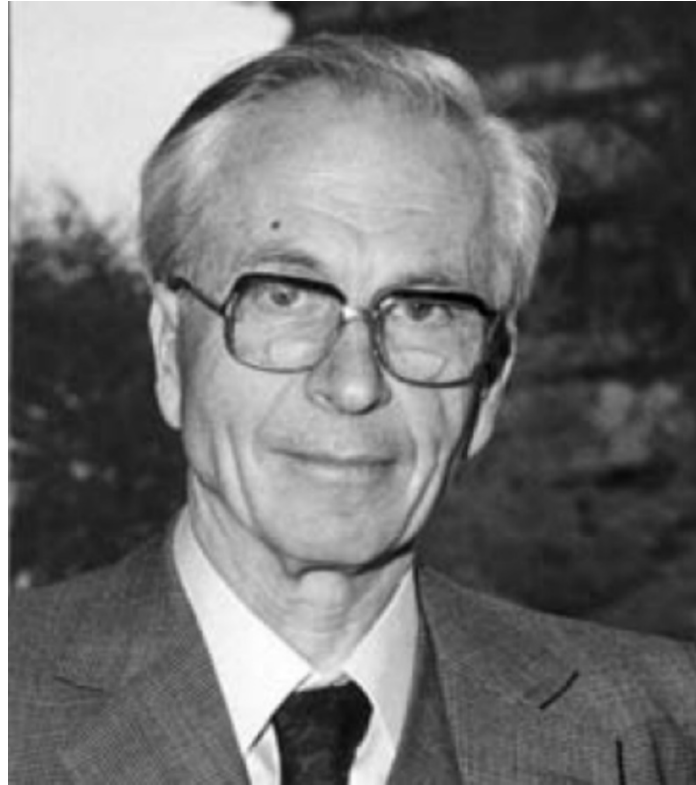
In collaboration with

S. Conti, S. Müller (Uni-Bonn); K. Karapiperis, J. Andrade (Caltech); A. Platzer, L. Stainier, A. Leygue (Central Nantes); R. Eggersmann, S. Reese (RWTH Aachen); P. Carrara, L. de Lorenzis (ETH Zürich)

University of Stuttgart, December 2, 2020

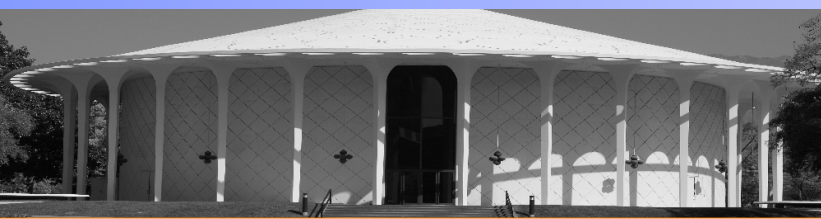
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IN MEMORIAM



Johann Hadji Argyris (1913-2004),
pioneer in the application of computer
methods to science and engineering

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A blast from the past!

Data-Driven Computing

Michael Ortiz

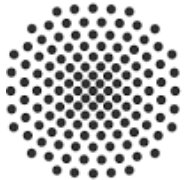
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

SimTech 2nd International Conference
on Simulation Technology,
University of Stuttgart, 26-28 March, 2018

A blast from the past!

- *Data-driven computing* is emerging as an alternative paradigm to model-based computing
- Data-Driven mechanics entails a *comprehensive reformulation* and generalization of the classical problems of mechanics and physics
- Data-driven computing can reliably supply *model-free* solutions from raw material data sets
- Data-driven computing is likely to be a growth area in an increasingly *data-rich world*
- Reliance on *fundamental data* makes material data fungible, mergeable, interchangeable: *Publicly editable material data repository? (Wikimat, a material data Wikipedia...)*

SimTech mission statement



University of Stuttgart



"With data-integrated simulation we are introducing a *new paradigm into simulation science* at the University of Stuttgart. We are reaching the limits of our traditional approaches, when it comes to simulating highly complex phenomena, for example in environmental issues, in digital human models, and in new materials, and we can only overcome these issues by integrating all the data which is available. We are convinced that the new methods emerging out of SimTech will *fundamentally change research and development in many scientific disciplines.*"

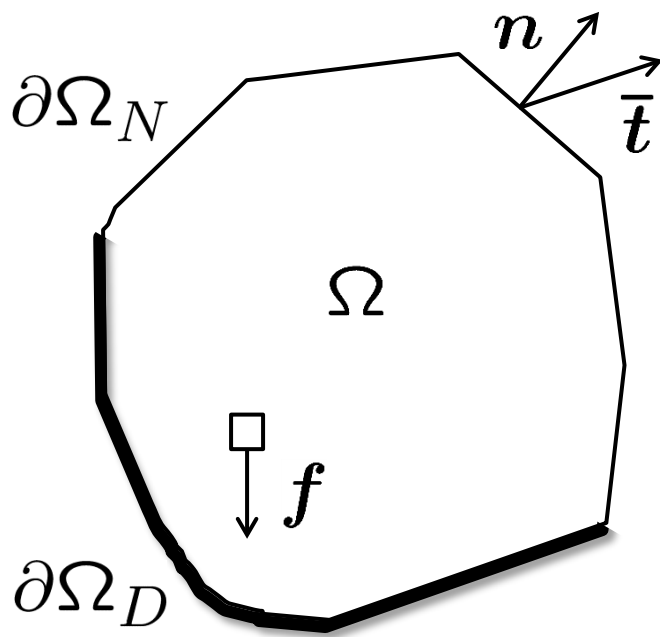
Data Science, Big Data...

- *Data Science* is the extraction of '*knowledge*' from large volumes of unstructured data¹
- 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...*

¹Dhar, 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:

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

- ii) Equilibrium + Neumann:

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

- iii) Material law: $\sigma(x) = \sigma(\epsilon(x))$

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:

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

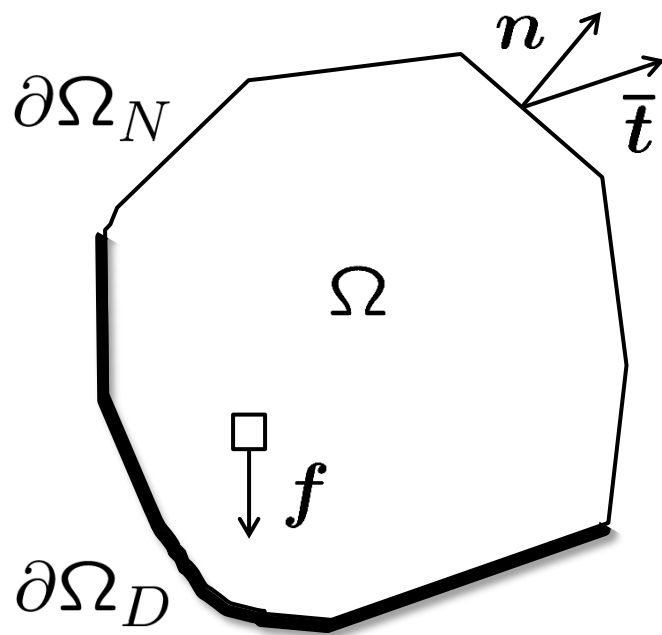
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Differential structure of field equations

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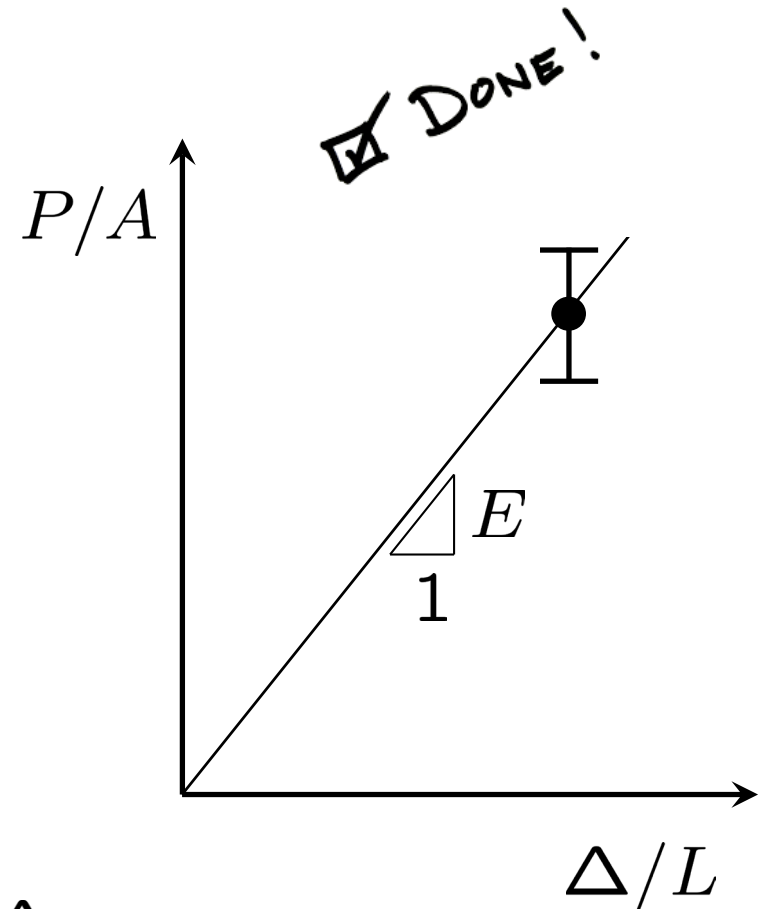
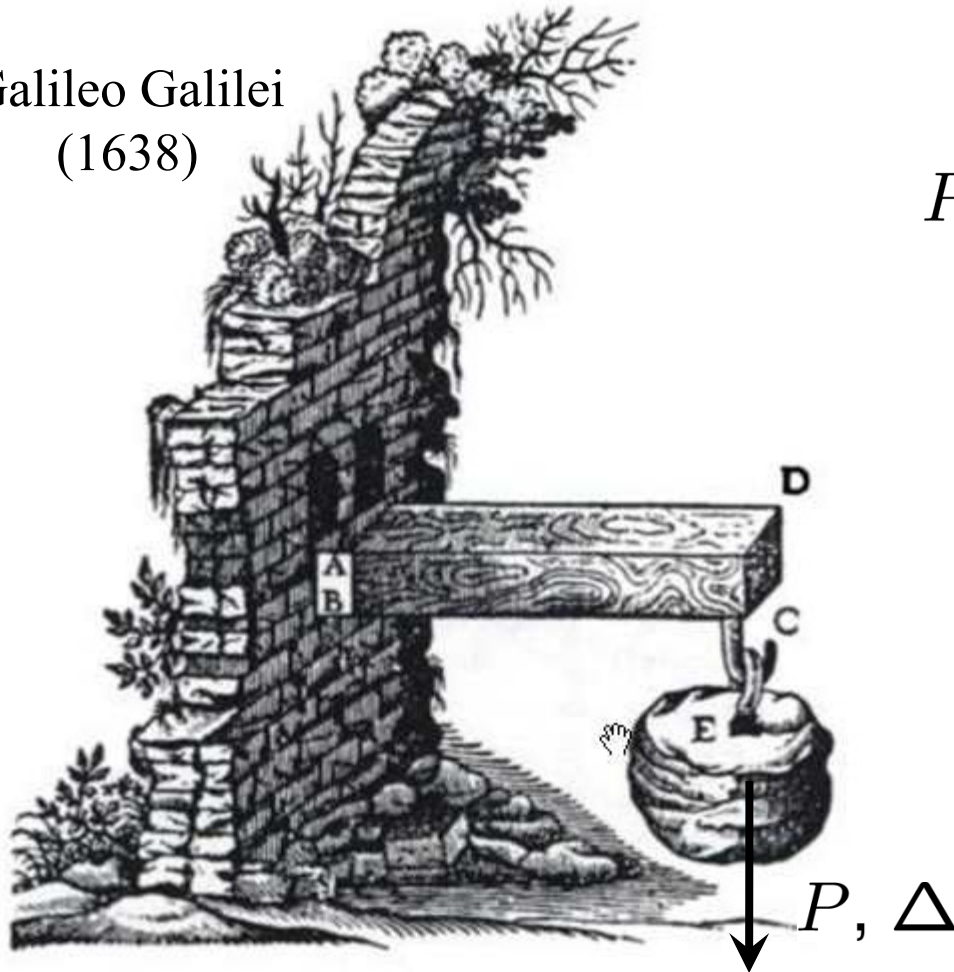
iii) Material law: $\sigma(x) = \sigma(\epsilon(x))$

Unknown! Epistemic uncertainty!

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

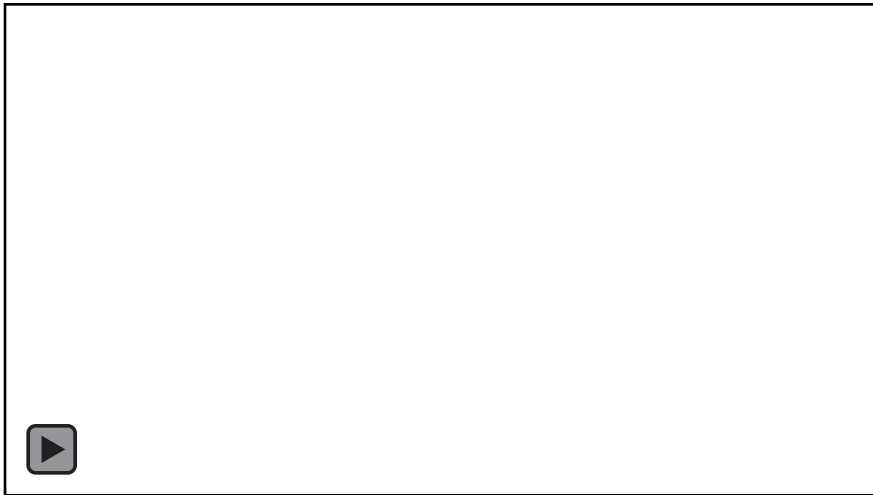
John Lambros, UIUC,

<https://lambros.ae.illinois.edu/moviesimages/>

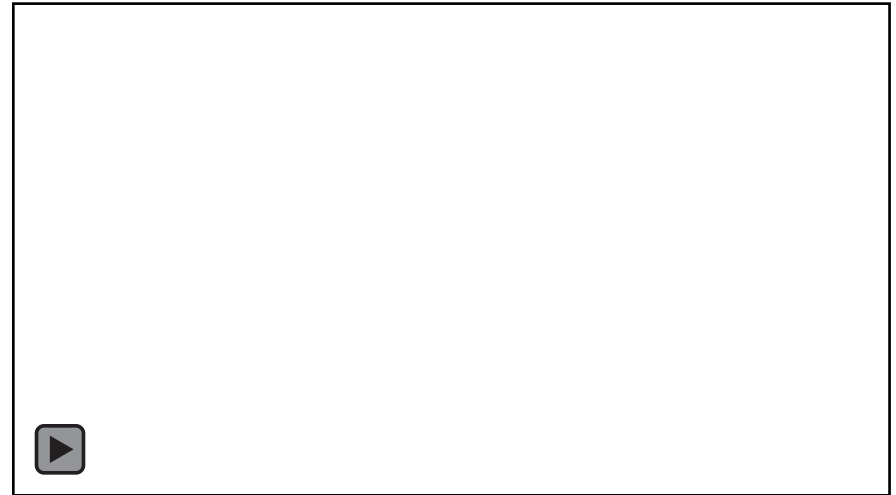
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3D tomographic reconstruction
of particles in battery electrode



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

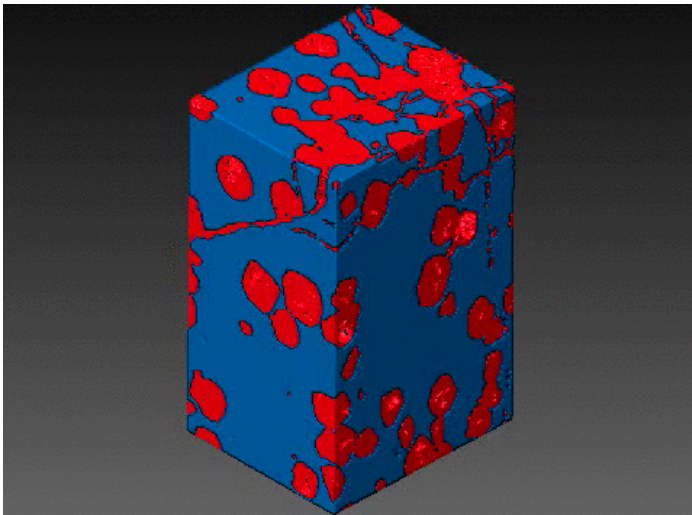
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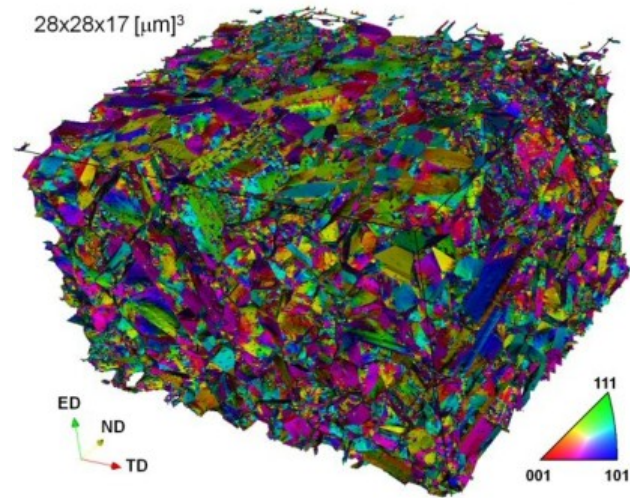
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The new data-rich world...

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



Two-phase μ CT analysis of Ti₂AlC/Al composite¹



3D EBSD microstructure in Cu-0.17wt%Zr after ECAP²

¹Hanaor *et al.*, *Mater Sci Eng A*, **672** (2019) 247.

²Khorashadizadeh, *Adv Eng Mater*, **13** (2011) 237.

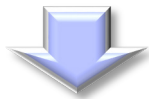
Adapting to a new data-rich world...

Classical Model-Based
Computational Science...

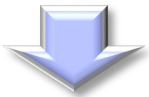


Alternative:
Model-Free
Data-Driven
Computing!

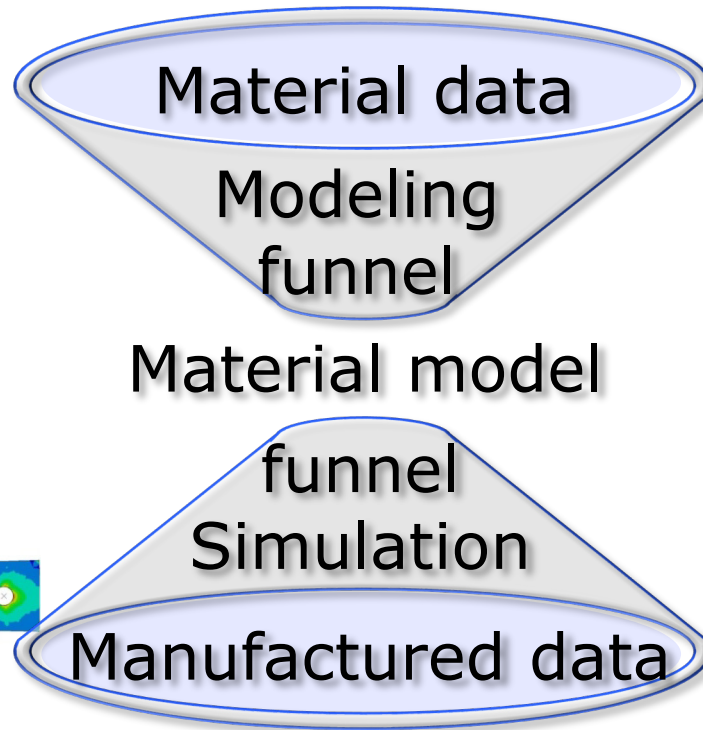
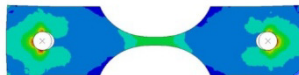
Modern
microscopy
generates
massive
data sets



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



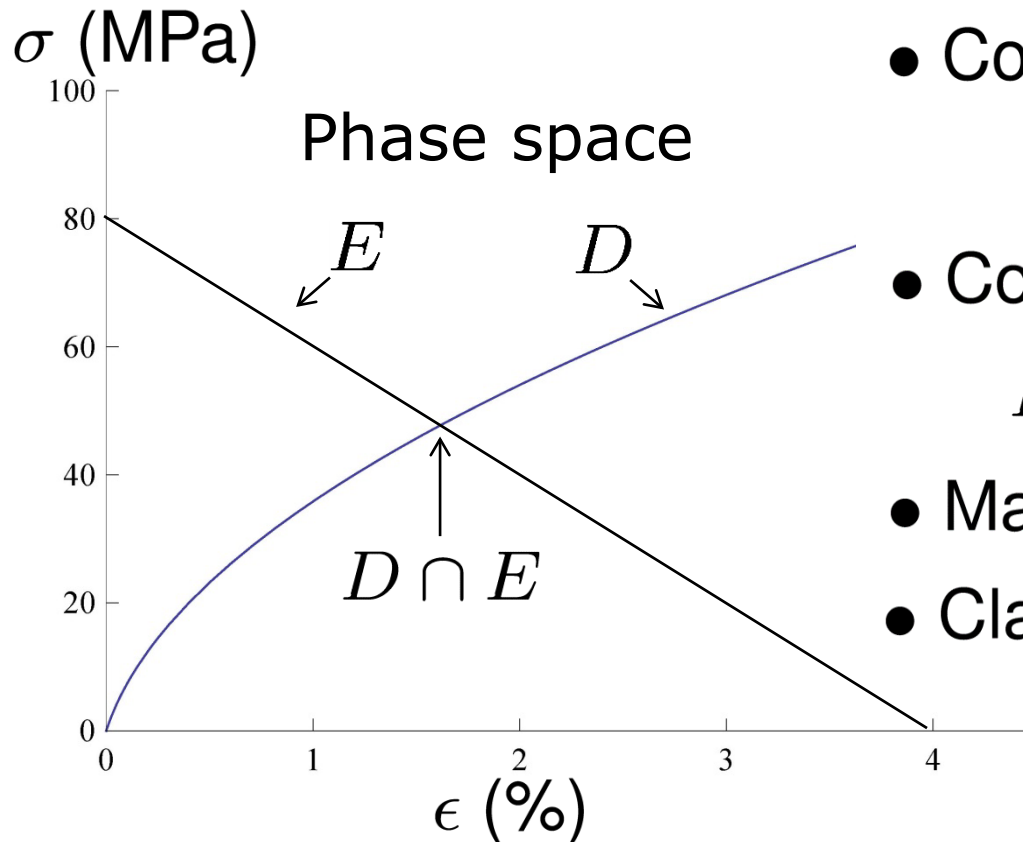
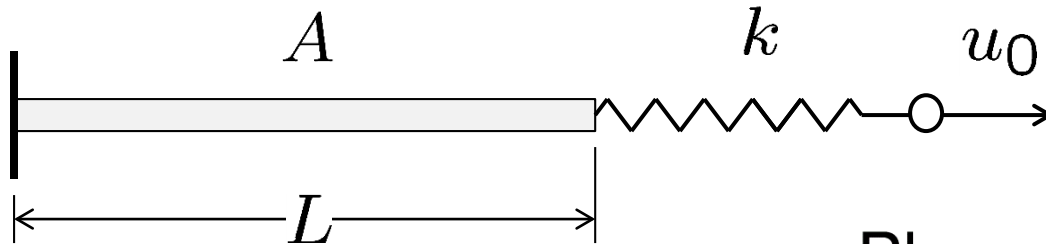
Modelling
entails
massive
loss of
information!



Set/solve
problems
directly
from data!

*Cut out the
modeling
middleman!*

Elementary example: Bar and spring



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

- Compatibility + equilibrium:

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

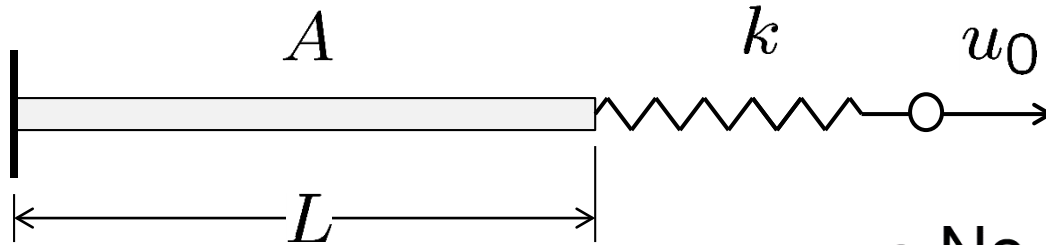
- Constraint set:

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

- Material data set: $D \subset Z$

- Classical solution set: $D \cap E$

Elementary example: Bar and spring

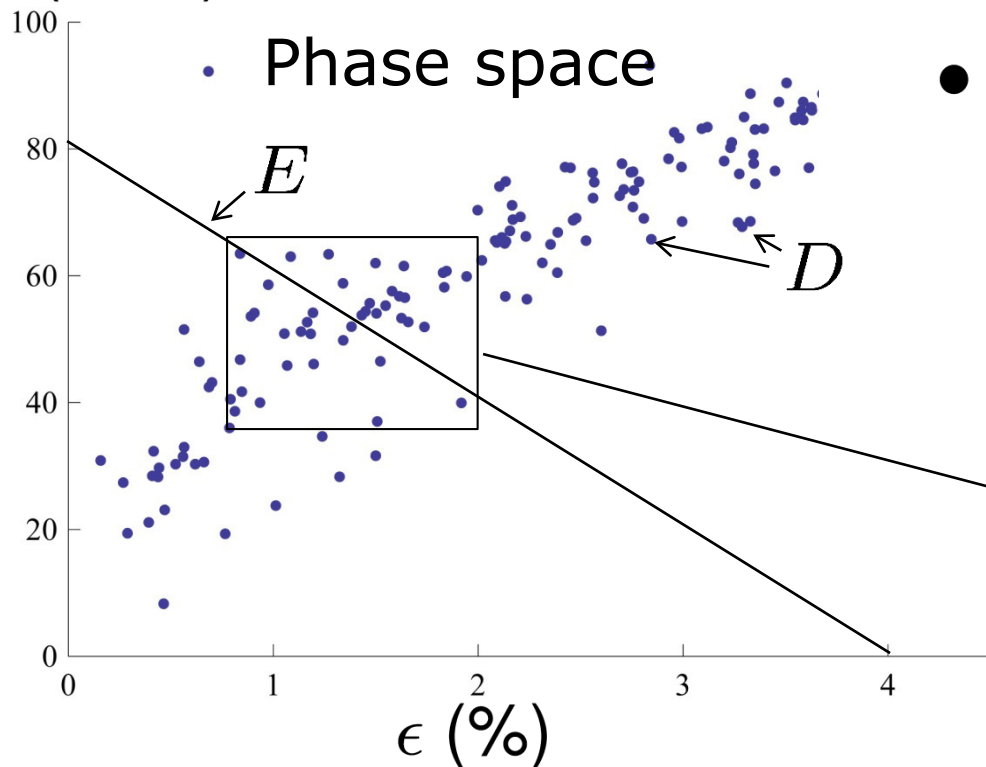


- No classical solutions!

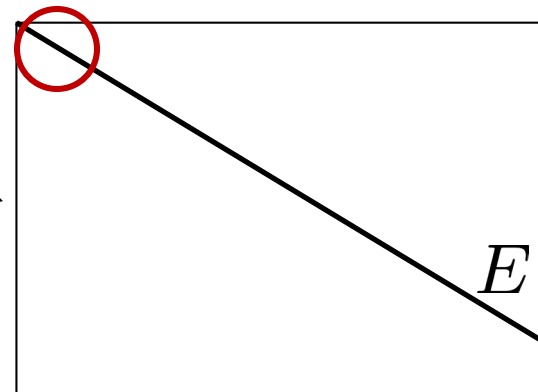
$$D \cap E = \emptyset$$

σ (MPa)

- Data-driven solution:



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



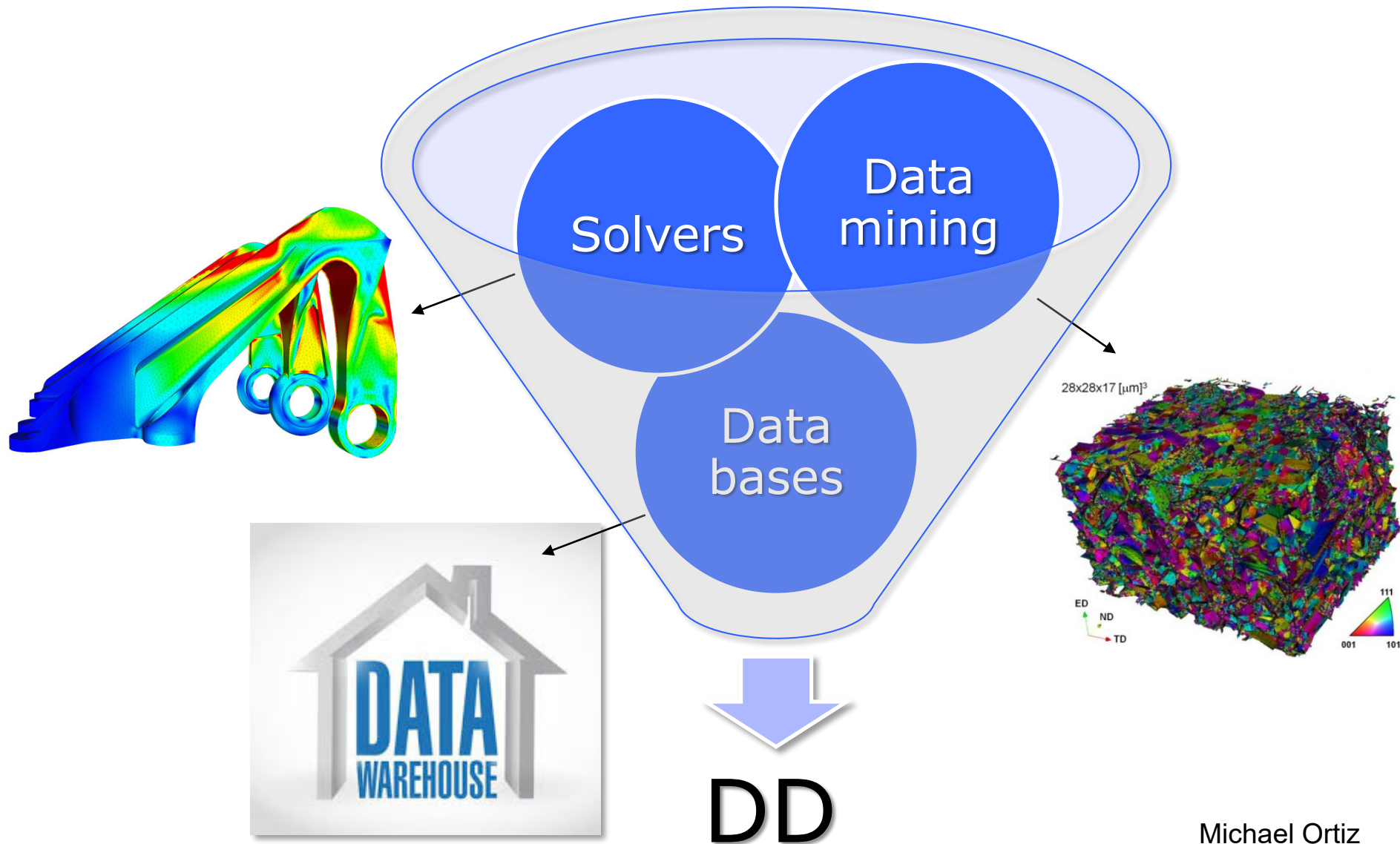
The general Data-Driven (DD) problem

- The *Data-Driven paradigm*¹: Given,
 - $D = \{\text{fundamental material data}\},$
 - $E = \{\text{compatibility} + \text{equilibrium}\},$Find: $\operatorname{argmin}\{d(z, D), z \in E\}$
- *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!*

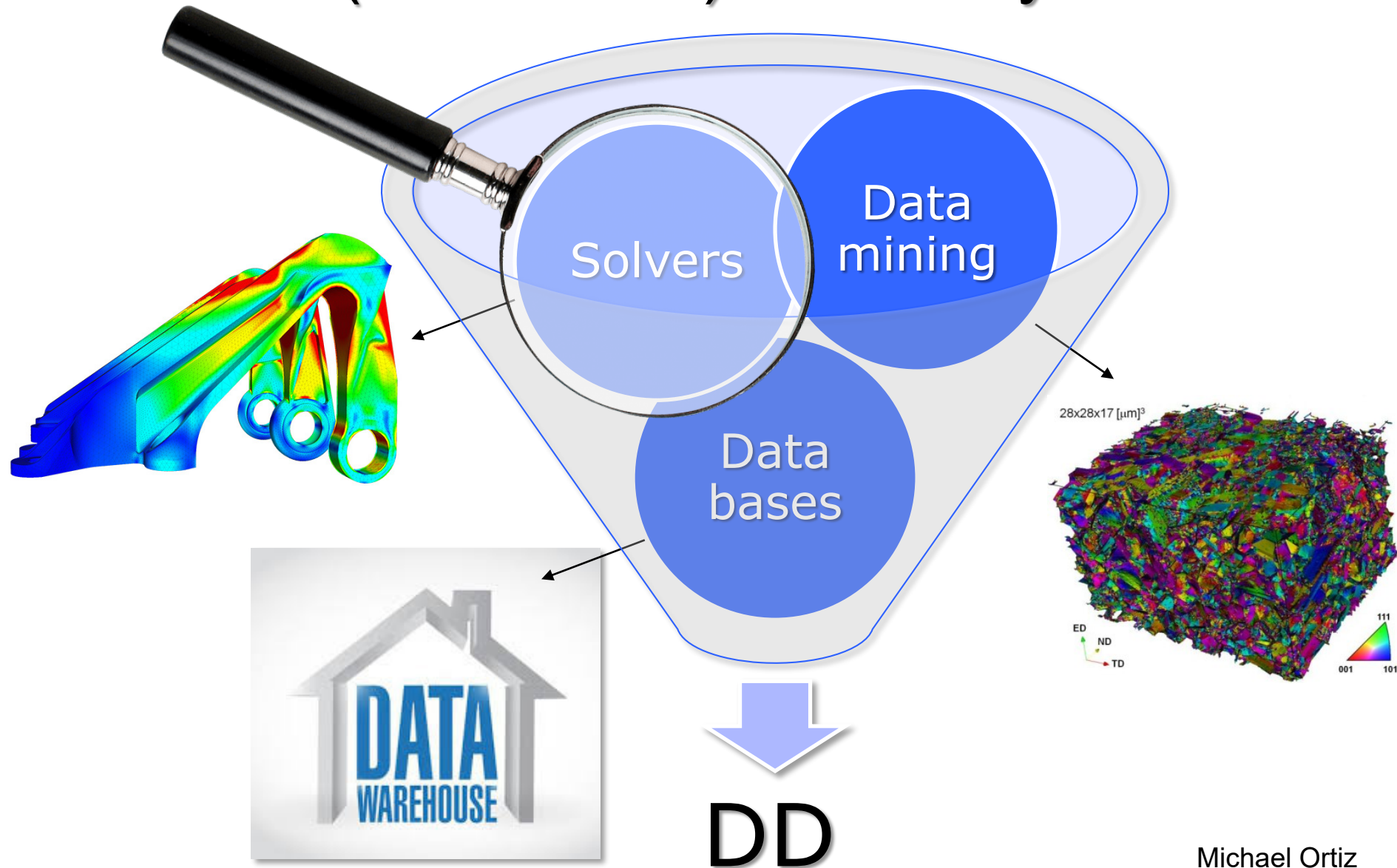
¹T. Kirchdoerfer and M. Ortiz (2015) arXiv:1510.04232.

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

The (model-free) DD ecosystem

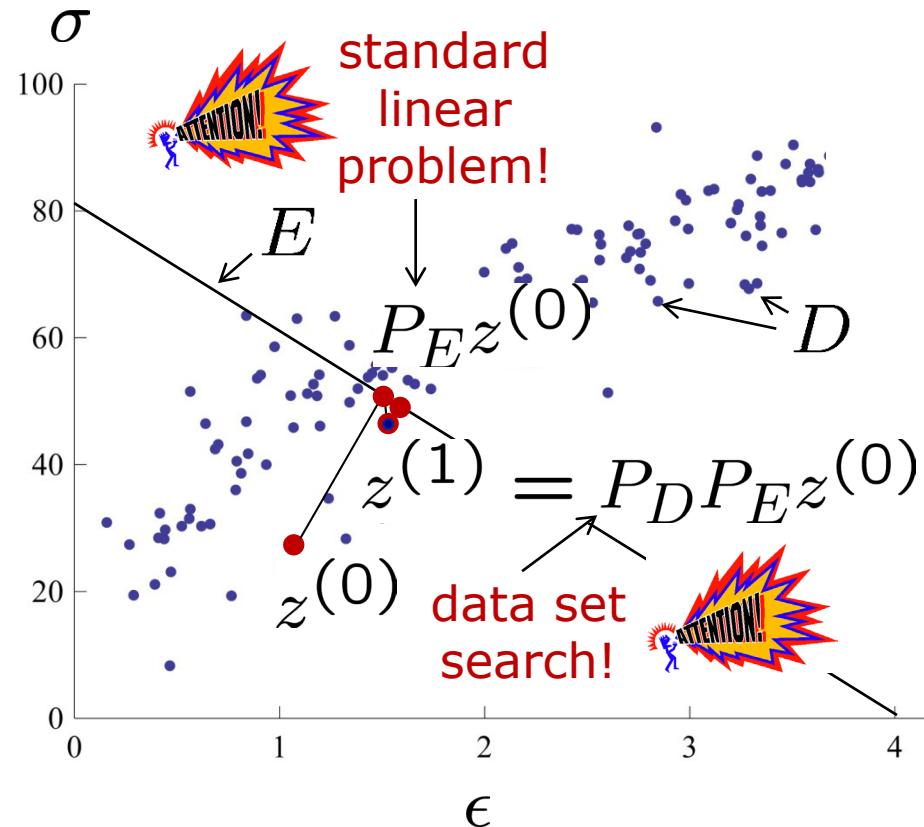
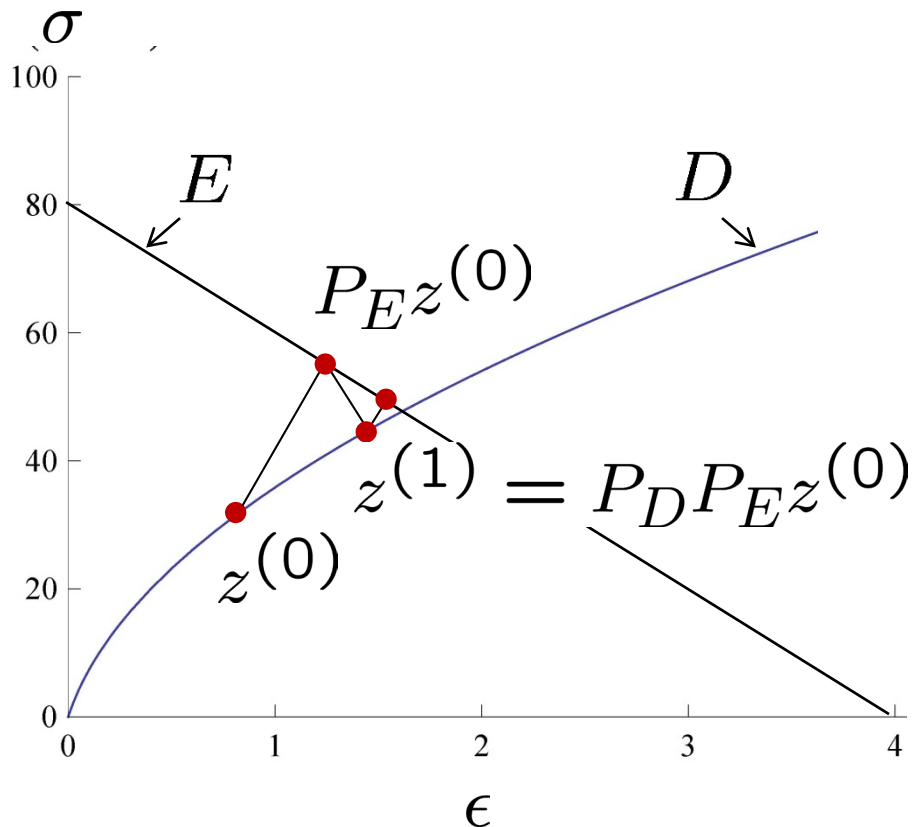


The (model-free) DD ecosystem



DD solvers: Fixed-point iteration

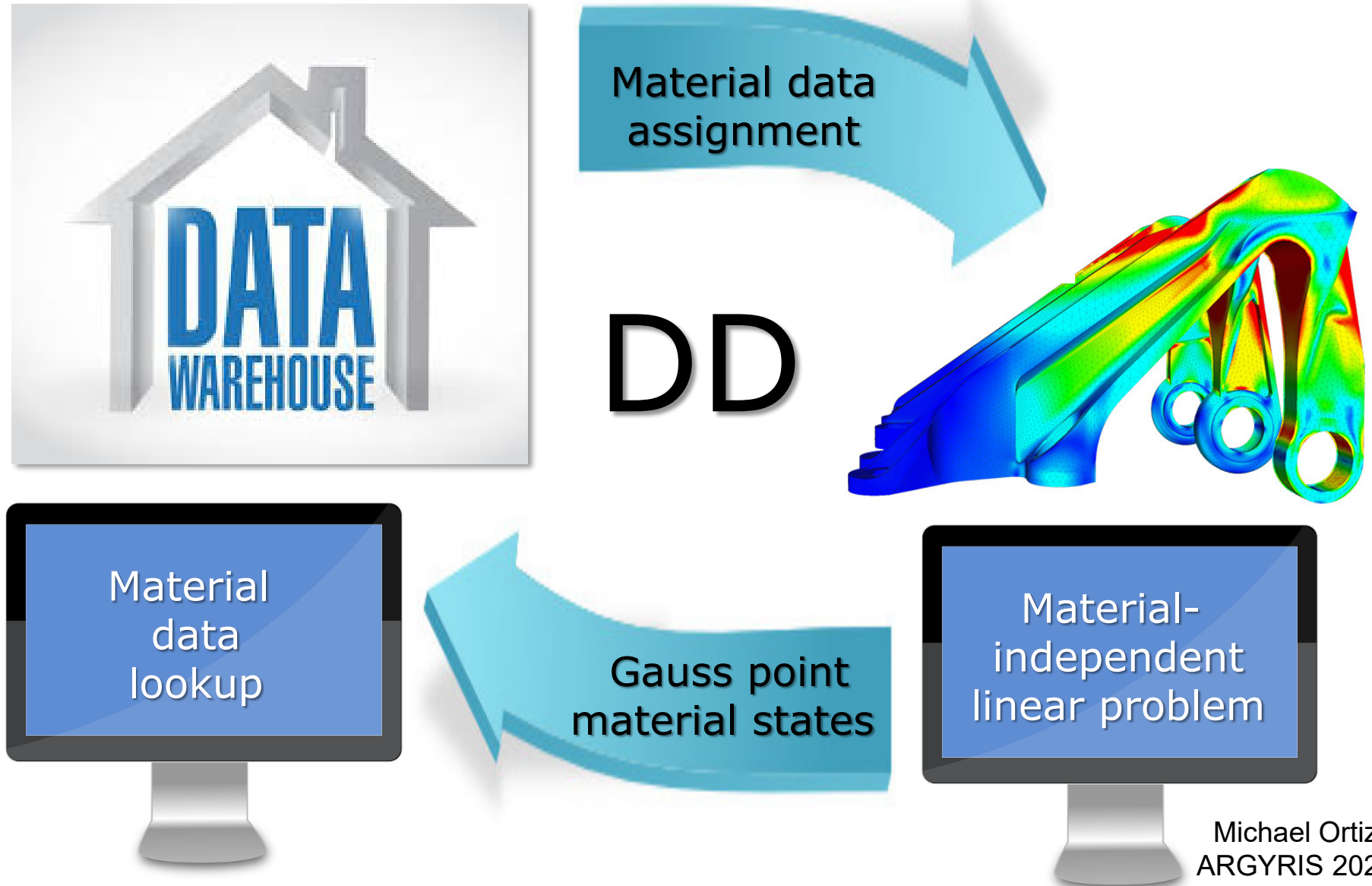
- Find: $\operatorname{argmin}\{d(z, D), z \in E\}$
- Fixed-point iteration¹: $z^{(k+1)} = P_D P_E z^{(k)}$



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

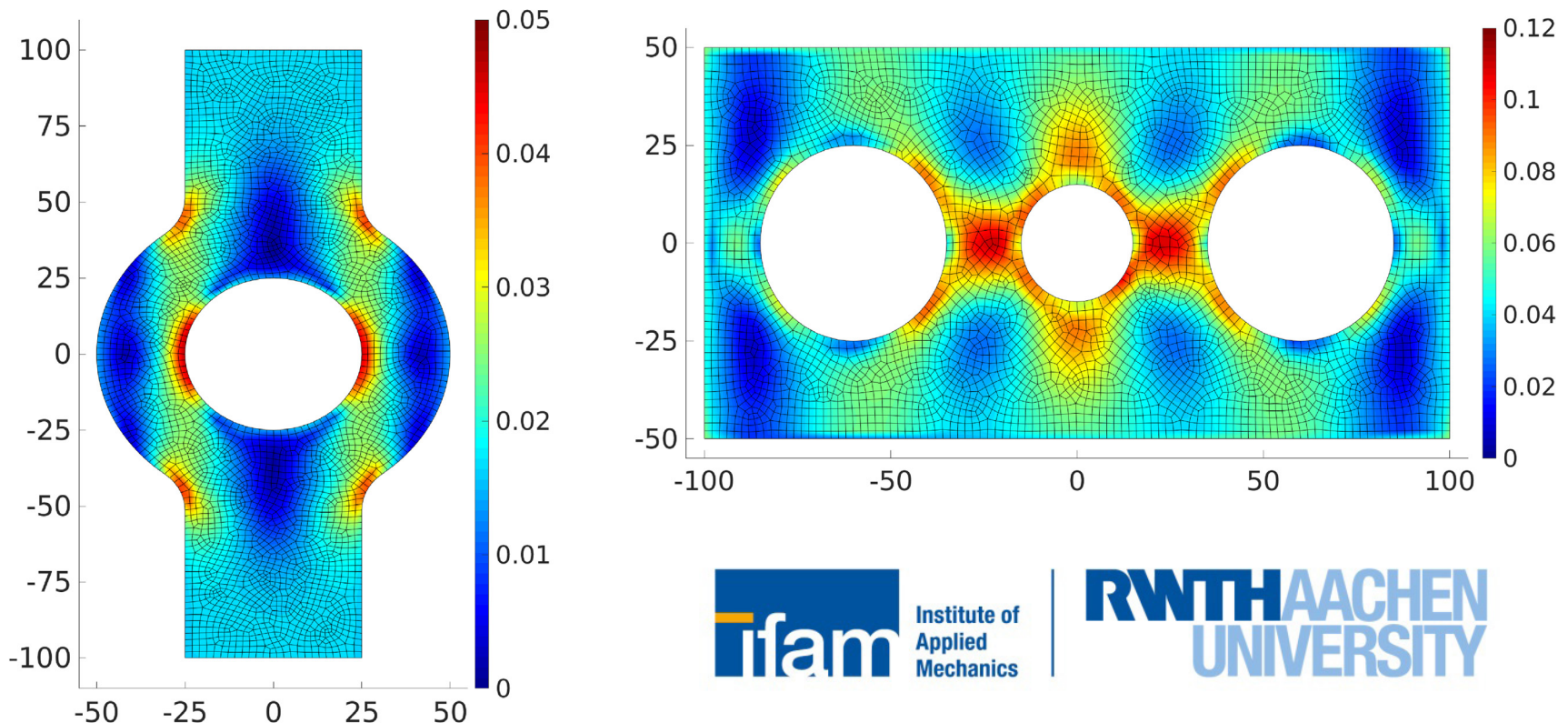
¹T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81–101

The DD information flow



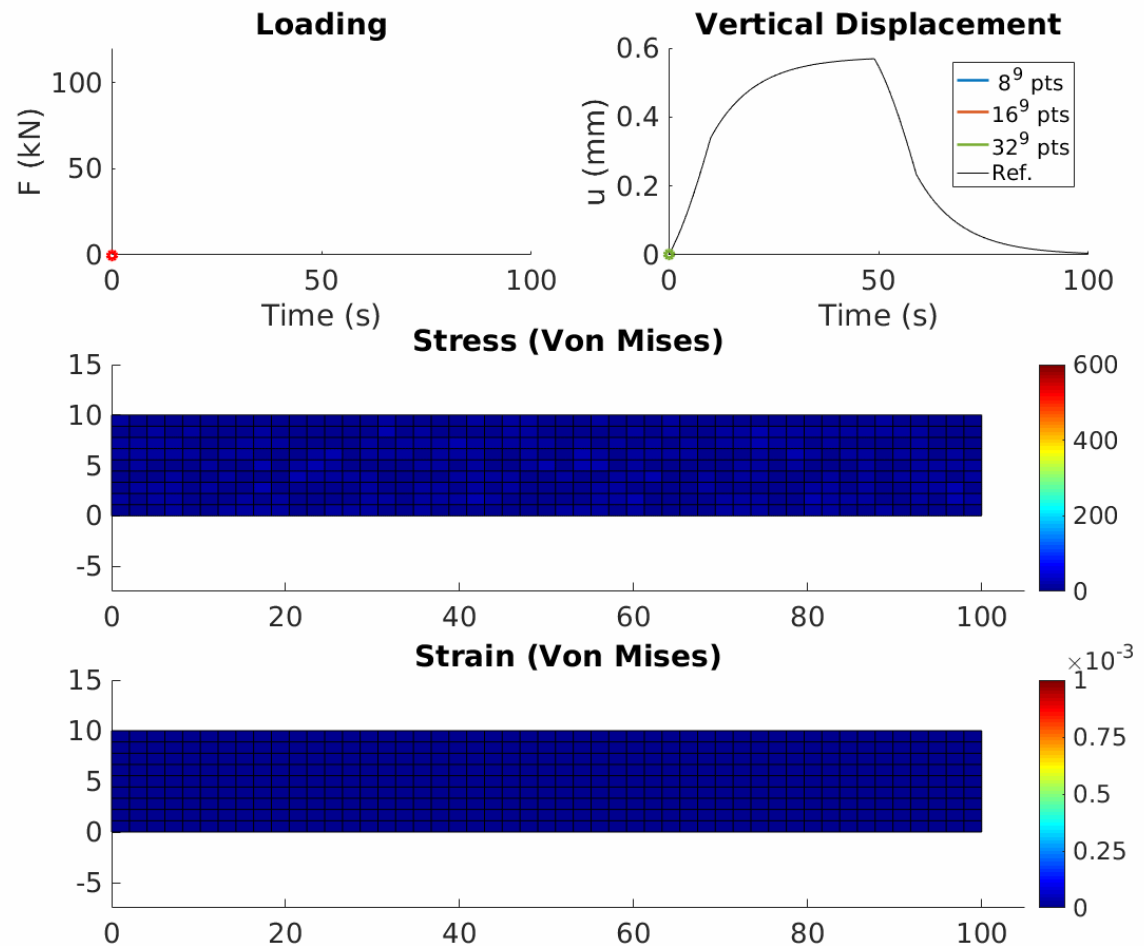
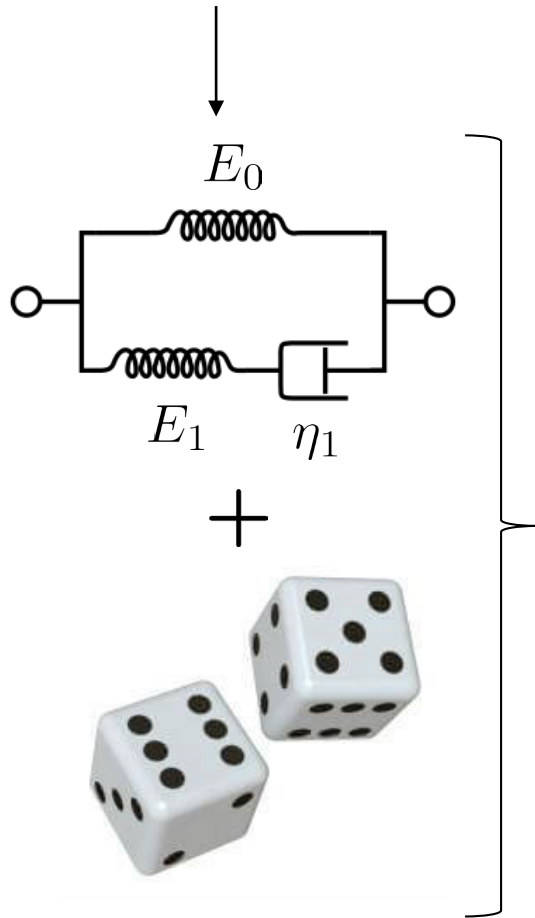
Data-Driven solvers and FE analysis

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



Data-Driven viscoelasticity

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



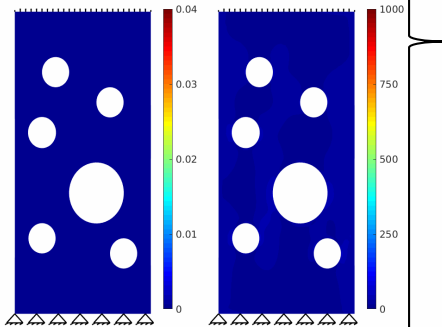
Data-Driven plasticity

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



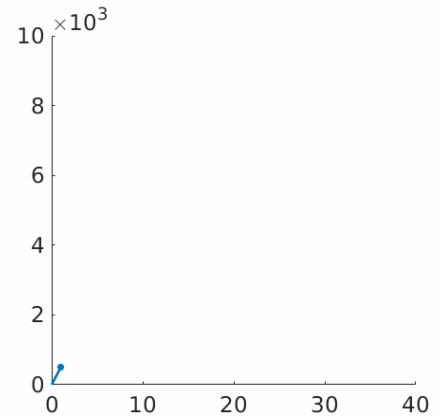
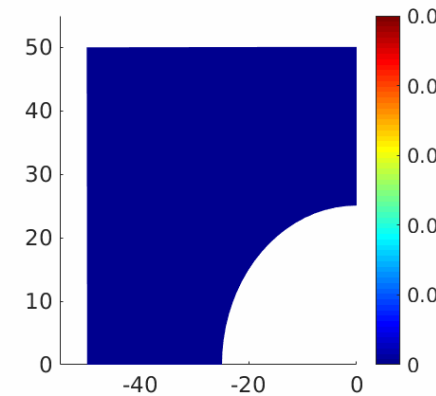
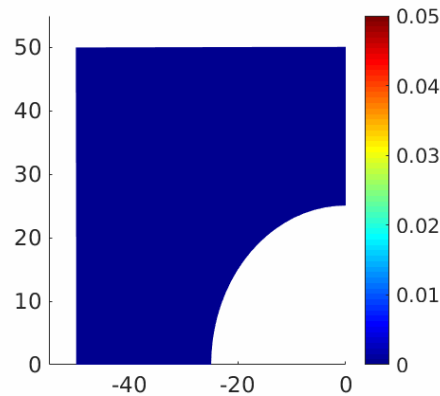
J2 plasticity
kinematic
hardening

+

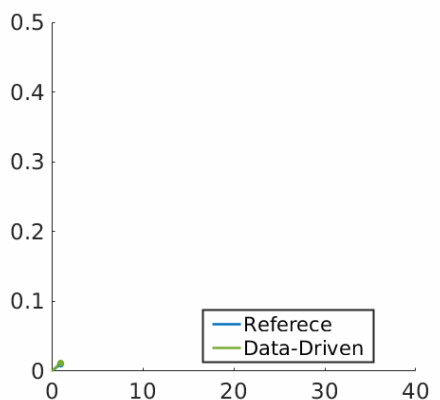
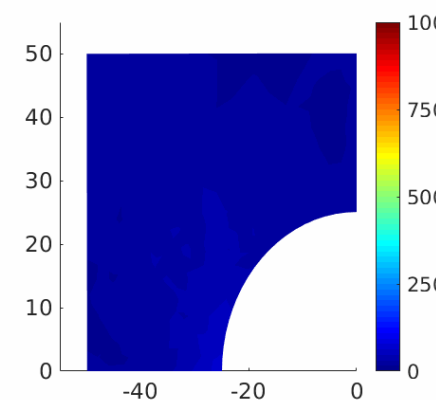
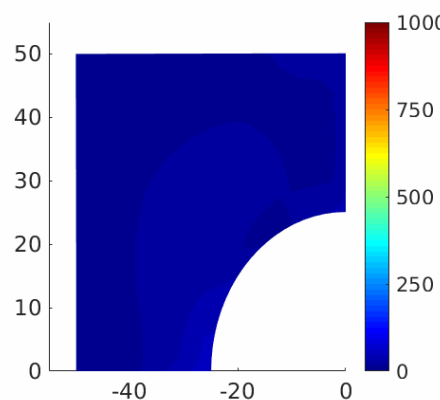


Virtual test

Strain (von Mises)



Stress (von Mises)



(R. Eggersmann & S. Reese, 2019)

(Model-Free) Data-Driven solvers

- Model-free DD computing is *achieving maturity*:
 - *Analysis*, existence of solutions, well-posedness¹
 - *Finite elasticity*, finite kinematics^{2,3}
 - *Dynamics*, time discretization⁴
 - *Noisy data*, clustering (k-means), outliers⁵
 - *Inelasticity*, viscoelasticity, plasticity⁶, fracture⁷
 - *Multiscale* data mining, model-free upscaling⁸
 - *Probabilistic extension*, model-free, prior-free
 - *Fast Data searching*, k-d trees, scalable ANN

¹Conti, S., Müller, S. & Ortiz, M., *ARMA*, **229** (2018) 79-123.

²L.T.K. Nguyen and M.A. Keip, *Comput. Struct.*, **194** (2018) 97–115

³S. Conti, S. Müller and M. Ortiz, *ARMA*, **237** (2020) 1–33.

⁴T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

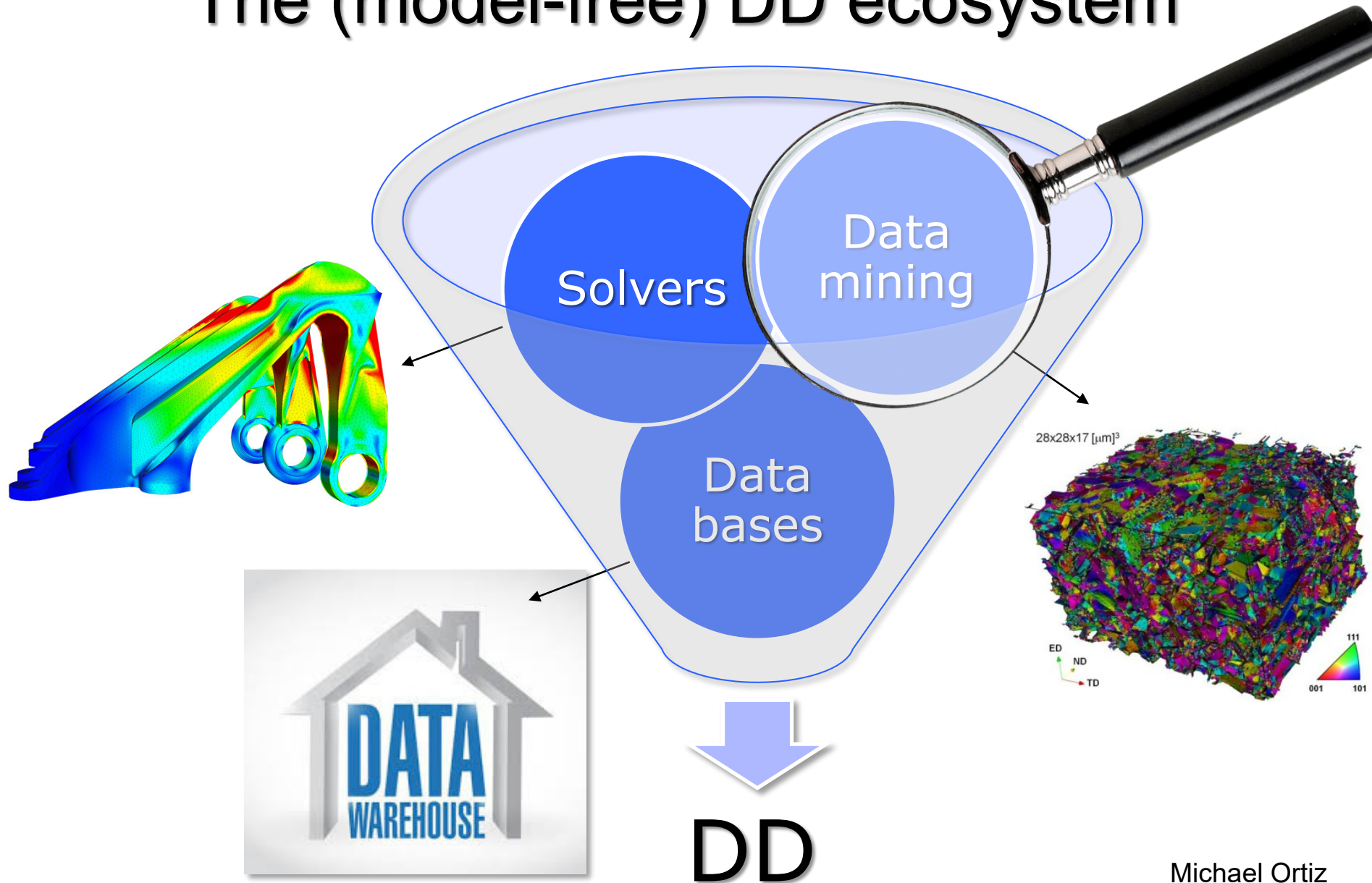
⁵T. Kirchdoerfer and M. Ortiz, *CMAME*, **326** (2017) 622-41.

⁶R. Eggersmann, S. Reese, L. Stainier, M. Ortiz, *CMAME*, **350** (2019) 81-99.

⁷P. Carrara, L. Lorenzis, L. Stainier, M. Ortiz, *CMAME*, **372** (2020) 113390. Michael Ortiz

⁸K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239. ARGYRIS 2020

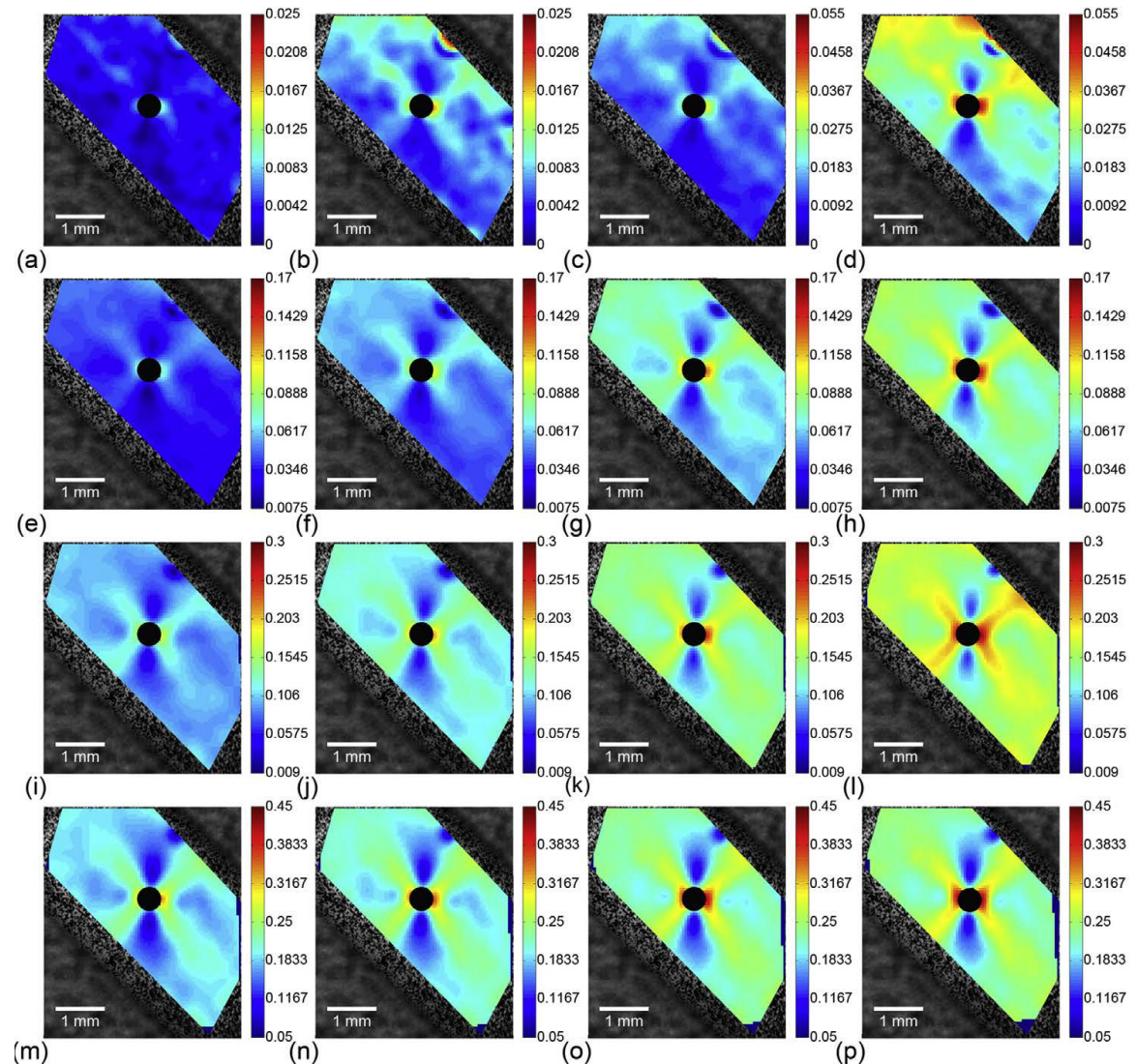
The (model-free) DD ecosystem



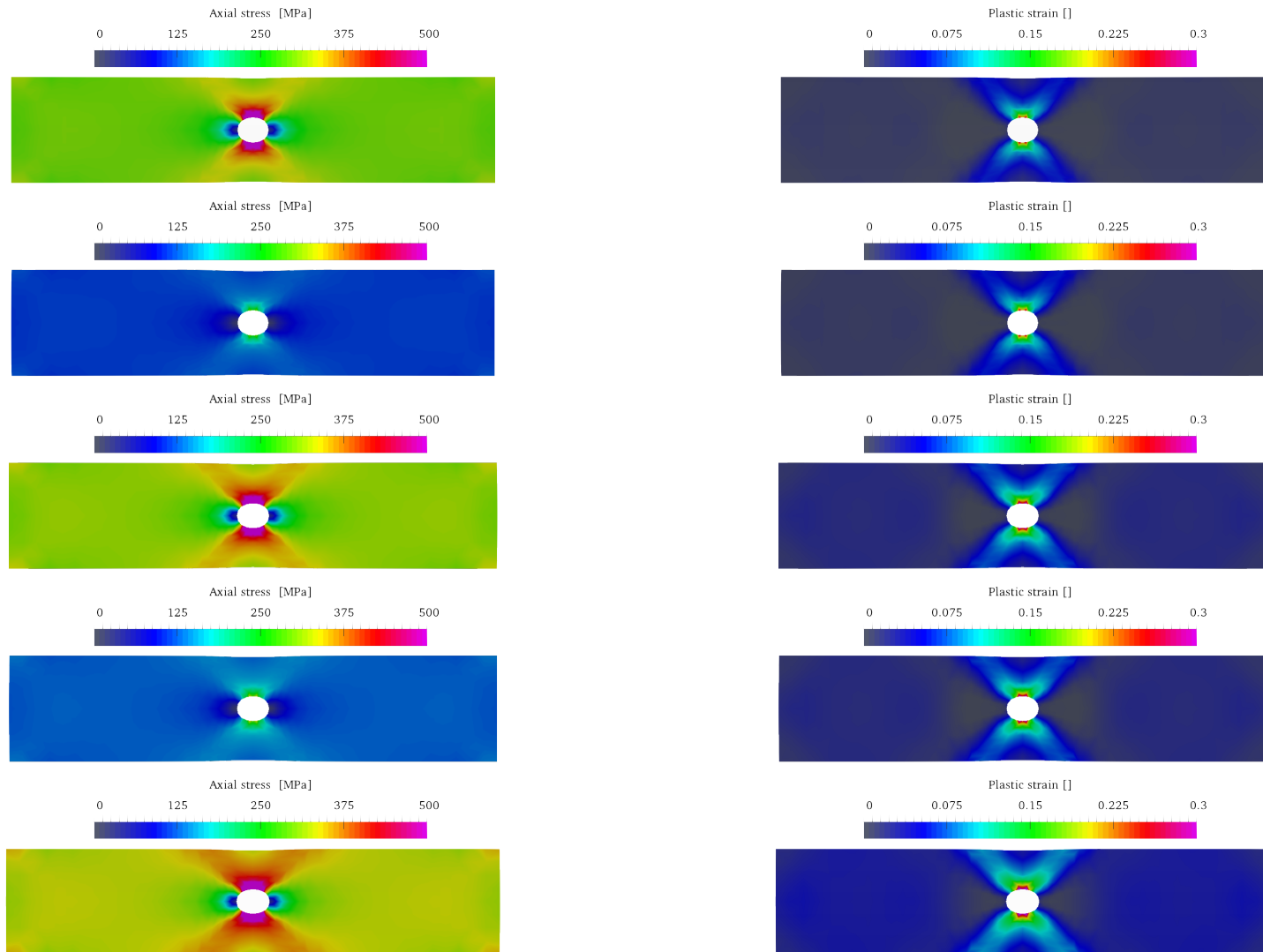
Full-field (DIC) microscopy data



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



Full-field (DIC) microscopy data

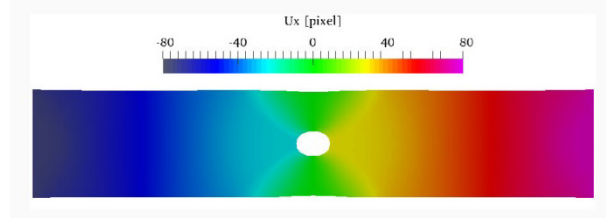


J. Rethore, HAL Id: hal-01454432, Feb. 2017.

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:

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

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

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

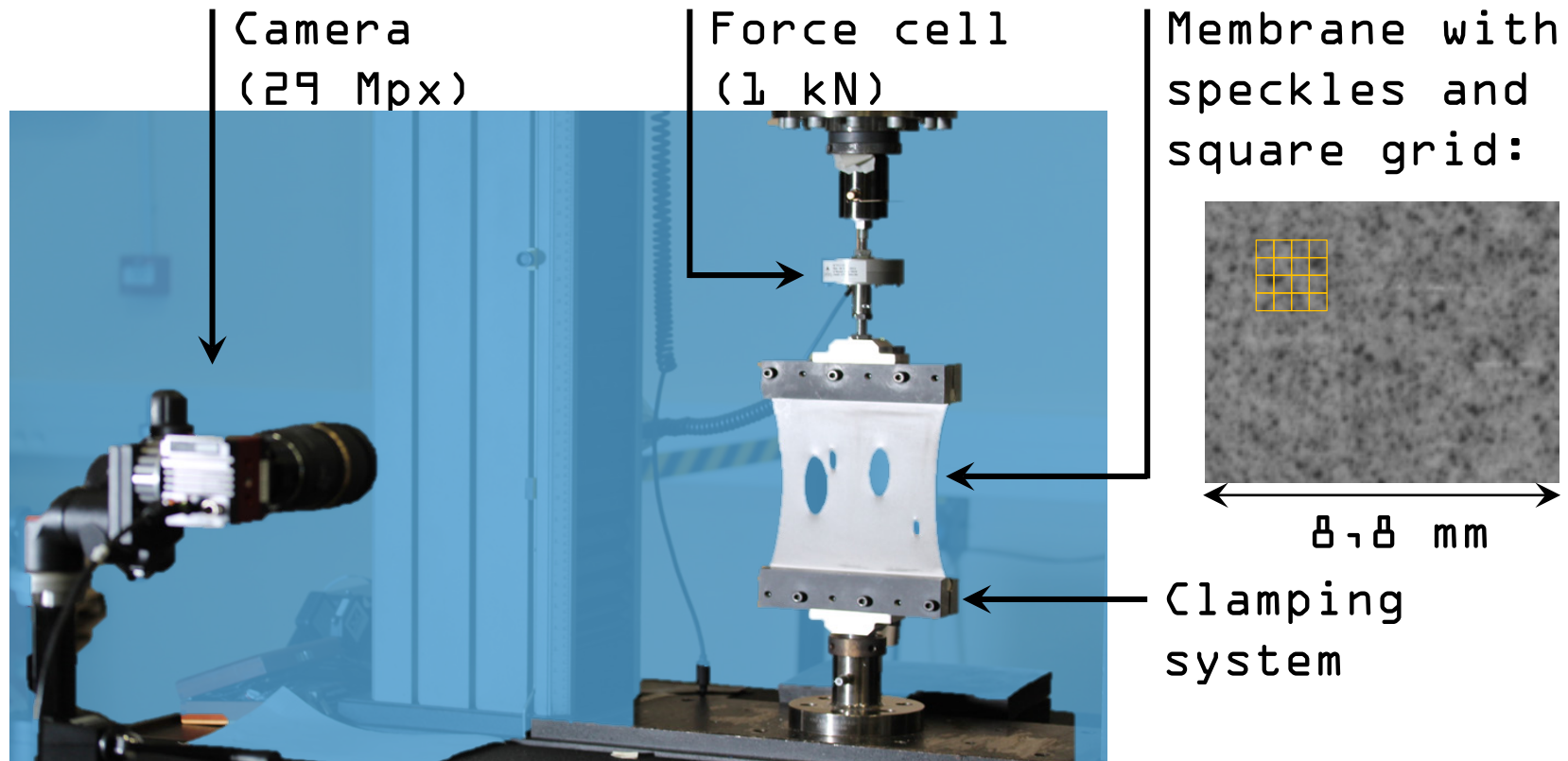
- DD self-consistent material-data identification:

Given D_{exp} :

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

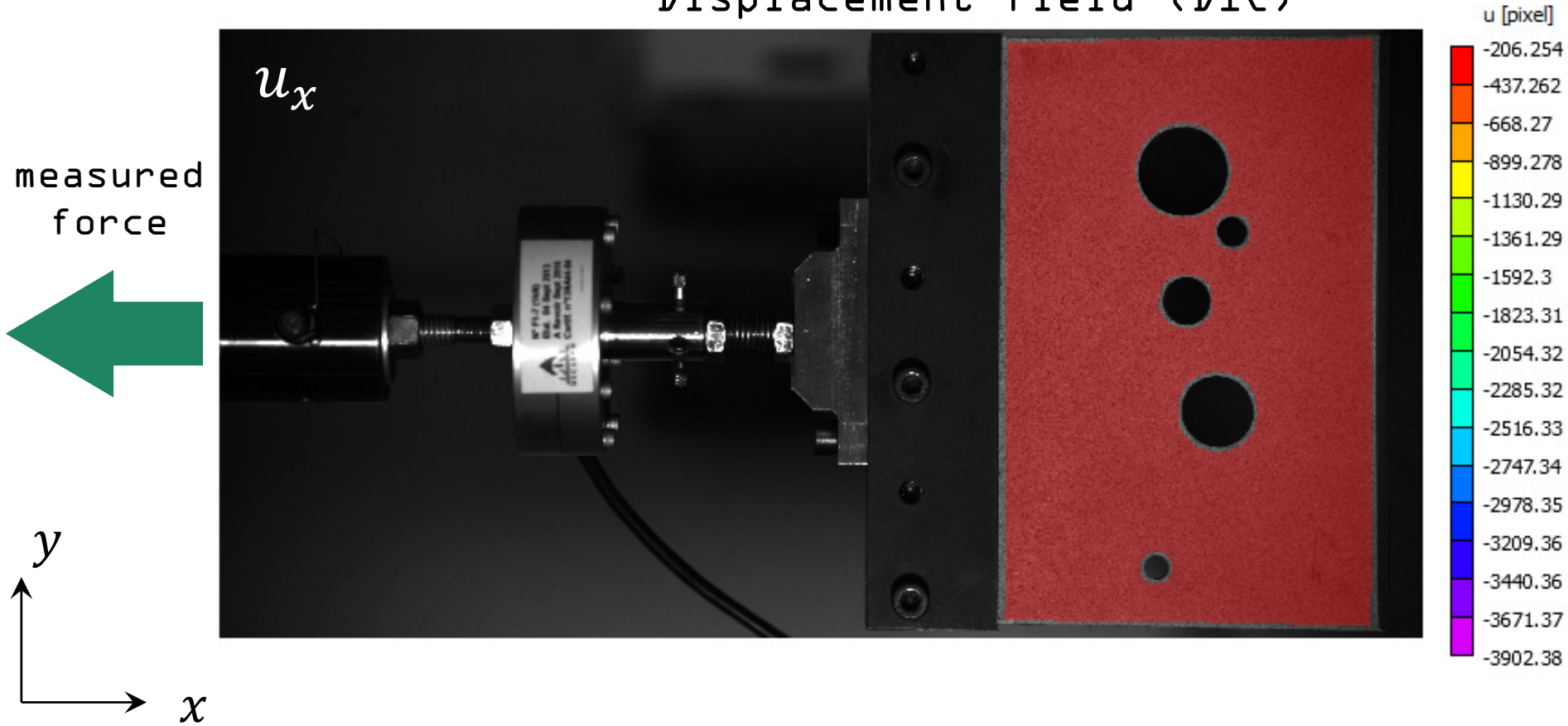
DDMI at Central Nantes

- Tests on perforated silicone sheets

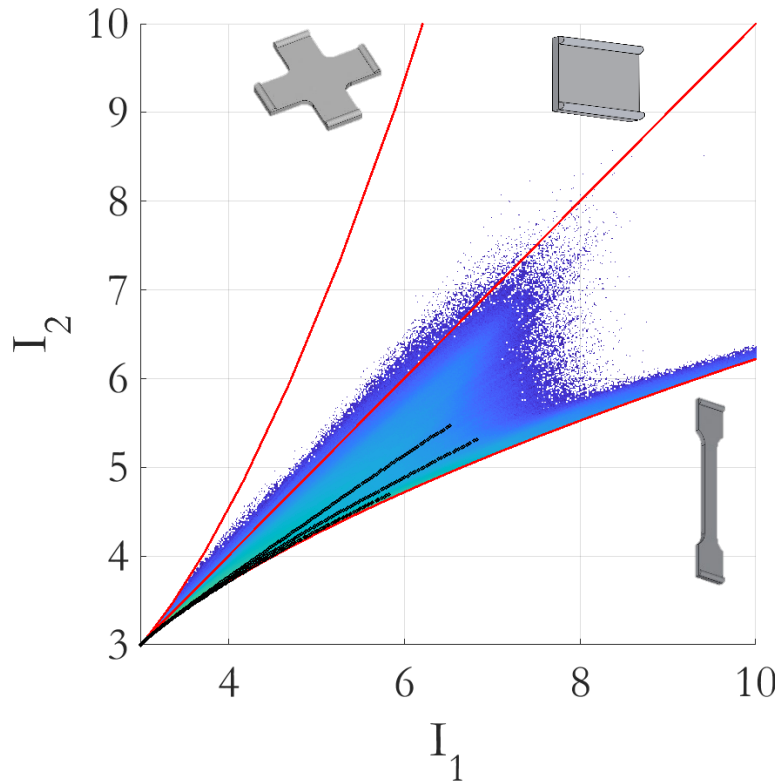
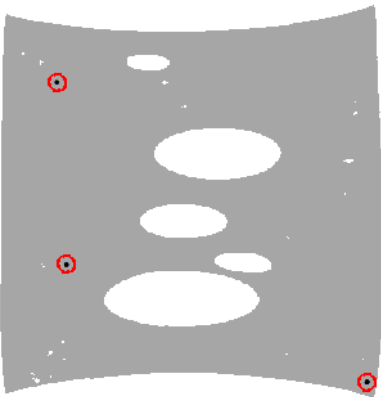


DDMI at Central Nantes

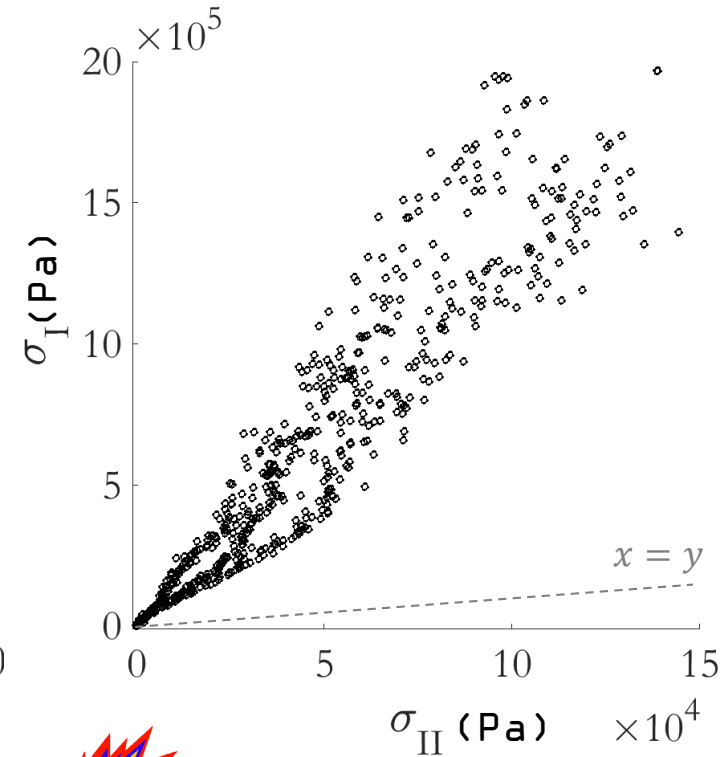
Displacement field (DIC)



DDMI at Central Nantes



Strain data

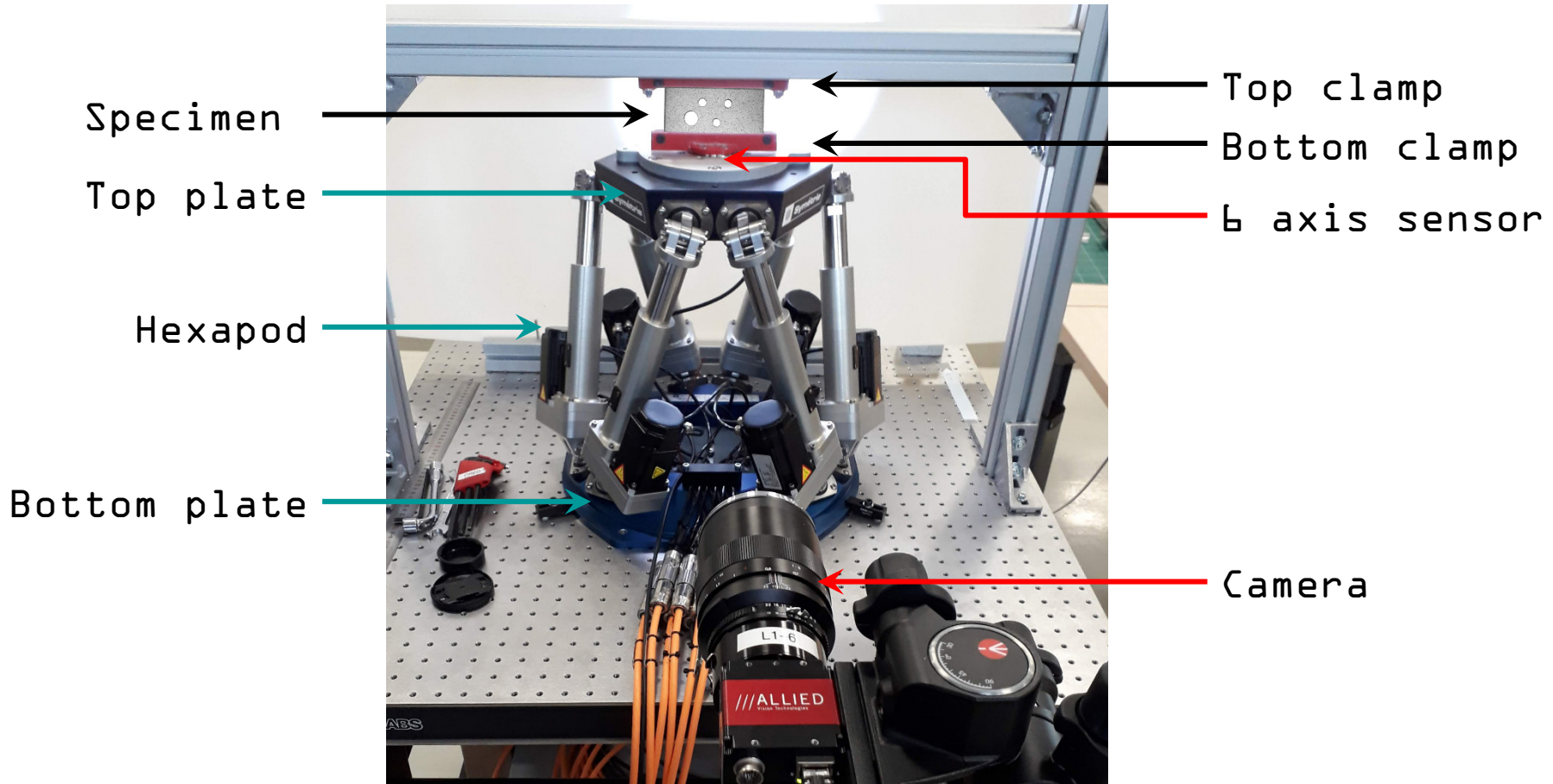


Stress data



DDMI at Central Nantes

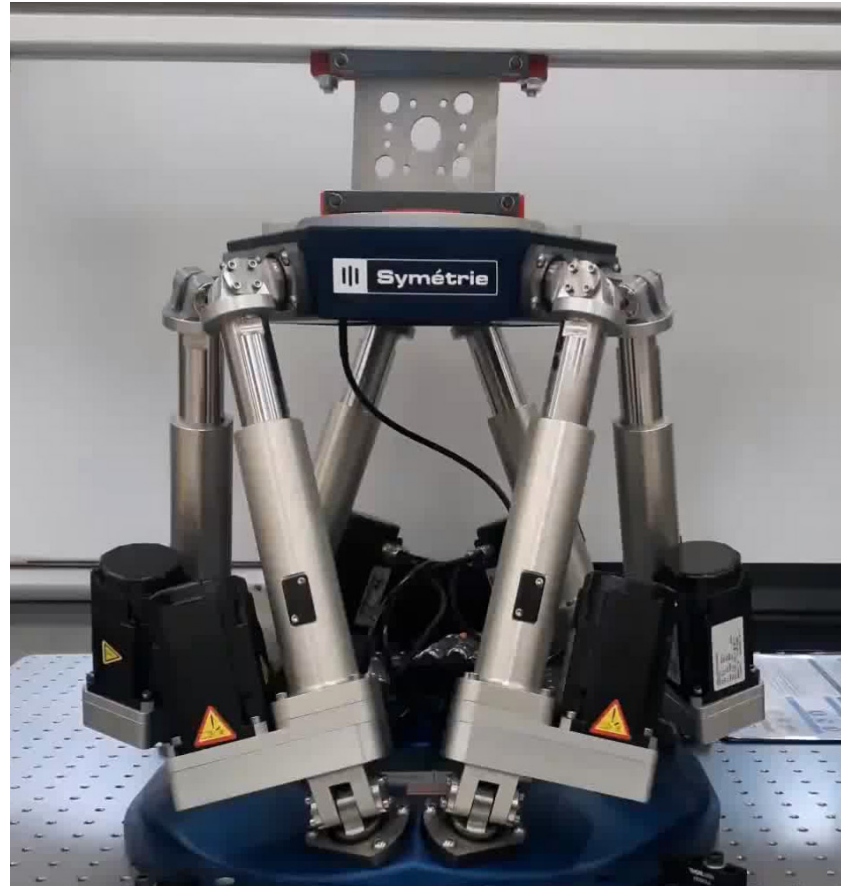
- Hexapod testing machine



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

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DDMI at Central Nantes



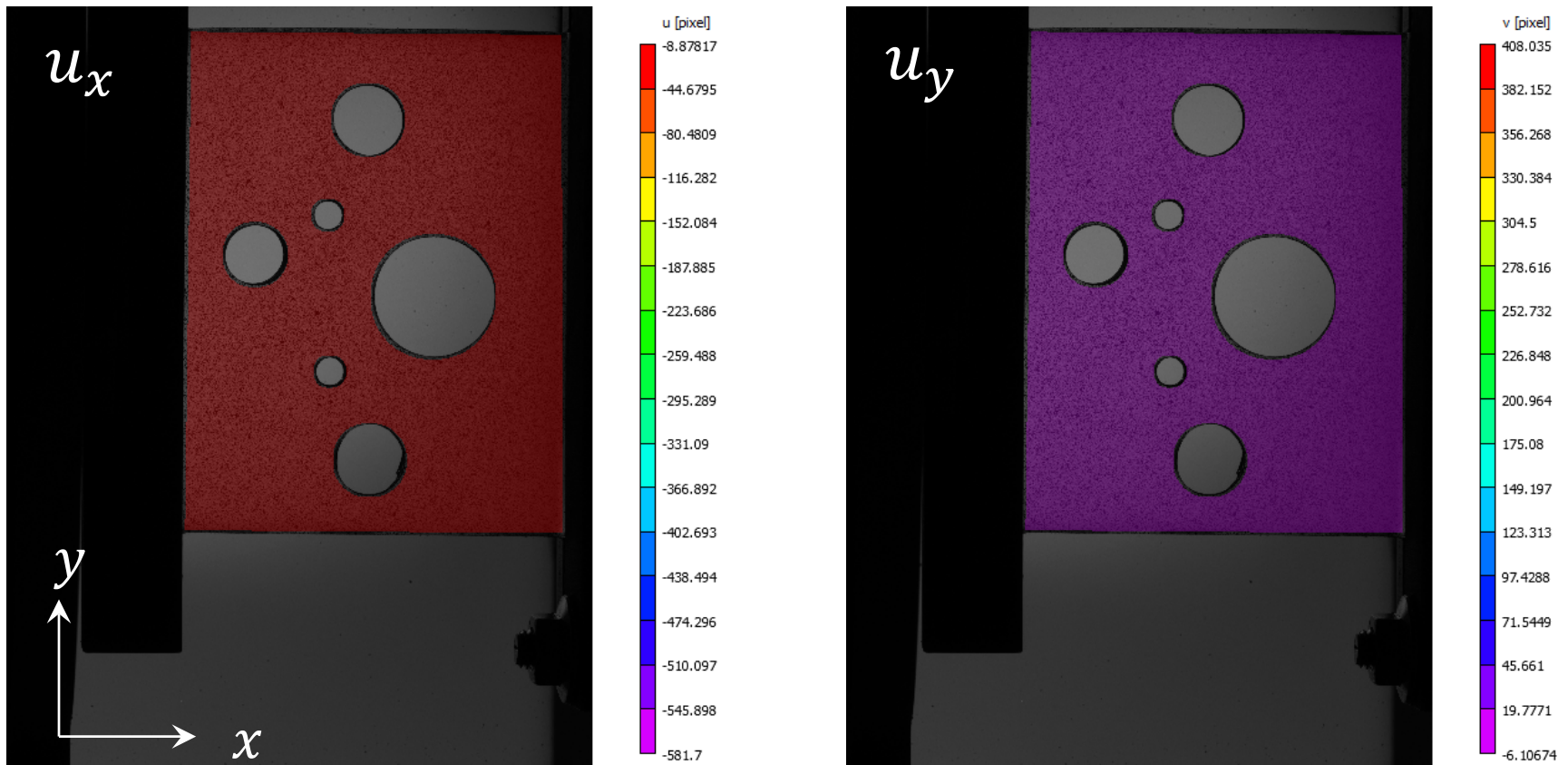
Hexapod in operation

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

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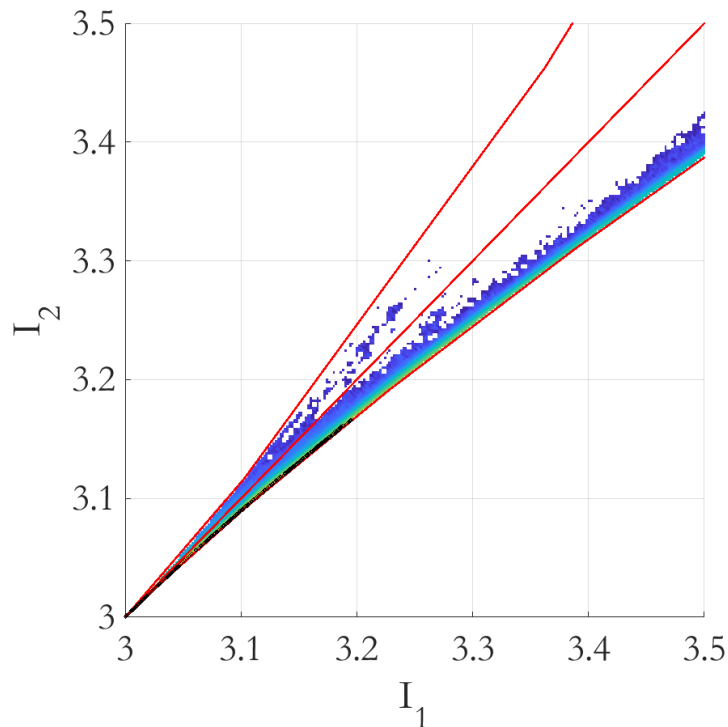
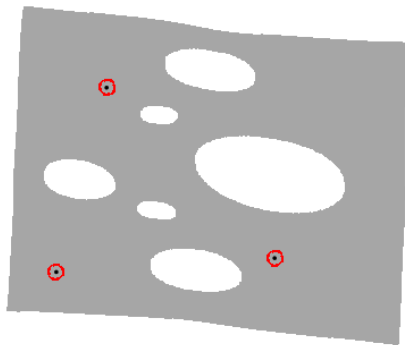
Displacement field (DIC)



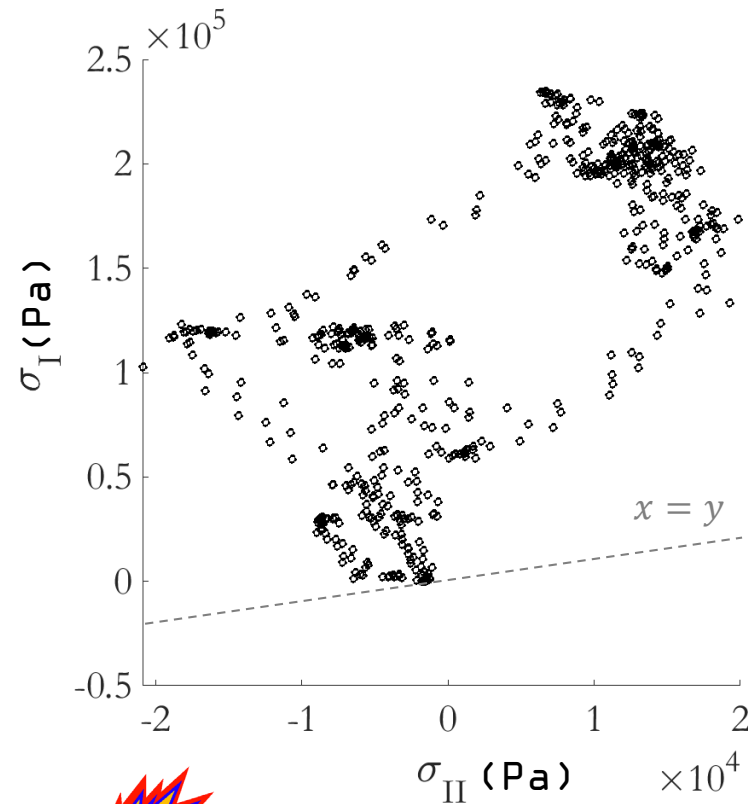
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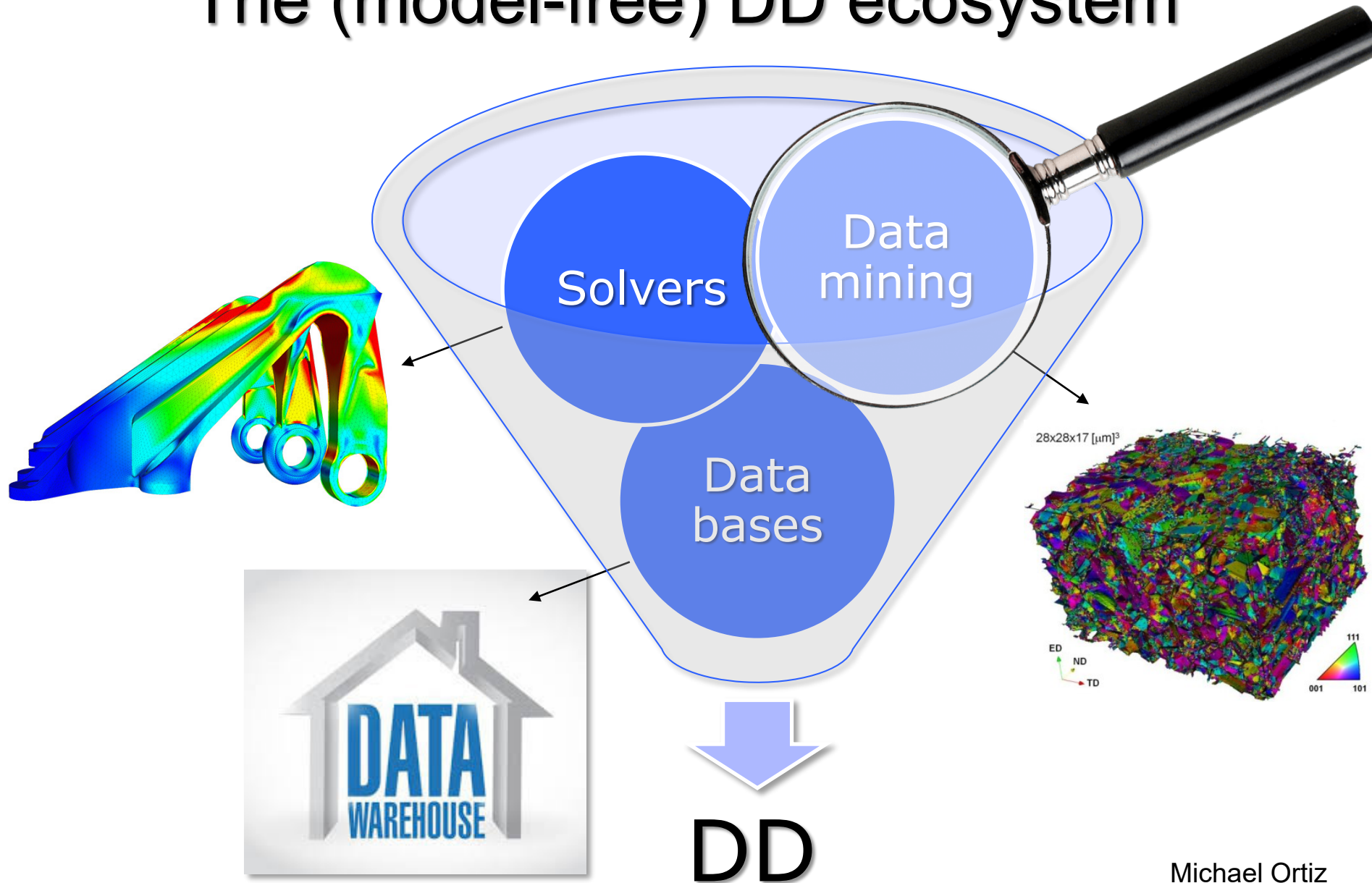


Strain data

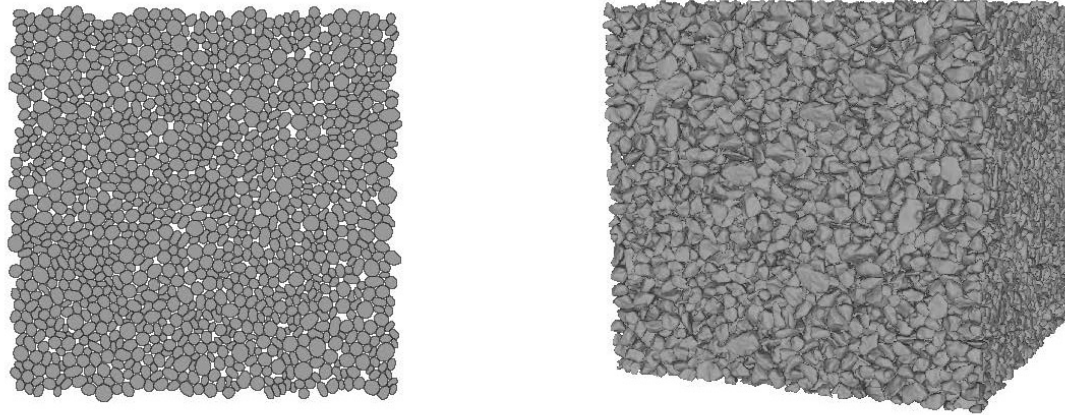


Stress data

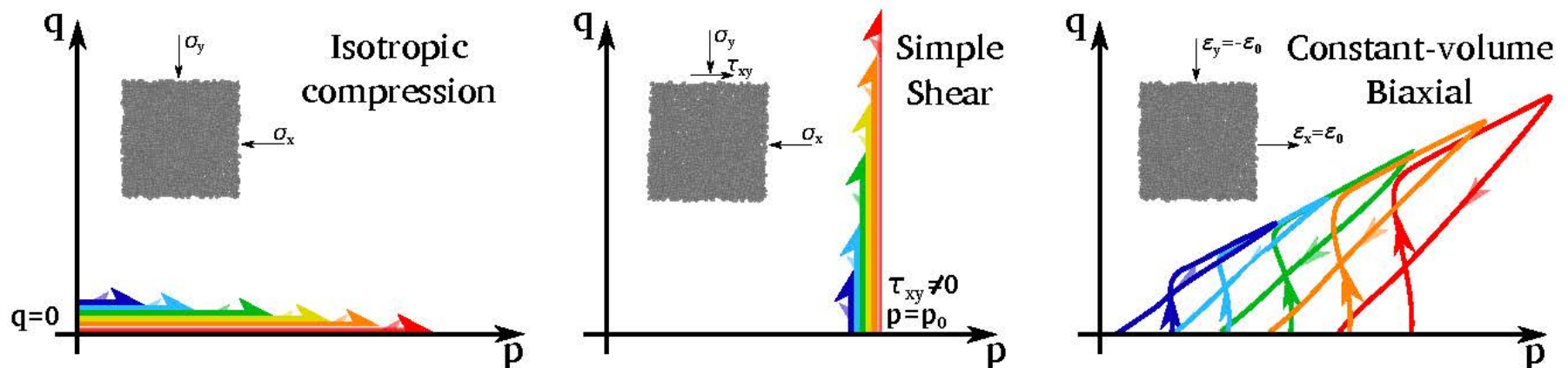
The (model-free) DD ecosystem



Multiscale data mining – Sand



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

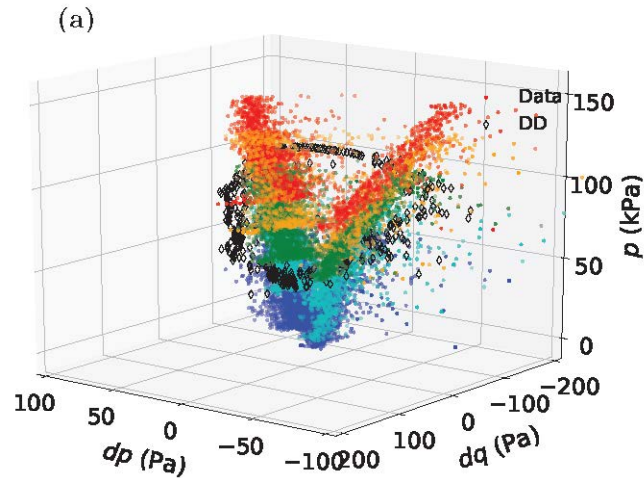
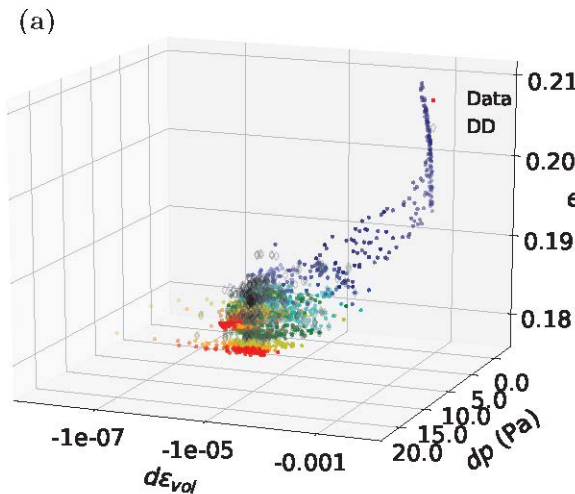


Stress paths for material point simulations and data mining

MICHAEL ORTIZ

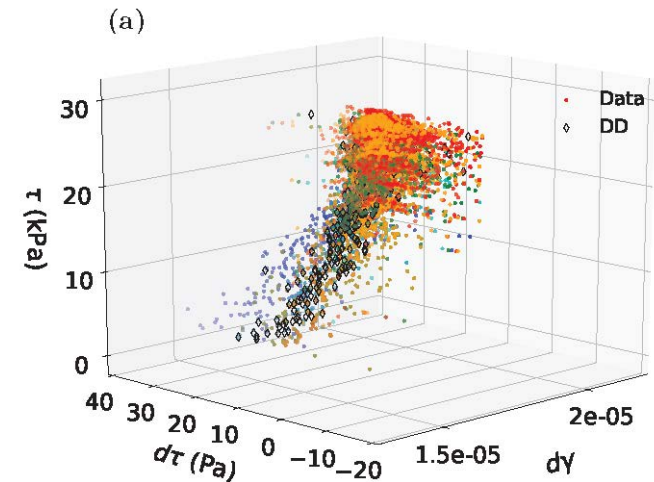
Multiscale data mining – Sand

Isotropic
compression



Biaxial
compression

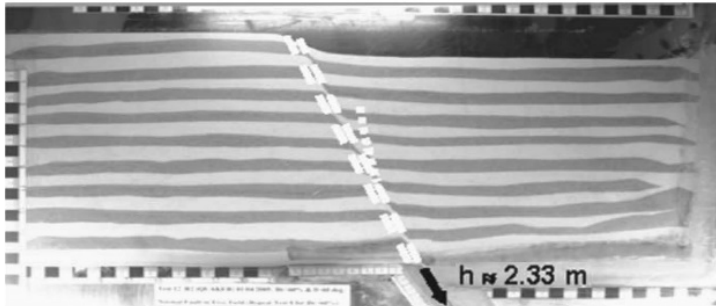
Simple
shear



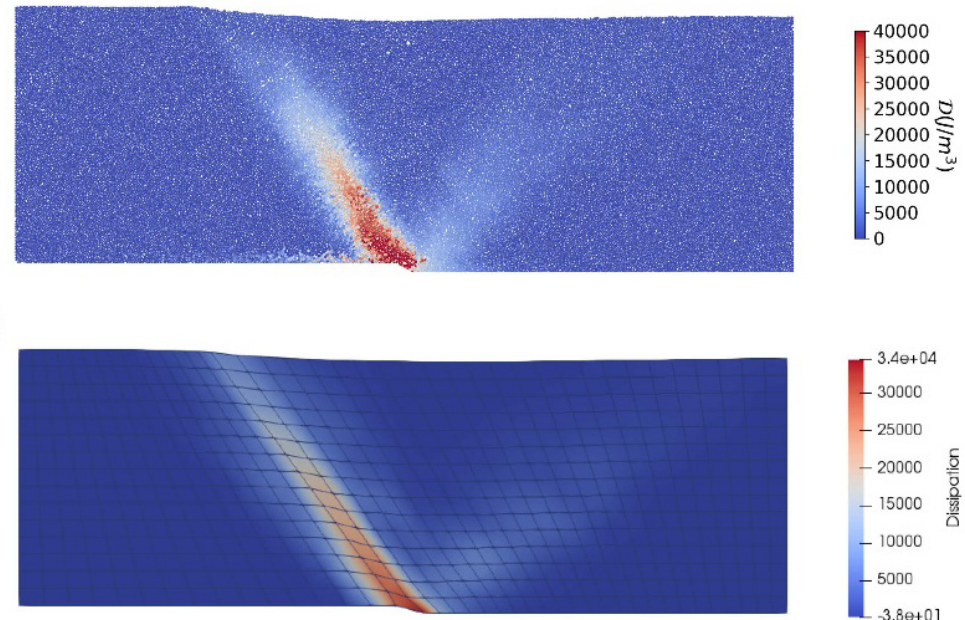
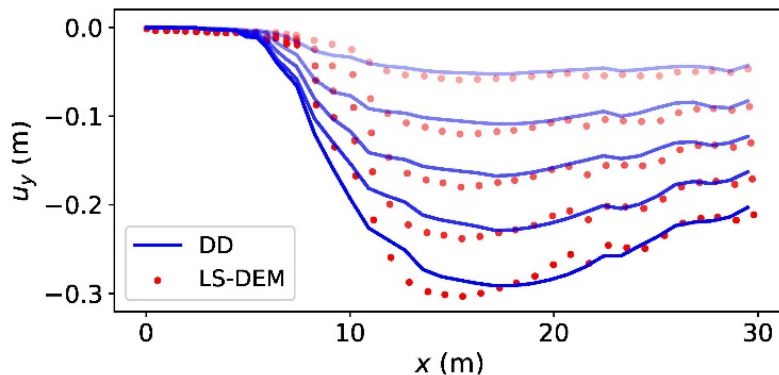
Data computed from
RVE LS-DEM calculations

Michael Ortiz

(Model-free) Data-Driven – Sand



Experimental fault rupture experiment
(Anastapoulos et al., 2007)

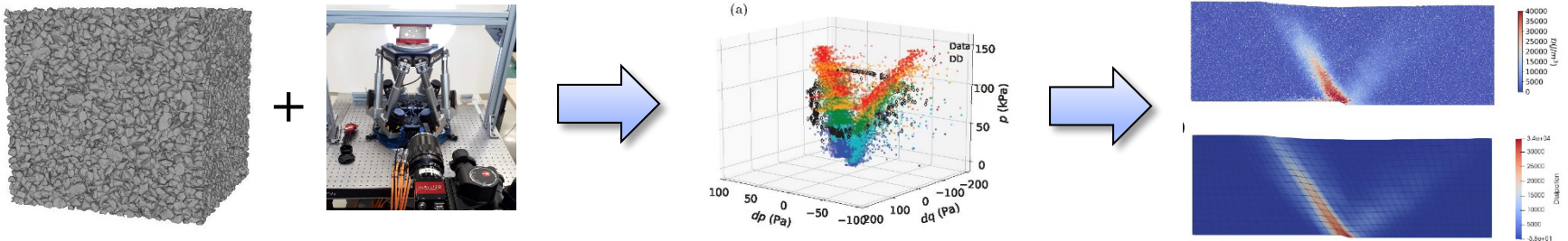


Top: LS-DEM simulation
Bottom: DD simulation

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

Data mining, generation, upscaling

- DDMI can extract data from *full-field experimental microscopy* (TEM, SEM, DIC, EBSD...)
- DDMI 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*

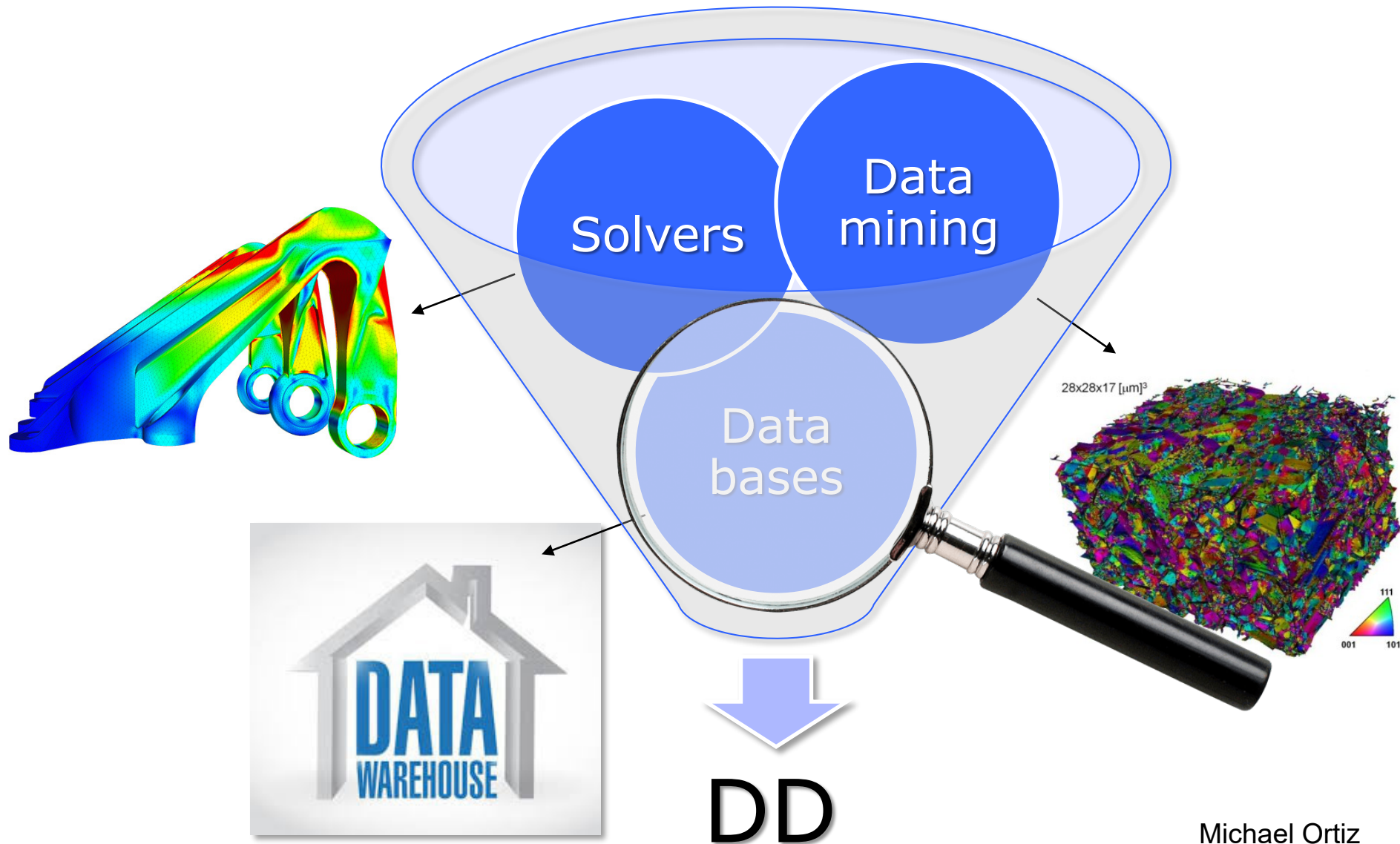


J. Rethore and A. Leygue, HAL Id: hal-01452494, Feb. 2017.

K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239. ARGYRIS 2020

Michael Ortiz

The (model-free) DD ecosystem



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 exceptional capacity for *organic growth*...
- *Publicly-editable material data repository! (Wikimat)*
 - *Fundamental data:*
 - *Stress-strain*
 - *Temperature-entropy*
 - *Gradients, rates*
 - *Tools/Scripts for interfacing with commercial FE packages*



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The Free Encyclopedia

Concluding remarks

- *The Model-Free Data-Driven 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!