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Model-Free Data-Driven Computing

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IUTAM SYMPOSIUM
ON DATA-DRIVEN MECHANICS
AND SURROGATE MODELING
Arts et Métiers Institute of Technology
Paris, October 28, 2022

Data-Driven computational mechanics

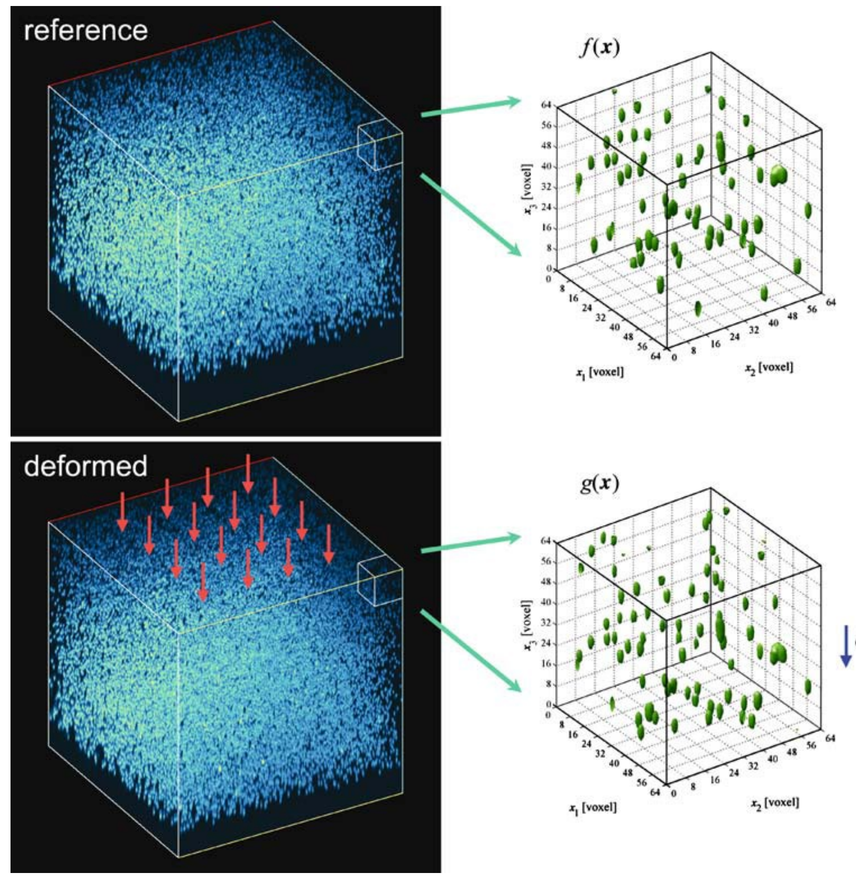
- Technological breakthroughs (internet, cheap storage, computer power, artificial intelligence…) are bringing about a *paradigm shift* in many fields (finance, marketing, political science…) regarding the *role of data*
- What's in it for *STEM*, *Scientific Computing*?
- Underlying premise: *Abundance of material data*

The new data-rich world of mechanics…

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

Digital Volume Correlation (DVC): Two confocal volume images of an agarose gel with randomly dispersed fluorescent particles before and after mechanical loading. The full displacement vector field is measured using 3D volume correlation methods.

C. Franck, S. Hong, S.A. Maskarinec, D.A. Tirrell and G. Ravichandran, *Experimental Mechanics* (2007) **47**:427–438.



The new data-rich world of mechanics…

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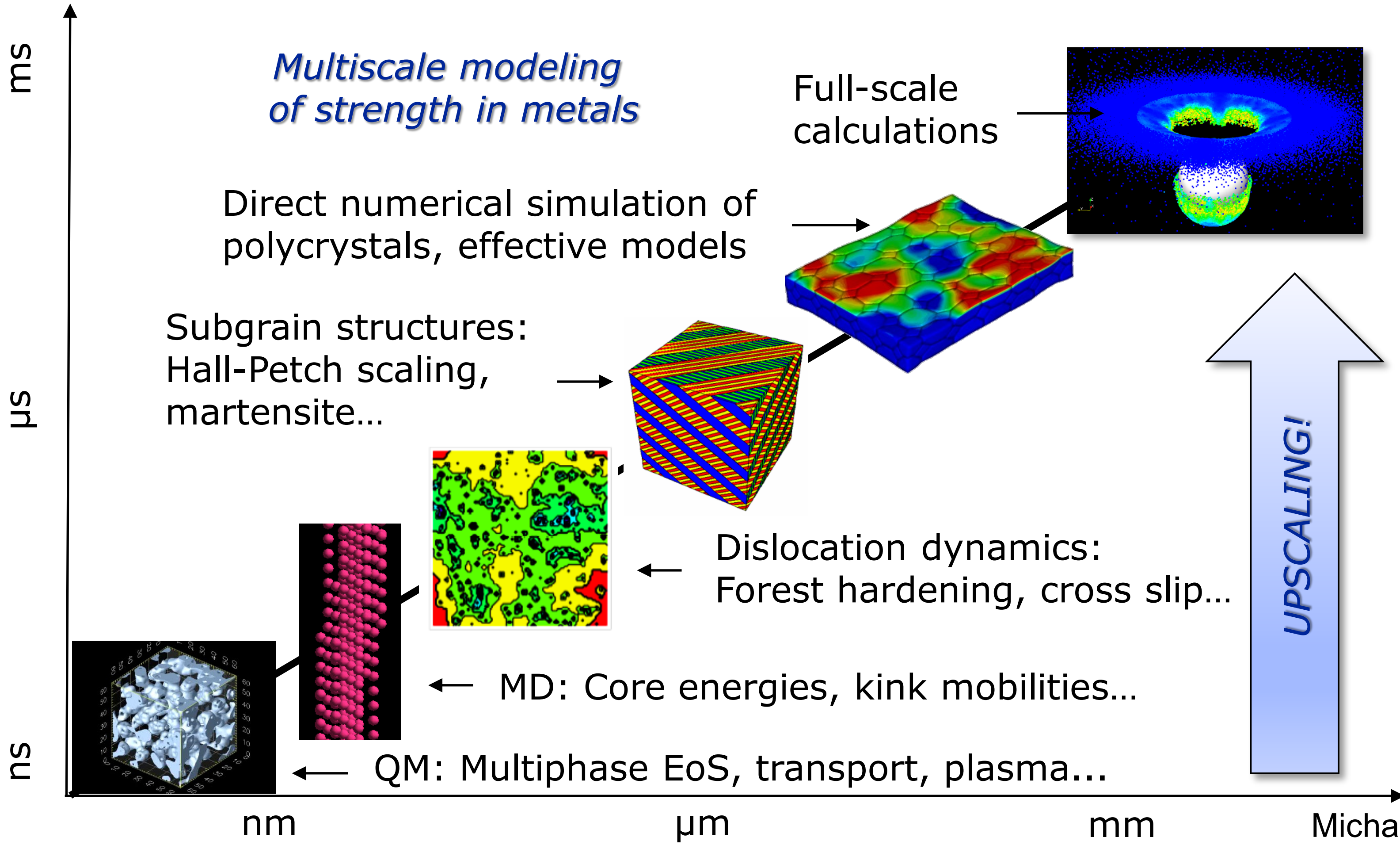

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The new data-rich world of EM…

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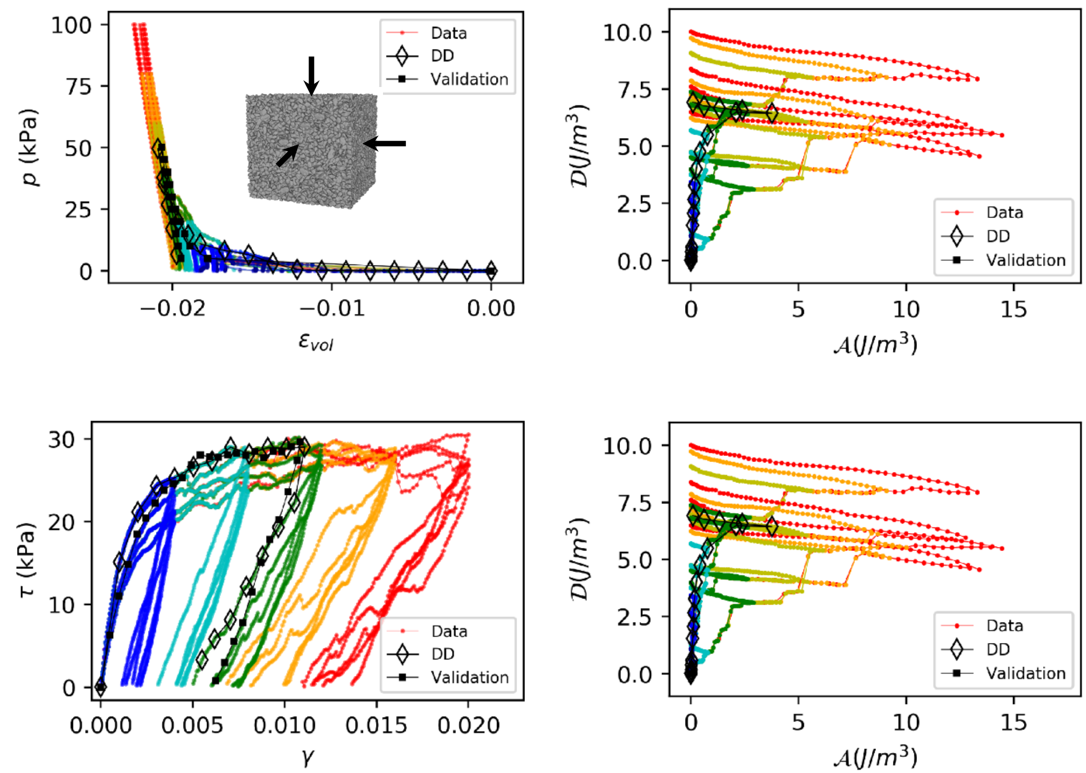
Granular matls. (dry sand): Level-Set Discrete Element Method (LS-DEM) simulation of granular material samples. 3D irregular *rigid particles* interact through *frictional contact*. Particle morphology described by level-set functions. Note calculation of *dissipation and free energy*.

Karapiperis, K., Harmon, J., And, E., Viggiani, G. & Andrade, J.E., *JMPS*, **144** (2020) 104103.

Karapiperis, K., Stainier, L., Ortiz, M. & Andrade, J.E., *JMPS*, **147** (2021) 104239.



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Data-Driven computational mechanics

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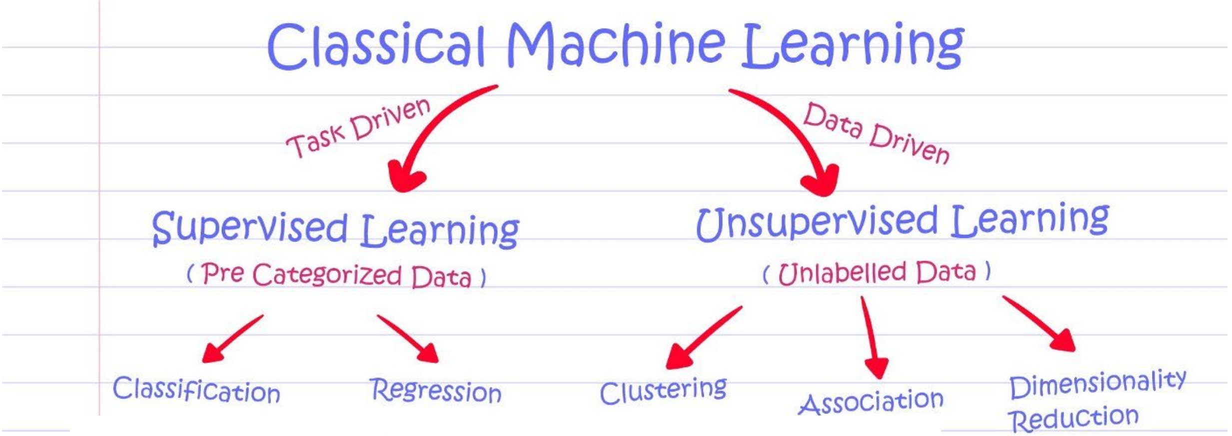
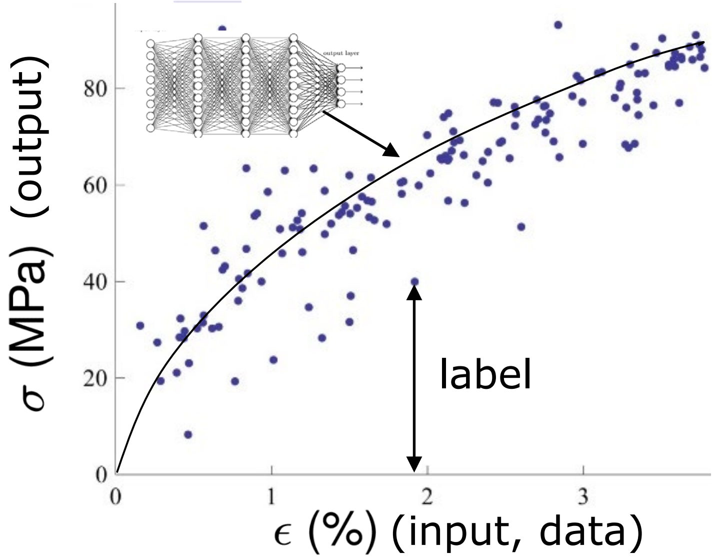
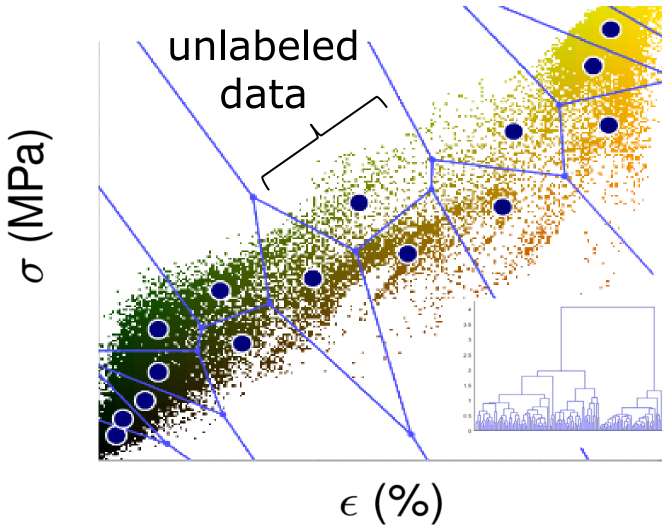
- What's in it for *STEM*, *Scientific Computing*?
- Underlying premise: *Abundance of material data*
- How does Data Science intersect with (*computational*) *mechanics?*

Supervised *vs*. unsupervised learning

- Challenge: Forge a *closer connection between data and predictions!*
- Fundamental dilemma: *To fit or not to fit* (that is the question)…







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The model-free Data-Driven paradigm

Definition (Data-Driven Problem)

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

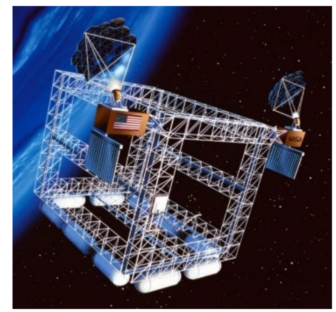
i) $D = \{\text{material data}\} \subset Z$,

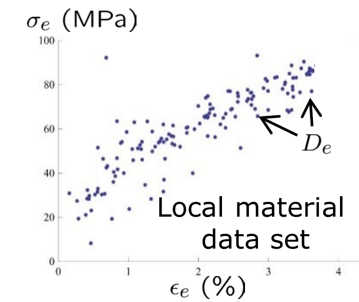
ii) $E = \{\text{field equations}\} \subset Z$,

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

Example (Structural mechanics)

$$Z = \{z := (\epsilon_e, \sigma_e)_{e=1}^m\}$$

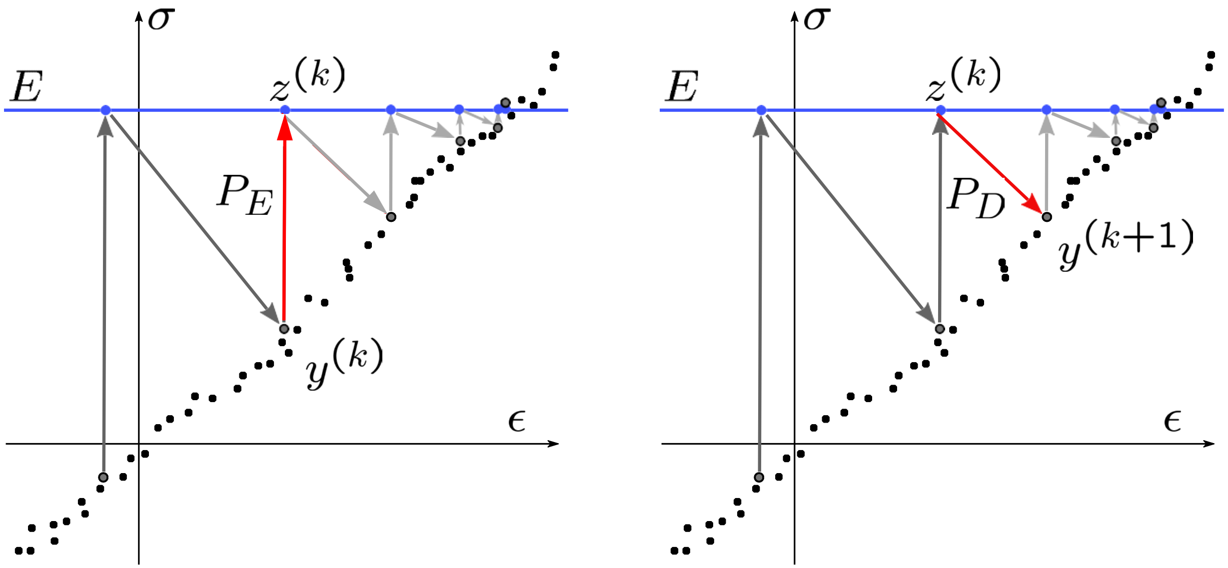




- Discussion:
  - Phase space Z determined by field equations
  - Fundamental data (model-independent) $=$ Points in phase space
  - No material modeling, no loss of information, no biasing of the data
  - DD problem generalizes and subsumes classical field-theoretical problems

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

Solvers: Fixed-point iteration



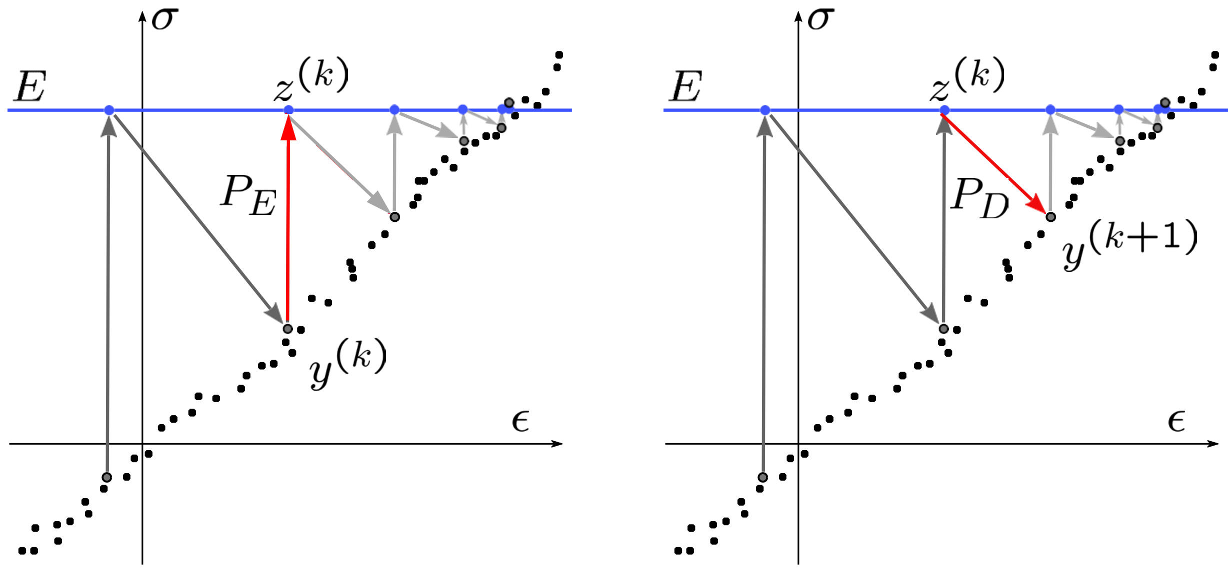
- Projection to E (inner minimization at fixed (ϵ', σ')): i) Enforce compatibility directly by writing $\epsilon = Bu$; ii) Enforce equilibrium through a Lagrange multiplier v,

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

- 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).

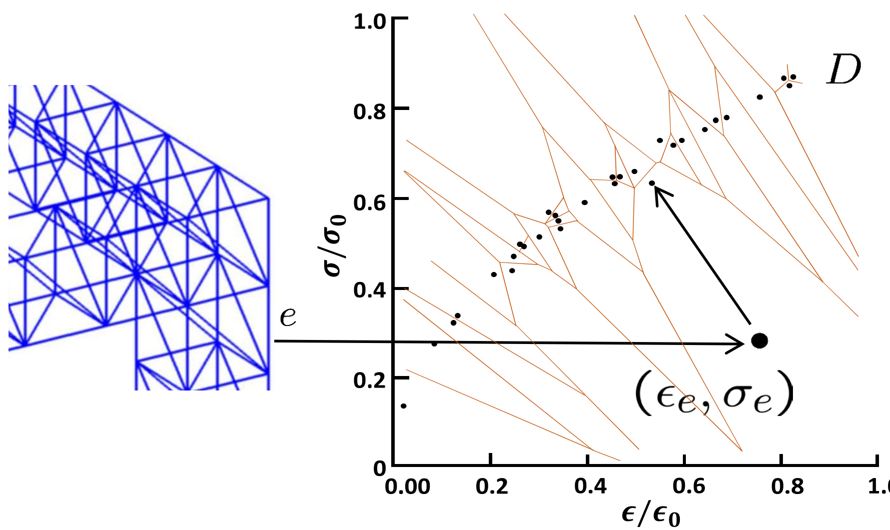
- DD leads to (material-independent) standardization of solvers.

Solvers: Fixed-point iteration

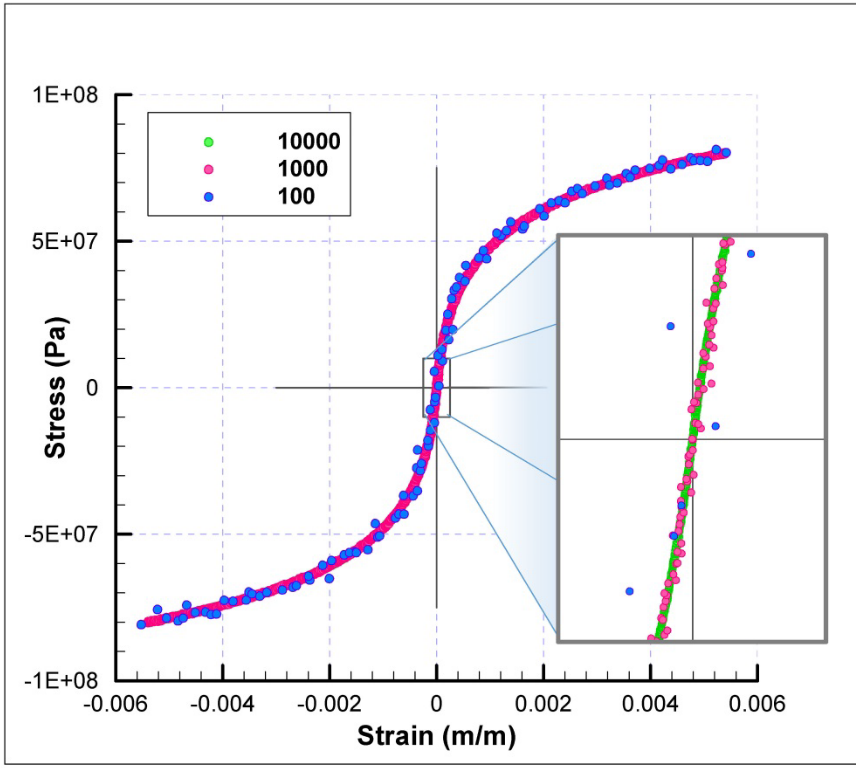


- Outer minimization: Projection onto (closest point in the) material data set D
- Fast searching algorithm
- Requires data structures
- 'Learning' structure of D
- Set-oriented (lossless) ML!

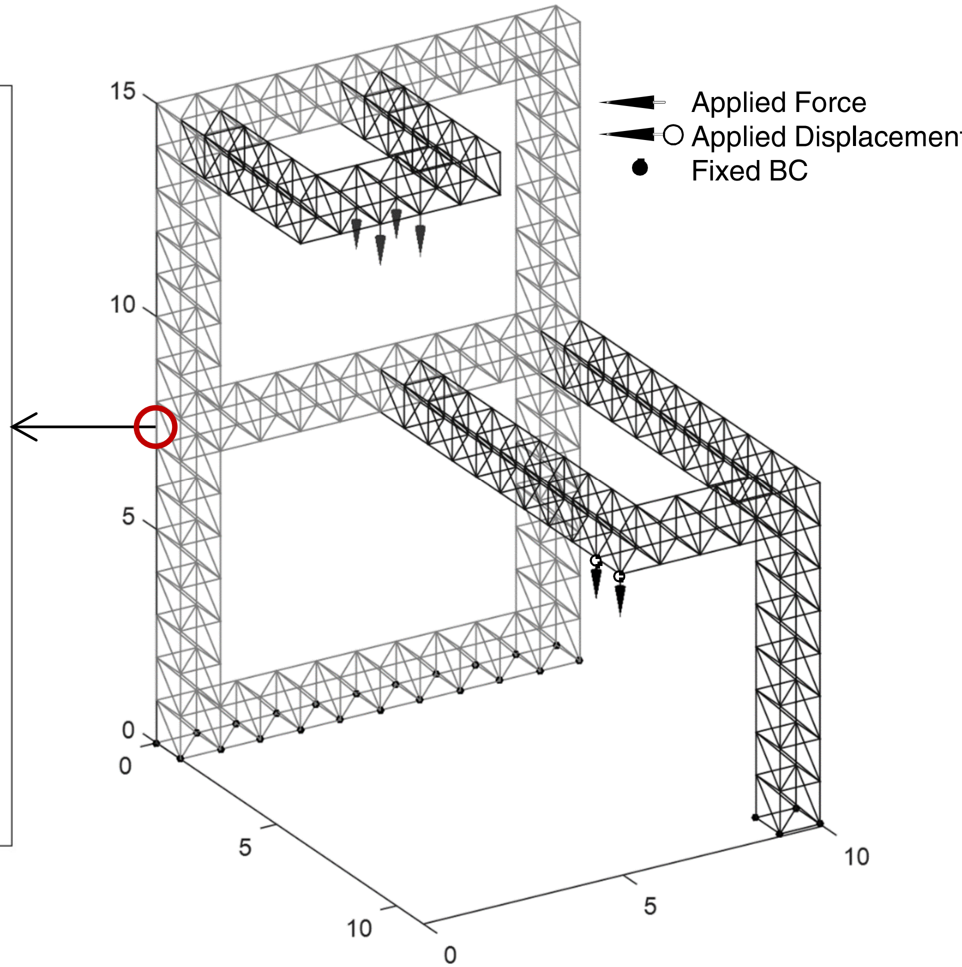
Unsupervised machine learning!



Convergence with respect to the data



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



3D truss structure

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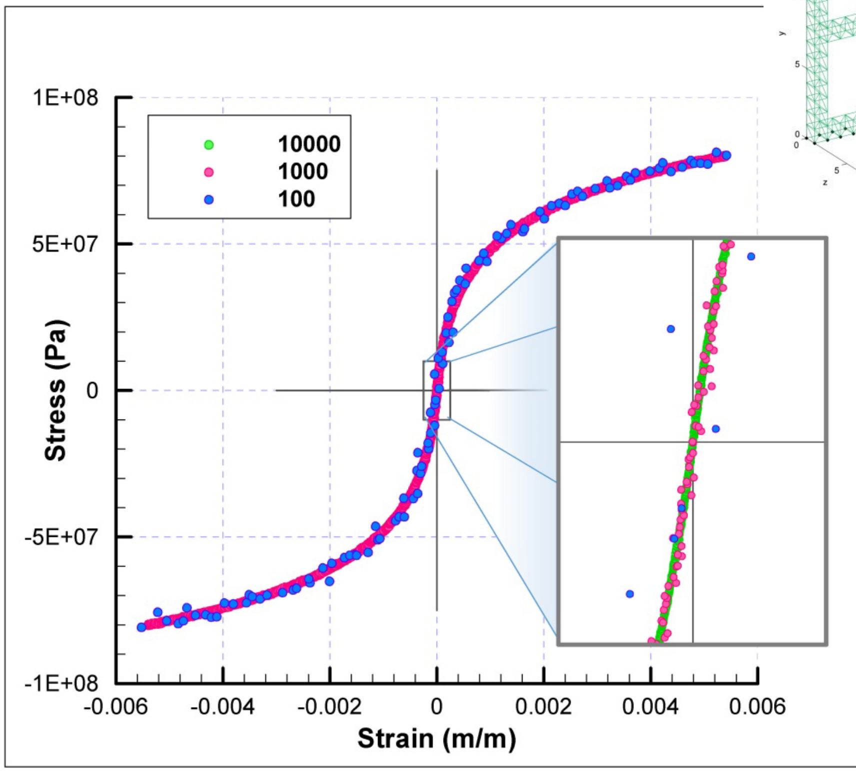
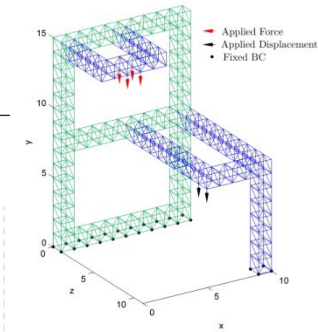
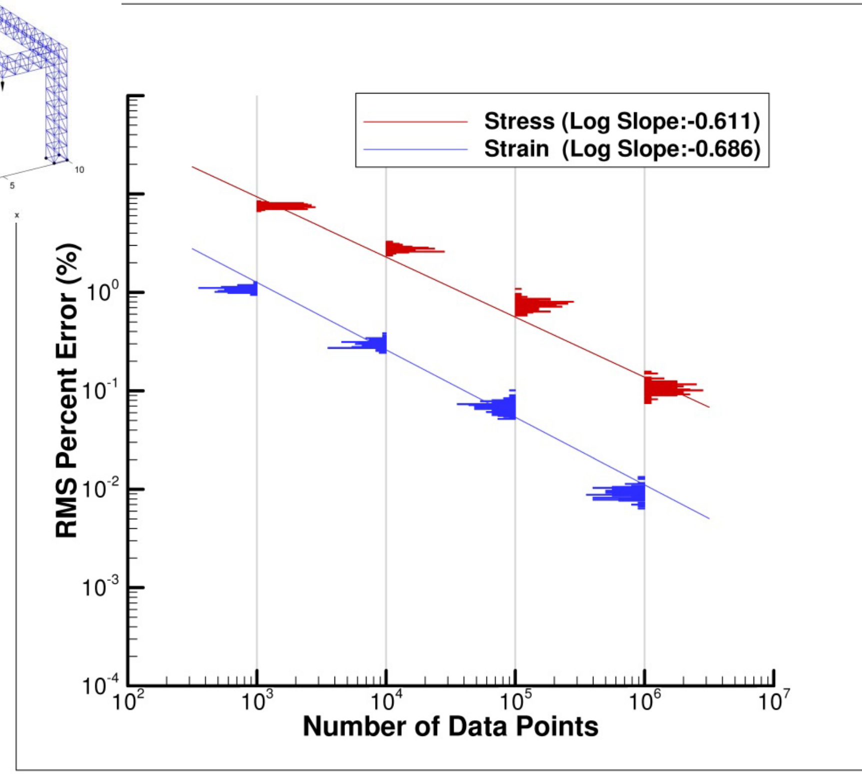
T. Kirchdoerfer and M. Ortiz, *CMAME*, **304** (2016) 81-101.

Convergence with respect to the data





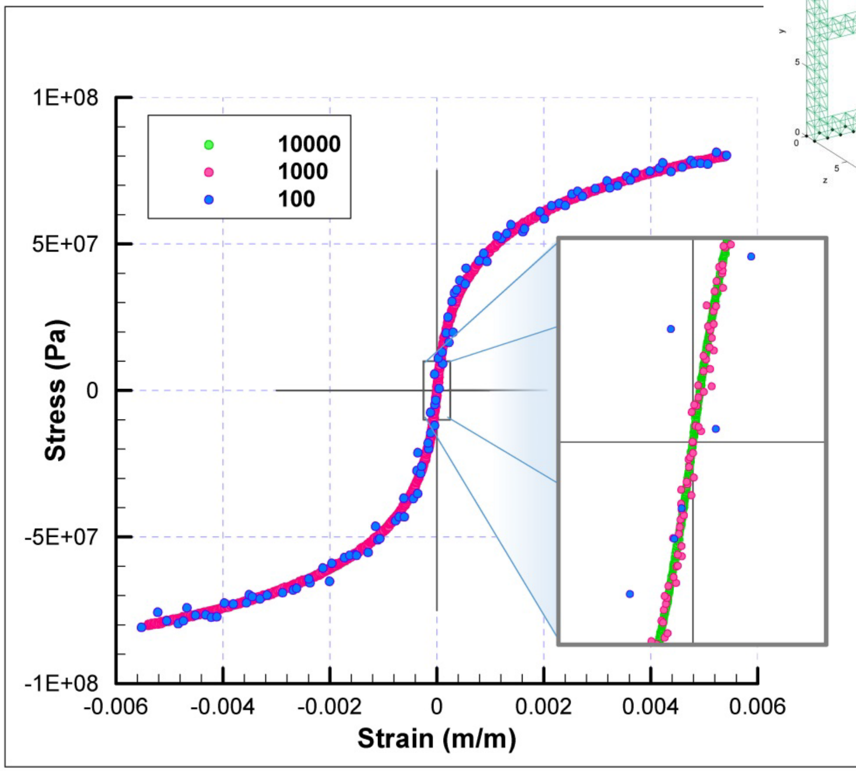


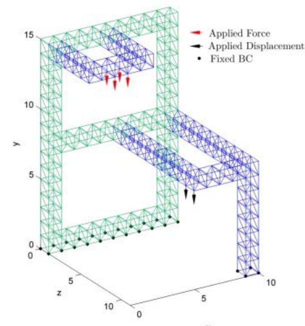
Sequence of
uniformly converging data sets
(increasing number of points, decreasing scatter)

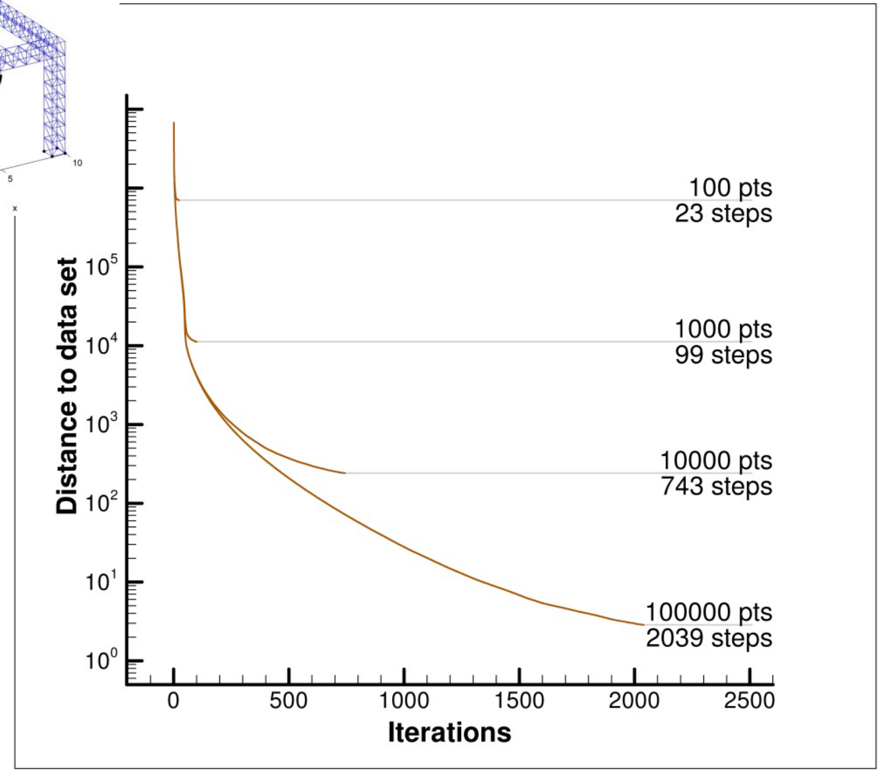
Convergence with respect to material data set towards solution of limiting problem (nonlinear elasticity)

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

Solvers: Fixed-point iteration





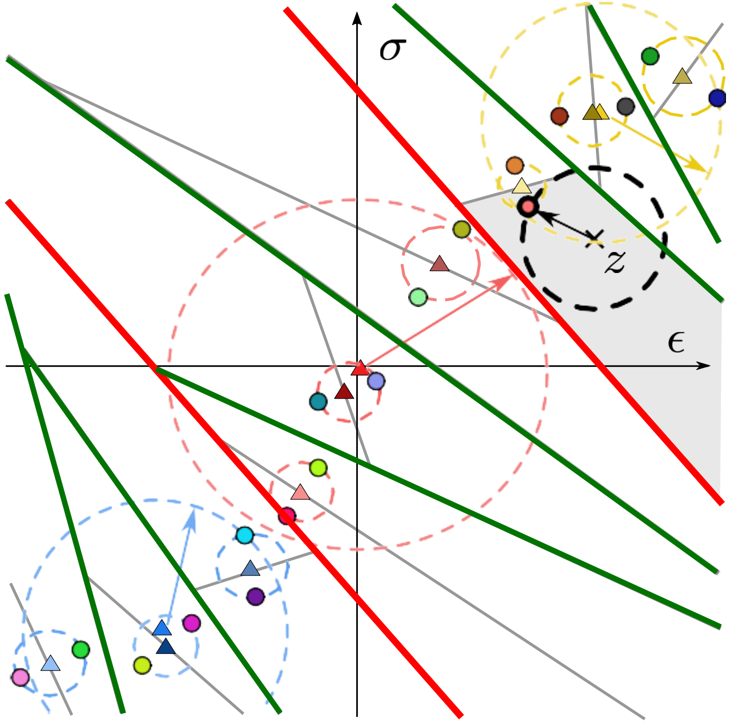


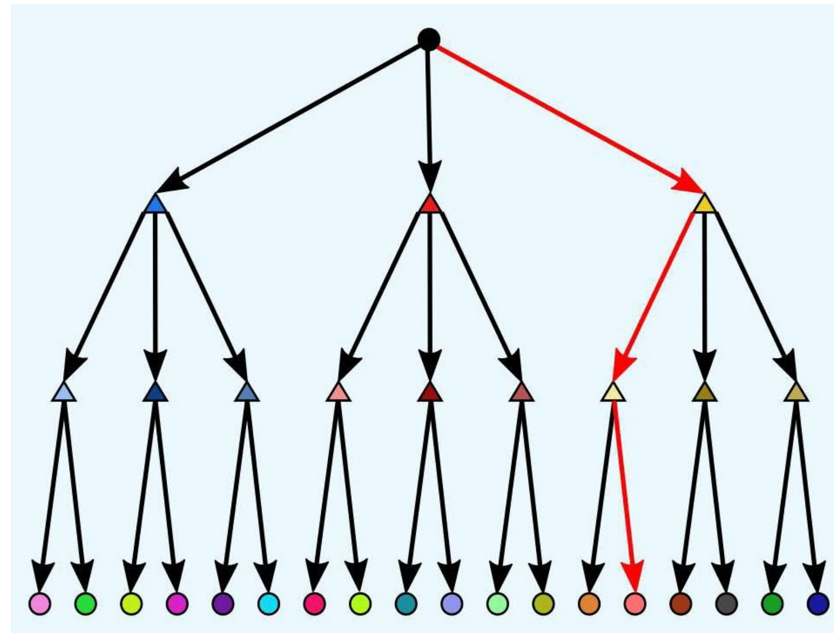
Sequence of *uniformly converging data sets* (increasing number of points, decreasing scatter)

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.

Navigating big material data sets (fast)

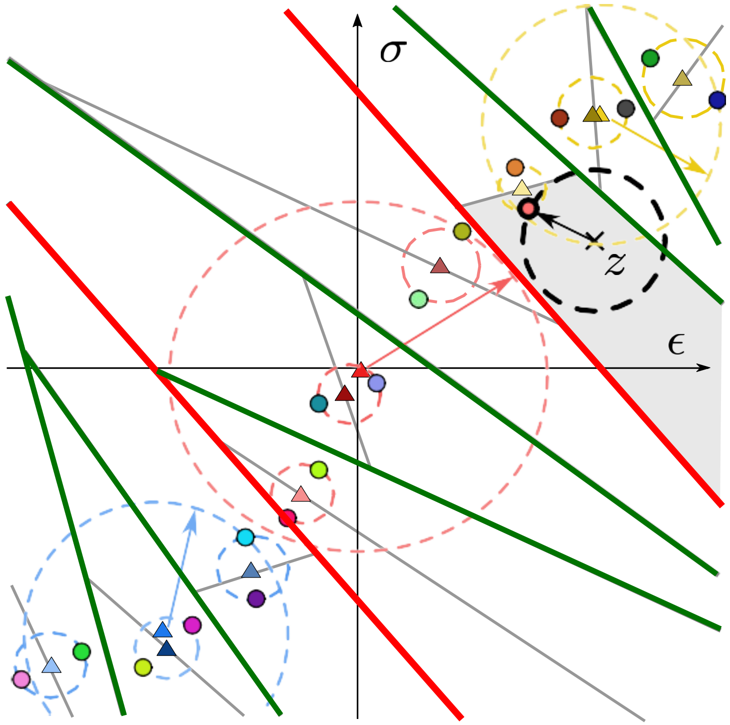


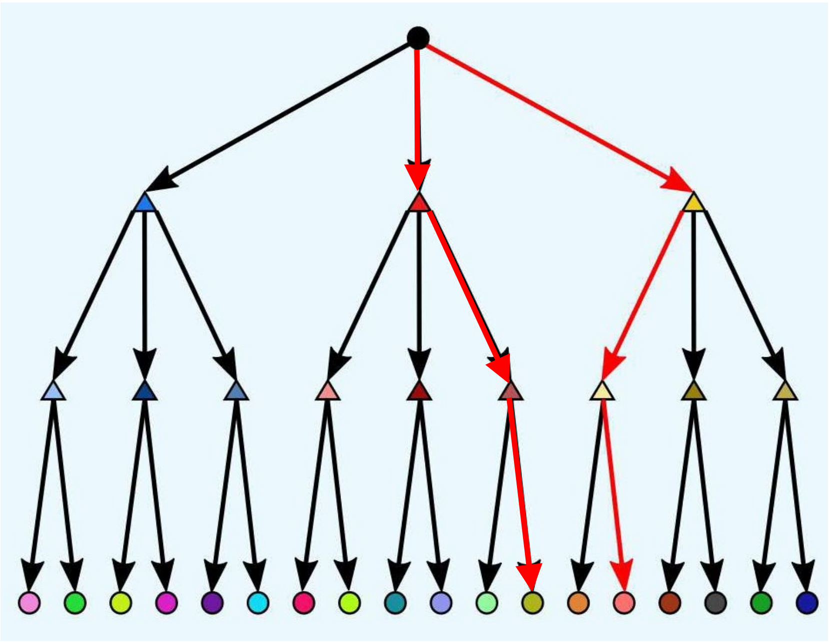


Nearest-neighbor tree traversal

- Material data sets can be very large, cannot do naïve linear lookups!
- *k-means clustering* aims to partition *n* points into *k* clusters in which each point belongs to the cluster with the *nearest mean* (centroid).
- *k*-means clustering can be applied *recursively* to define a *k-means tree*
- *Queries* can be executed by *traversing* the *k*-means tree along *nearest neighbors* or approximate nearest neighbors (*backtracking*)

Navigating big material data sets (fast)





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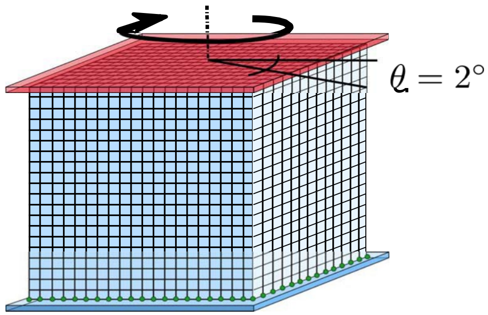
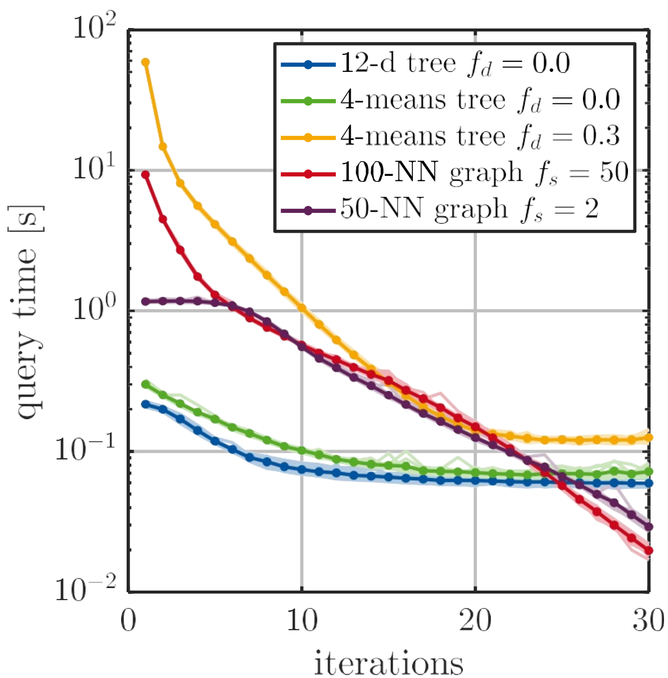
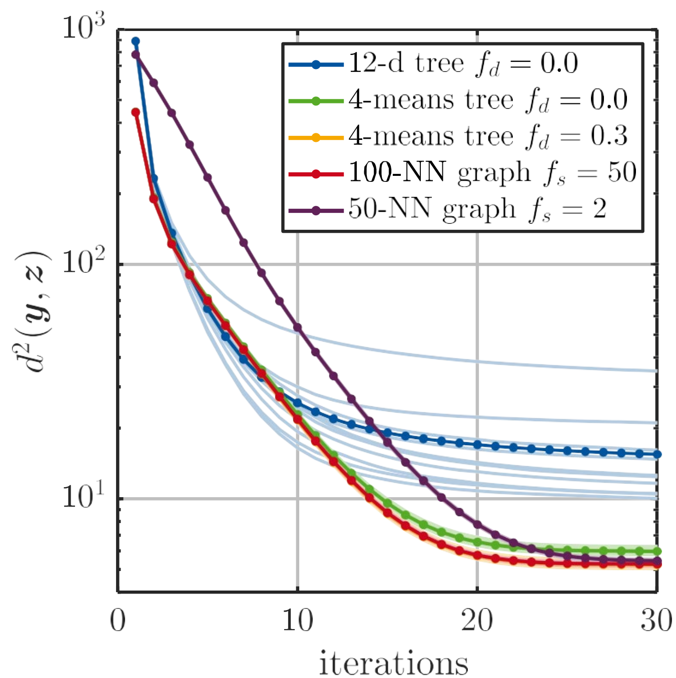
Benchmark problem: Torsion of cube



- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- *100 million material data points*





Comparison of search algorithms:
kd-tree, k-means and kNN graph algorithms

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

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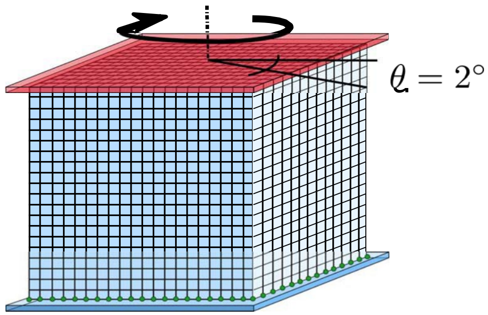
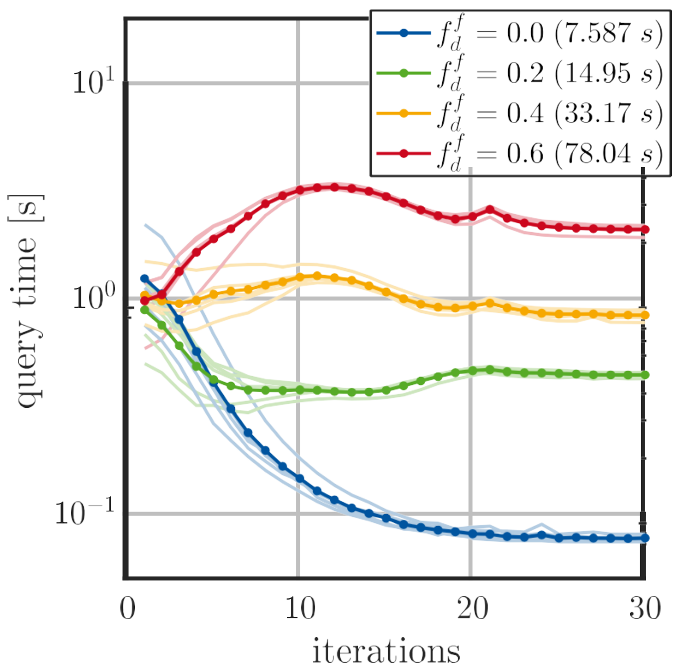
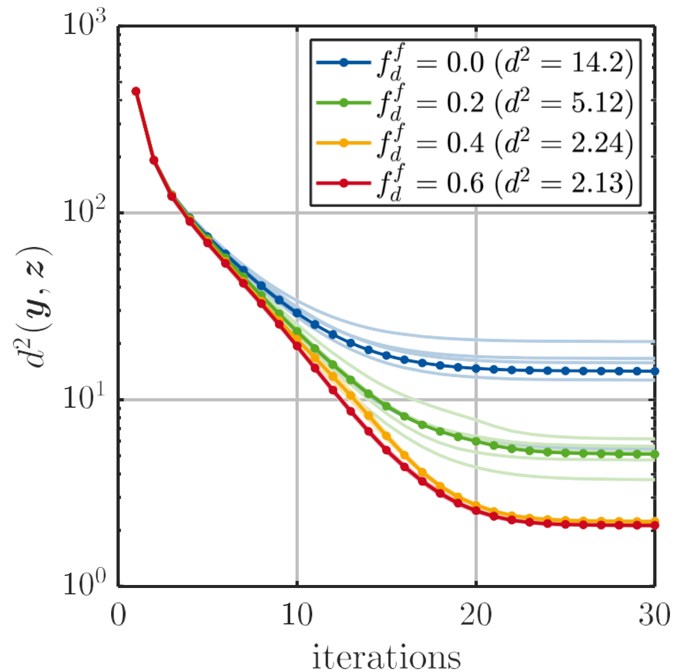
Benchmark problem: Torsion of cube



- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- *1 billion material data points*





k-means with different degrees of backtracking.
search accuracy set to increase with DD iteration

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

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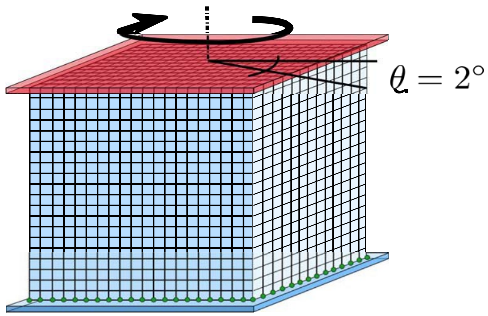
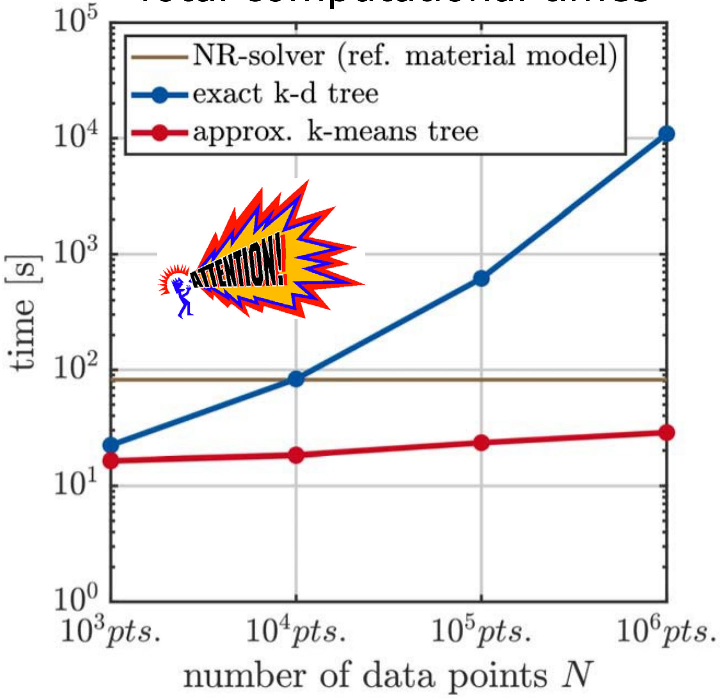


- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- 10^3-10^6 material data points

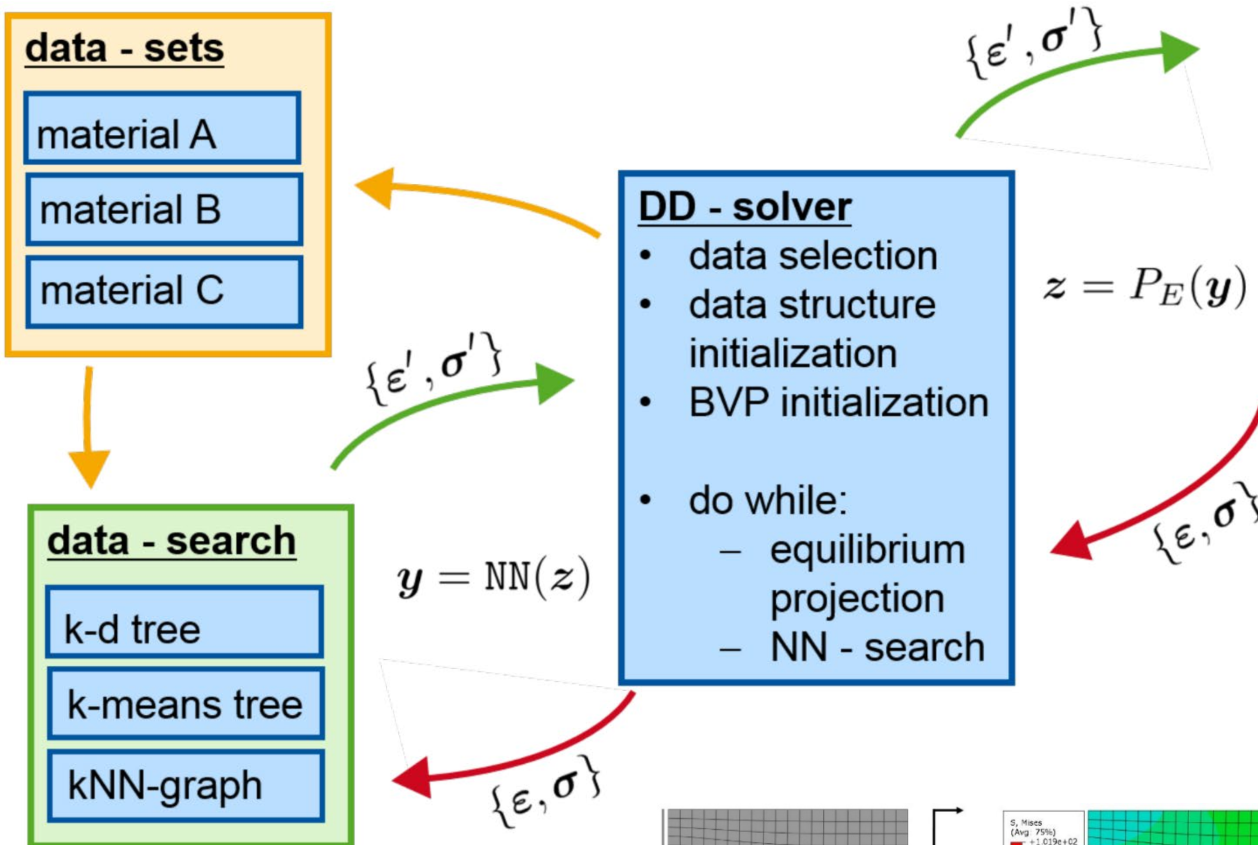
Total computational times



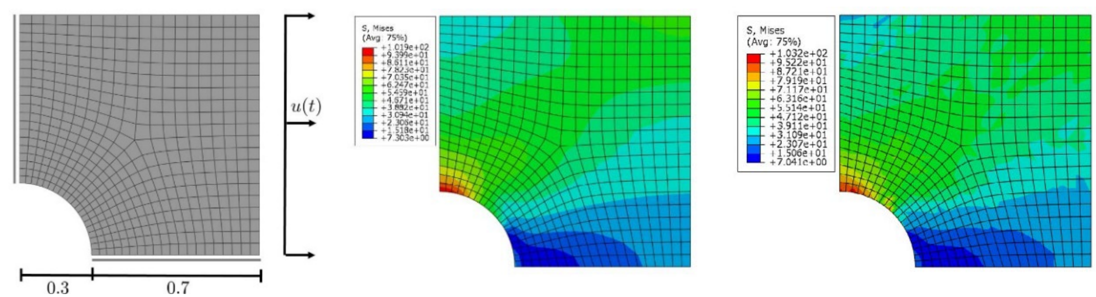
- *DD solver beats Newton-Raphson!*
- DD requires the solution of linear FE problems only (projection P_E to the admissible set E)
- System matrix can be factorized once and for all at the outset
- Load increments require back-substitution operations only
- Newton-Raphson requires repeated assembly and factorization of stiffness matrix
- *DD factorization advantage offsets data-searching overhead!*

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

Implementation into commercial software



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



Model-free Data-Driven solvers can be easily implemented using commercial software and scripts

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

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- What's in it for *STEM*, *Scientific Computing*?
- Underlying premise: *Abundance of material data*
- How does Data Science intersect with (*computational*) *mechanics?*
- Where do the data come from? *Data acquisition!*

RVE data acquisition – Adaptive Learning

0 Initial database

$\mathcal{D}^{(0)}$

DDCM simulation

1 Mechanical response

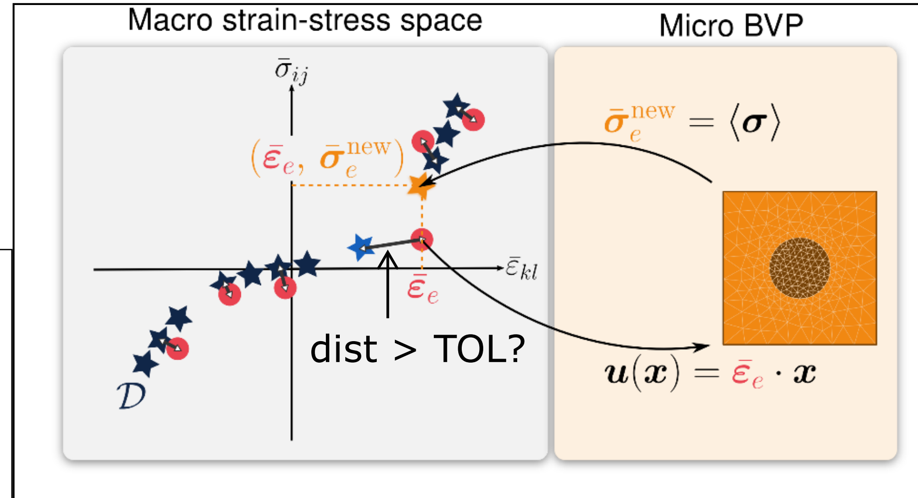
$\{(\bar{\boldsymbol{\varepsilon}}_e, \bar{\boldsymbol{\sigma}}_e)\}_{e=1}^{M}$

select isolated points

2 New database

$$\mathcal{D}^{(j+1)} = \mathcal{D}^{(j)} \bigcup_{e \in I} (\bar{\boldsymbol{\varepsilon}}_e, \bar{\boldsymbol{\sigma}}_e^{\text{new}})$$

$j \leftarrow j + 1$

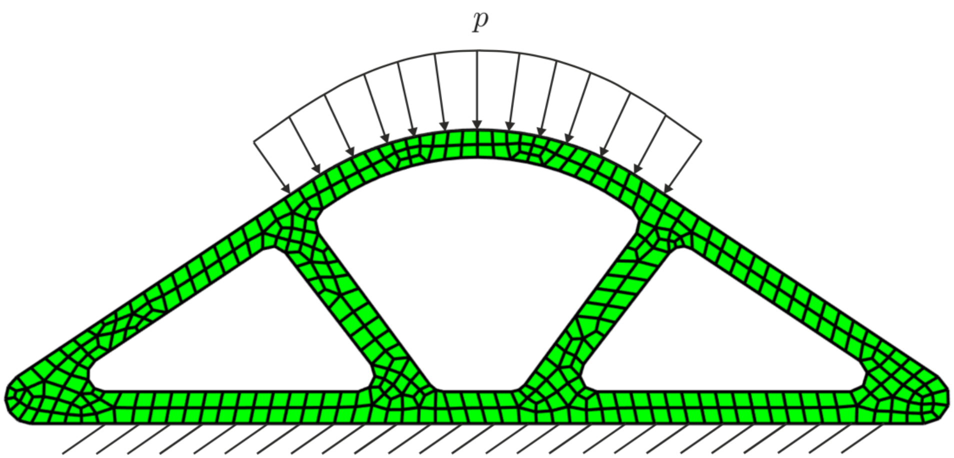


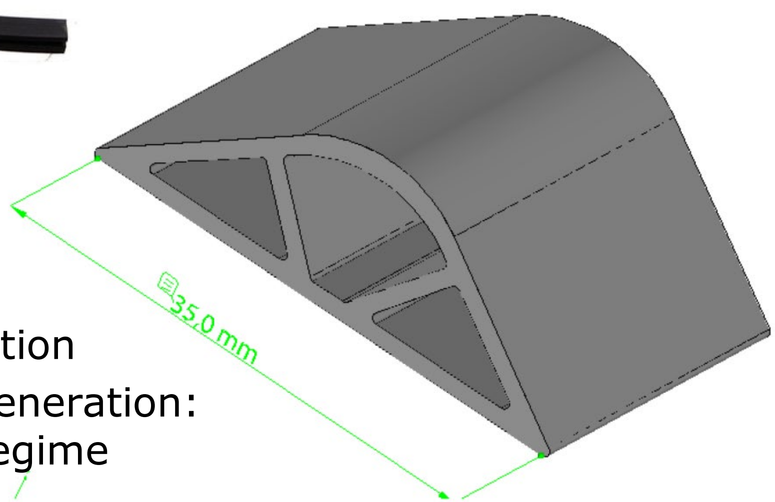
- *Generate new data from RVE when local state dist(z_e ,D) > TOL!*
- Areas of *poor coverage* in the material data set are detected by DD solver, filled in *on-the-fly* as needed
- Material data set adapted to solution (*goal-oriented adaptive learning*)
- *Concurrent multiscale analysis* with *material data re-use* (unlike FE^2)

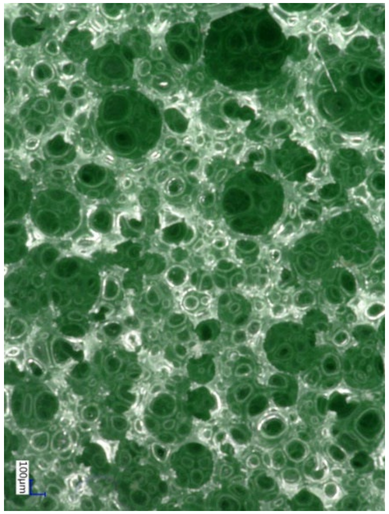
A. Platzer, Ph.D. Dissertation, l'École Centrale de Nantes, 2020.

Adaptive Learning – Elasticity

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







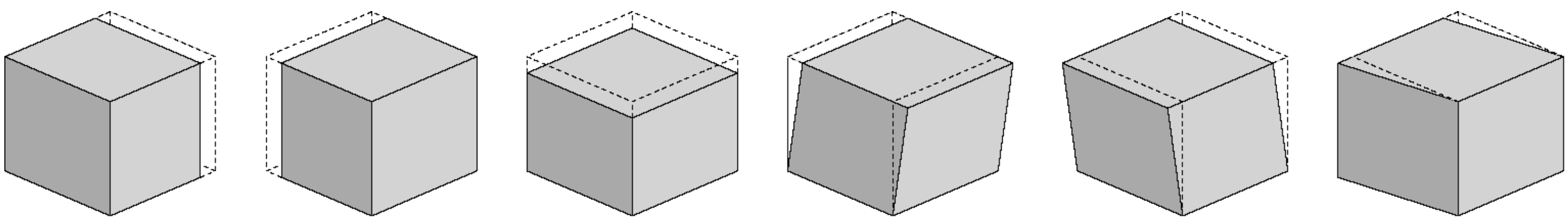
microstructure

- Open-cell foam
- Isotropic material
- 3D analysis/simulation
- Microscopic data generation: linear/non-linear regime

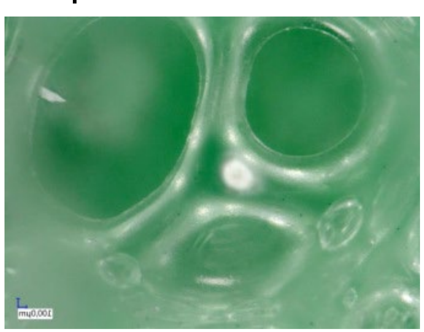
T.F. Korzeniowski and K. Weinberg, *CMAME*, **400** (2022) 115487.

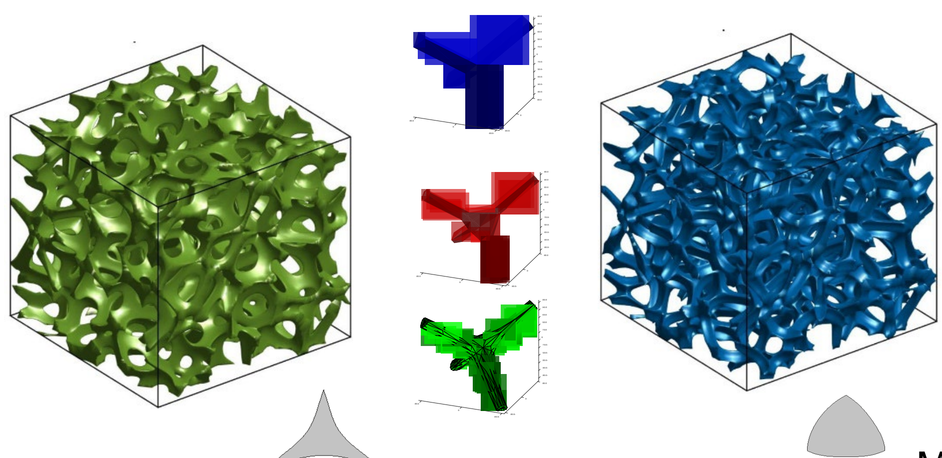
Adaptive Learning – Elasticity

- Data sets: $\mathcal{D} = \{(\epsilon, \sigma)\}$, or $\mathcal{D} = \{(F, P)\}$, or $\mathcal{D} = \{(C, S)\}$.
  1. apply deformation
  2. compute RVE and determine average stress
  3. collect data pairs
- *Can generate macroscopic data on demand as required!*
- Six different loading cases (unit loads)



- 3D open-cell foam RVEs:





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

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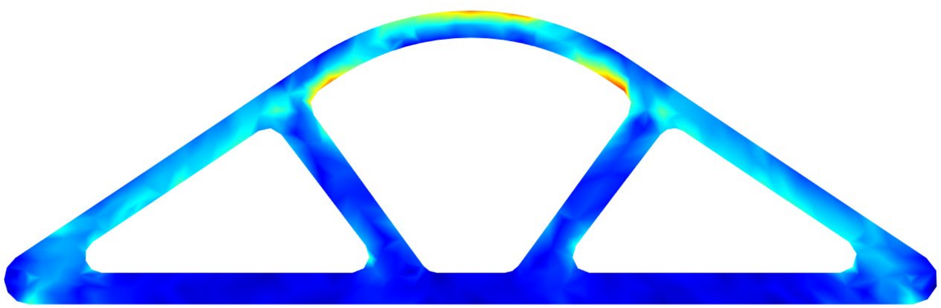
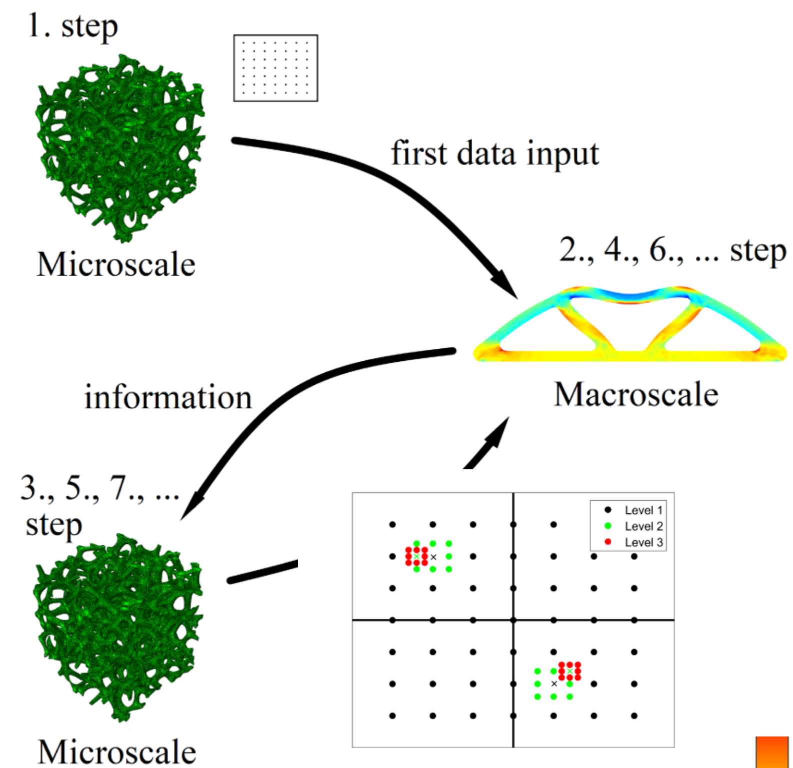
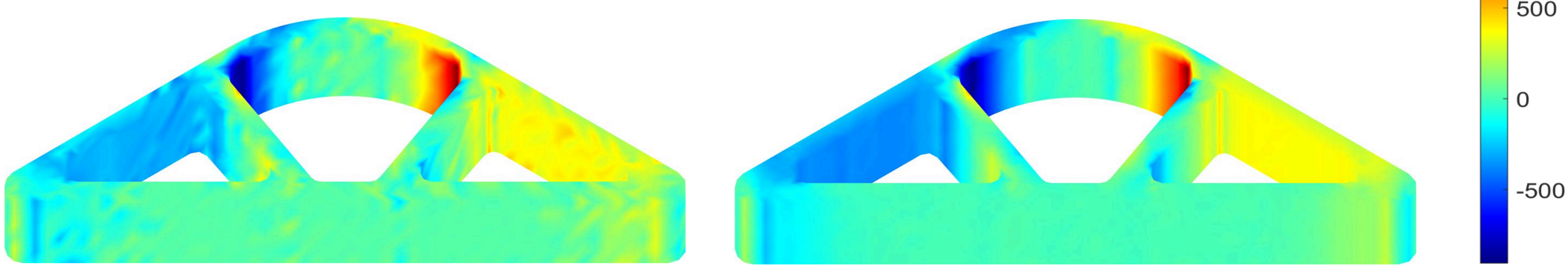
Adaptive Learning – Elasticity

- 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



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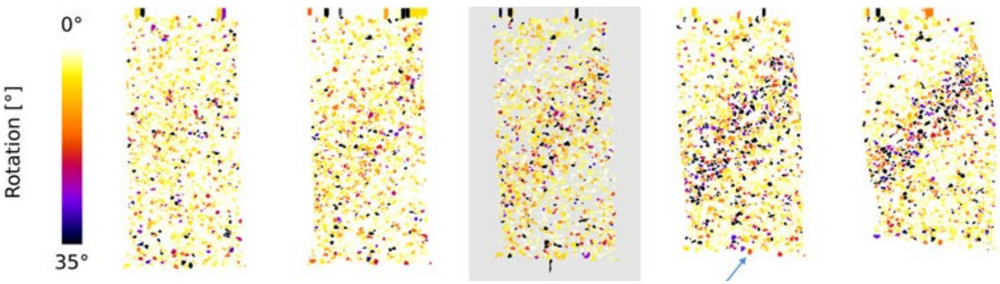
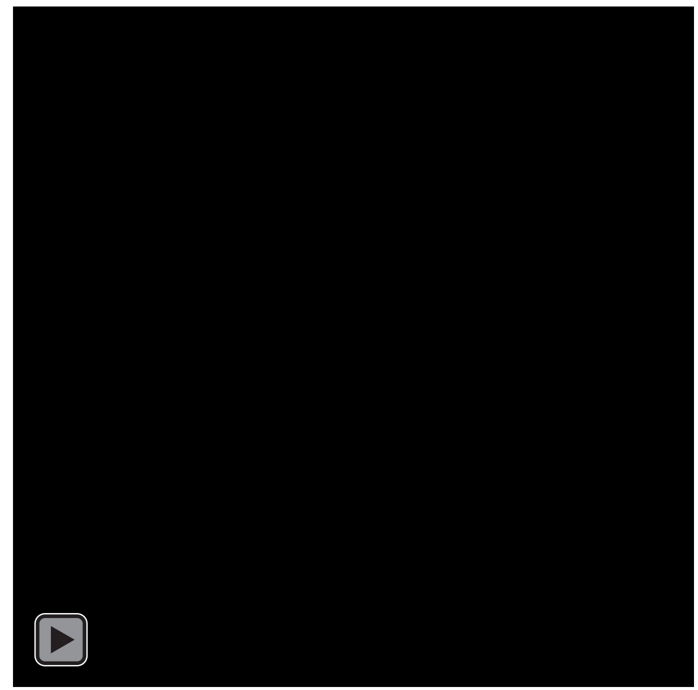
Adaptive Learning – Plasticity



RVE
generation



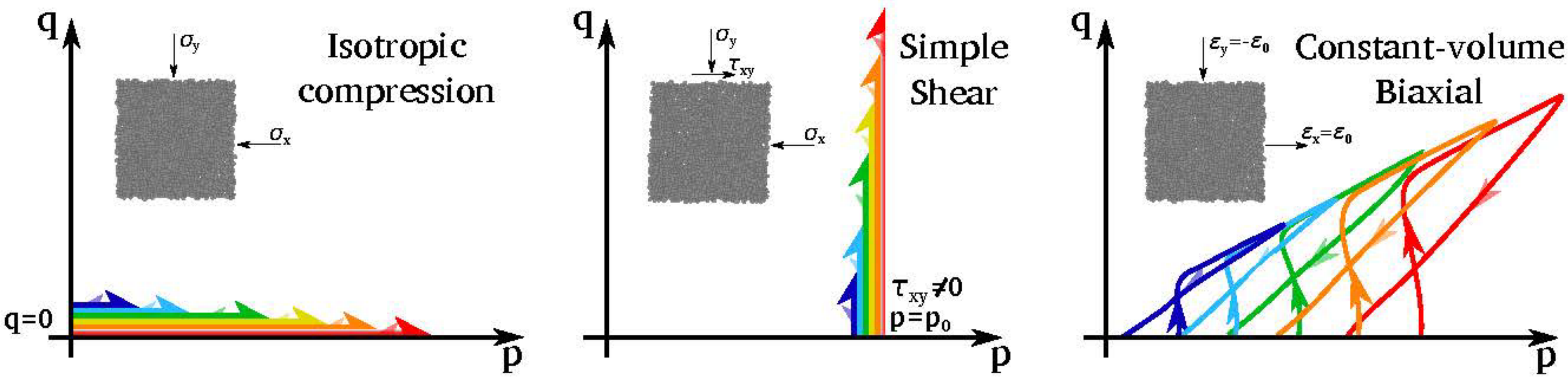
Triaxial compression test,
angular Hostun sand,
100 kPa confining pressure,
11 mm x 22 mm samples
in latex membrane.
Particles tracked by XRMT.
Failure occurs by
shear banding

Andò, E., *et al*.,
Acta Geotech., **7** (2012) 1-13.

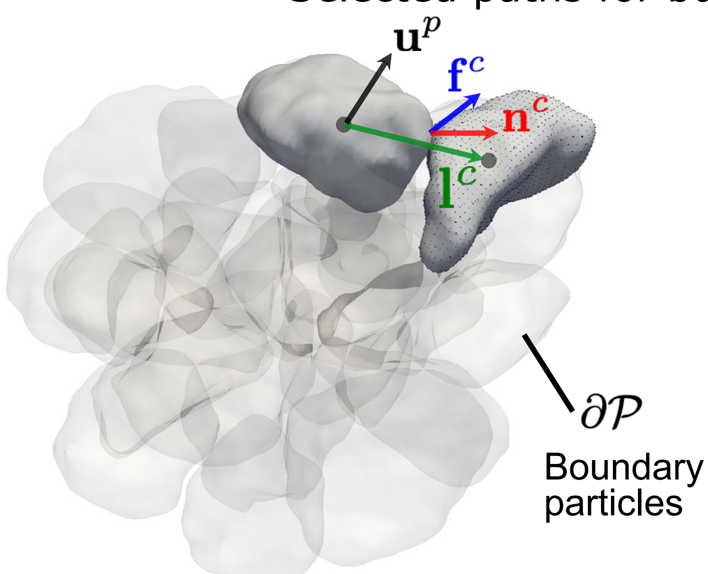
Kawamoto, R., Andò, E., Viggiani, G., Andrade,
J.E., *JMPS*, **91** (2016) 1-13.

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

Adaptive Learning – Plasticity



Selected paths for building the material data repository



$$
\left\{
\begin{aligned}
\boldsymbol{\varepsilon} &= \frac{1}{2V}\operatorname{sym}\Big(\sum_{p\in\partial\mathcal{P}} \mathbf{u}^p \otimes \mathbf{n}^p\Big) \\
\boldsymbol{\sigma} &= \frac{1}{V}\operatorname{sym}\Big(\sum_{c\in\mathcal{C}} \mathbf{f}^c \otimes \mathbf{l}^c\Big) \\
\mathcal{A} &= \sum_c \mathcal{A}^c = \frac{1}{2V}\sum_c \Big(\frac{\|\mathbf{f}^c_\mathbf{n}\|^2}{k_n} + \frac{\|\mathbf{f}^c_\mathbf{t}\|^2}{k_t}\Big) \\
d\mathcal{D} &= \sum_c d\mathcal{D}^c = \frac{1}{V}\sum_c \mathbf{f}^c_t \cdot d\mathbf{u}^{c,slip}
\end{aligned}
\right.
$$

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

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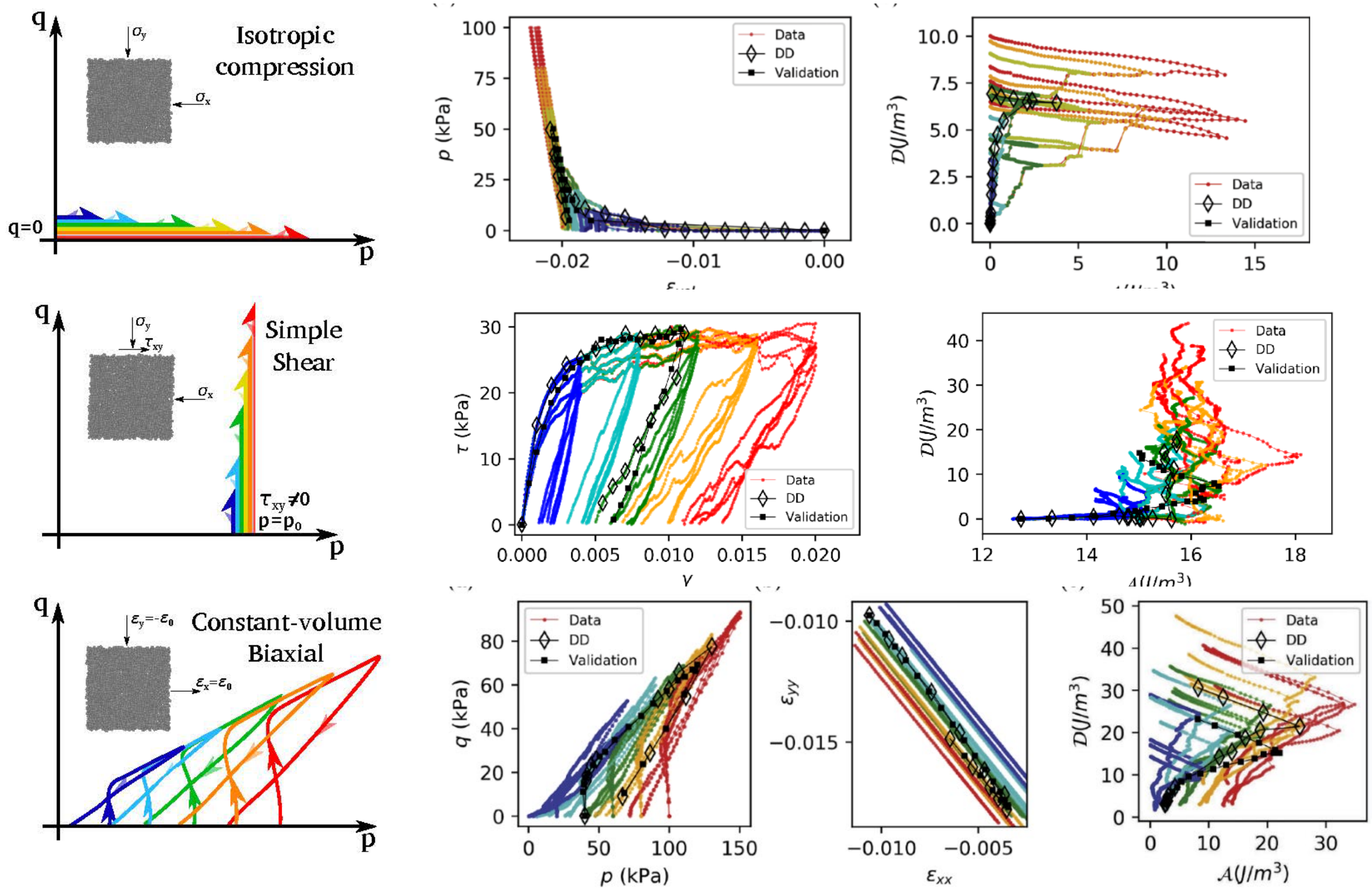
Adaptive Learning – Plasticity



path

stress-strain

energy-dissipation

Compilation of path data for Hatsun angular sand computed from RVEs using LS-DEM

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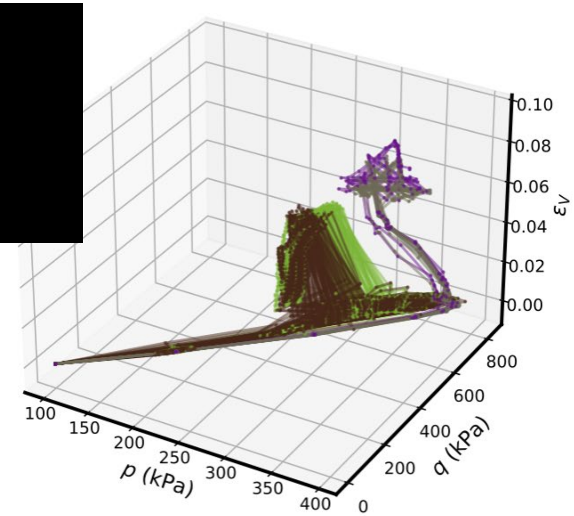
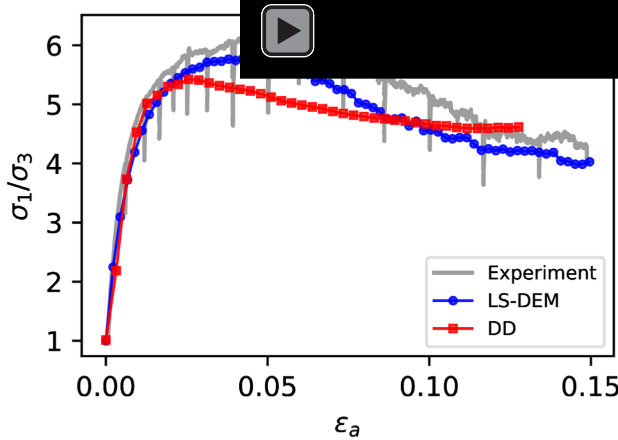
K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239.

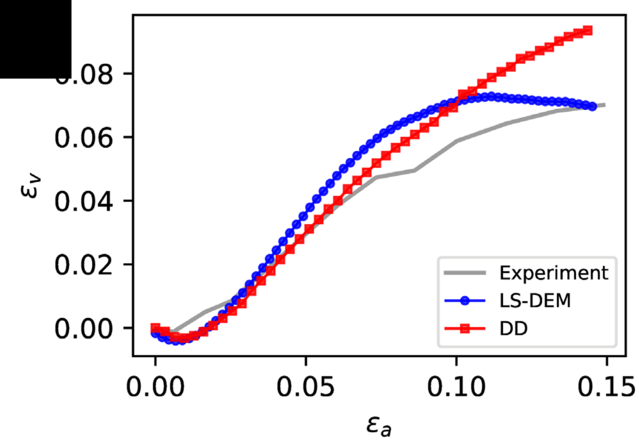
Adaptive Learning – Plasticity

LS-DEM



Clustering of mechanical paths traversed in the initial DD simulation





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

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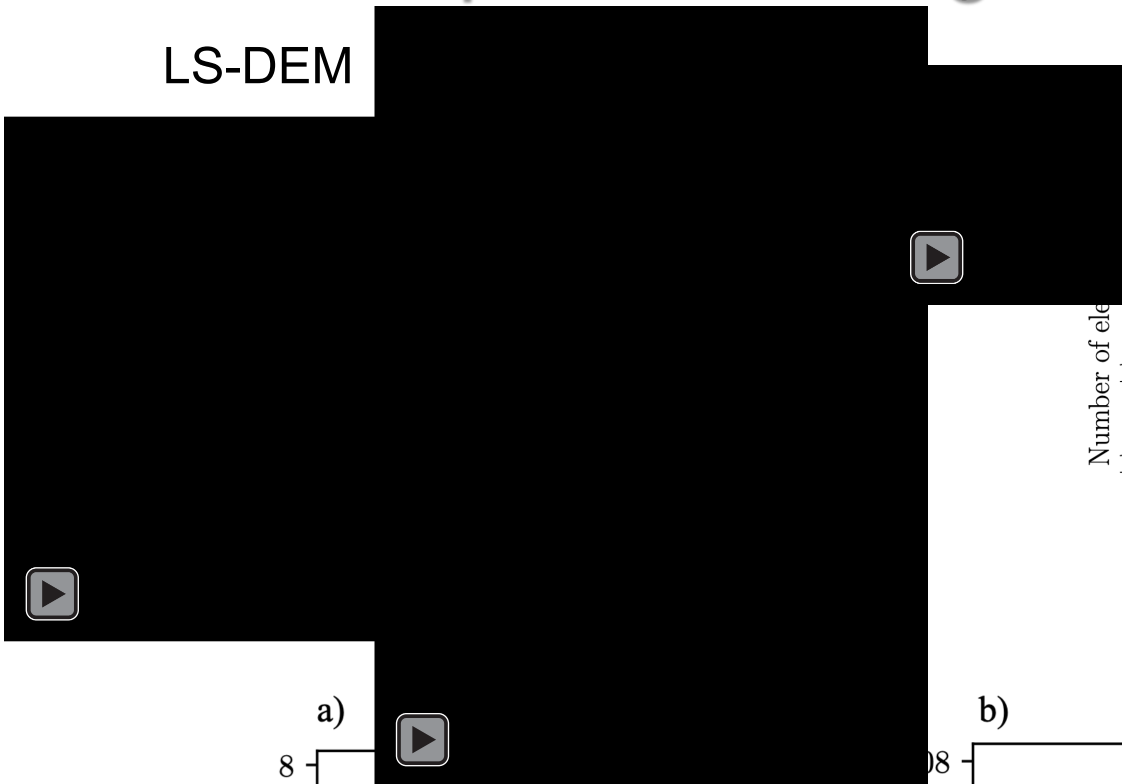
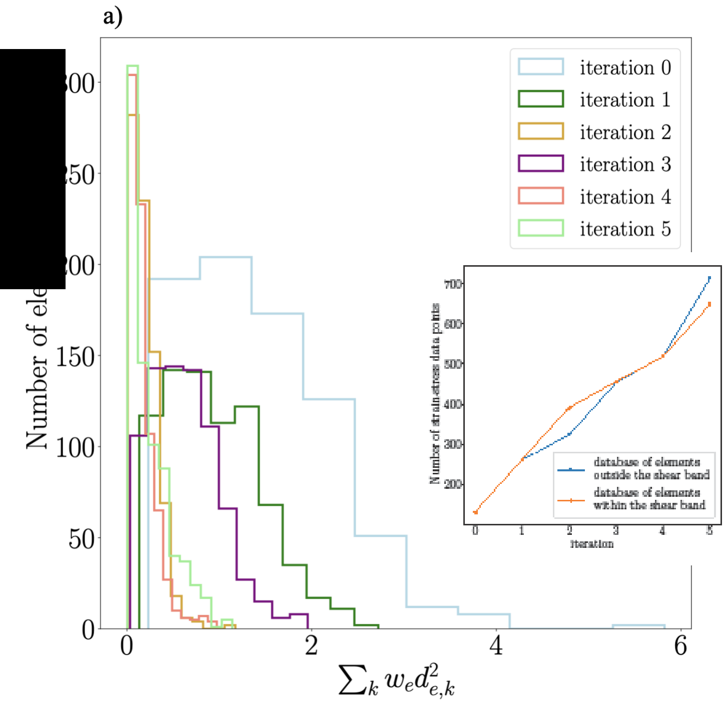
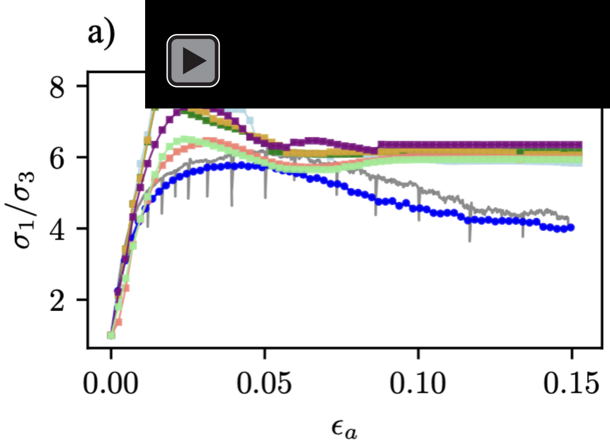
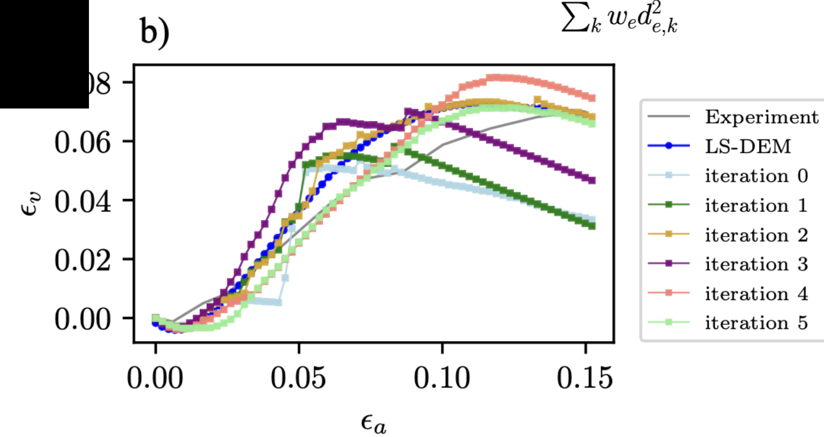
Adaptive Learning – Plasticity

LS-DEM









Results of adaptive learning iteration
(courtesy A. Gorgogianni, Caltech)

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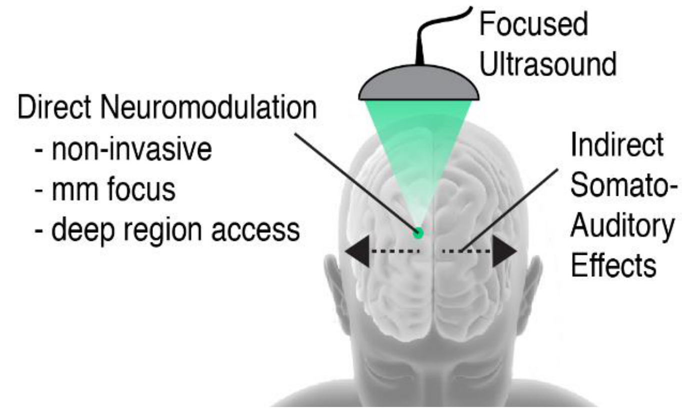
Concurrent data acquisition: Towards DD patient-specific UNM

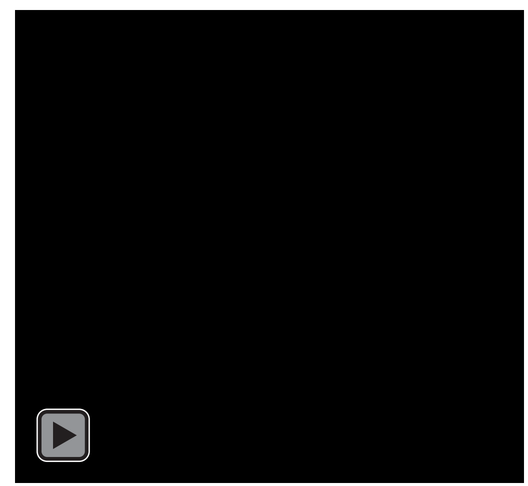
- *Ultrasonic neuromodulation* (UNM) is a novel non-invasive technique that uses *low intensity focused ultrasound* (LIFU) to stimulate the brain.
- First proposed in 2002 by A. Bystritsky as possibly having therapeutic benefits.
- W. Tyler and team discovered UNM is able to stimulate high neuron activity.
- UNM is currently used clinically to treat neurological disorders and improving cognitive function.
- Optimizing UNM therapies in a clinical setting requires *advanced patient-specific data-acquisition and simulation capability*.

Bystritsky A., USPTO patent 7,283,861, 2002.

Tyler, W.J., Tufail, Y., Finsterwald, M., Tauchmann, M.L., Olson, E.J., Majestic, C., PLoS One. 2008;3(10):e3511.

Salahshoor, S., Shapiro, M. and Ortiz, M. Appl. Phys. Lett. **117**, 033702 (2020)

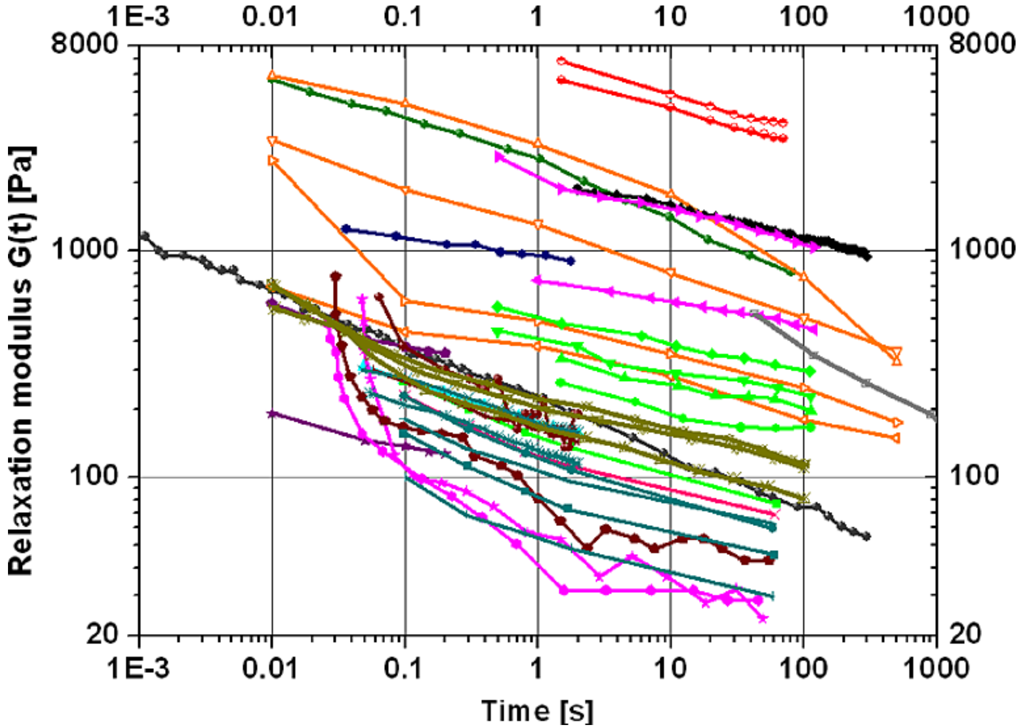




3D FE simulation of Pressure waves under Transcranial LIFUS (100 kHz).

Towards DD patient-specific UNM

- *Complexity* and *variability* of brain viscoelasticity defy effective *ad hoc* modeling!



In vitro relaxation modulus versus time from literature survey. Curves were obtained from either compression or shear quasi-static experiments.

Chatelin, S., Constantinesco, A., Willinger, R., "Fifty years of brain tissue mechanical testing: from in vitro to in vivo investigations." *Biorheology*. 2010;**47**(5-6):255-76.

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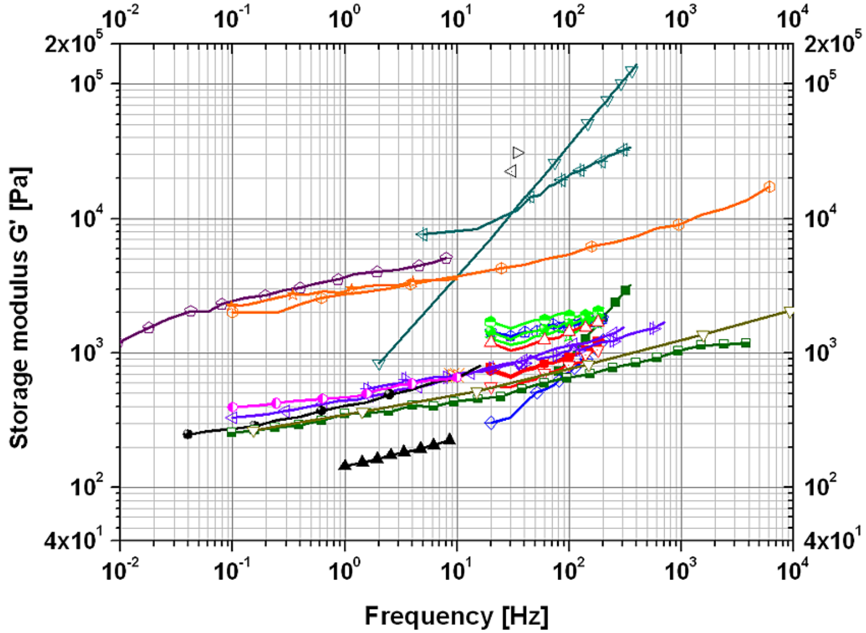
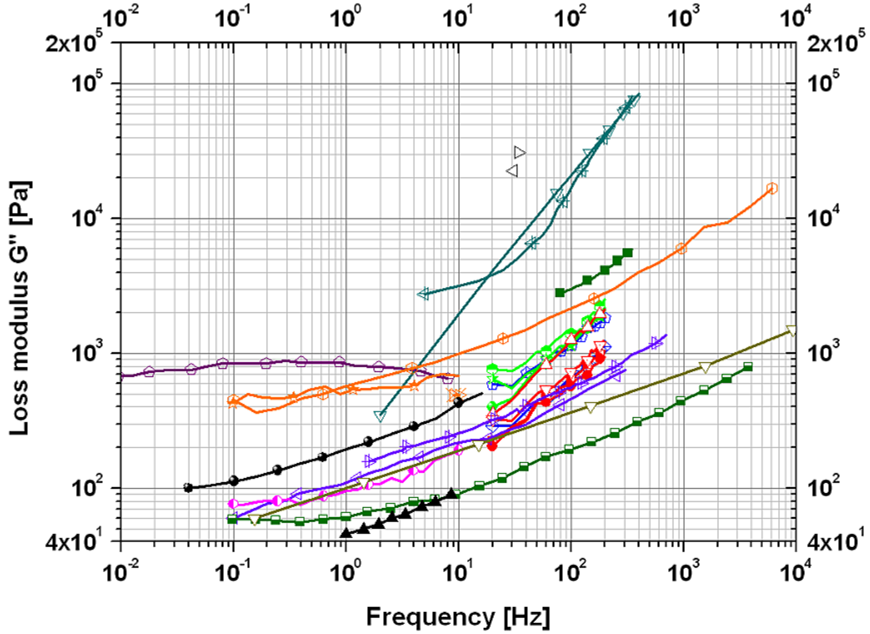


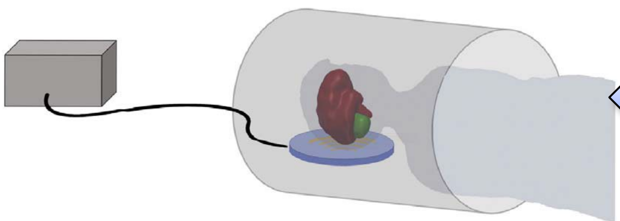


Storage and loss moduli of brain tissue compiled from literature survey of *in vitro* dynamic frequency sweep tests in shear.

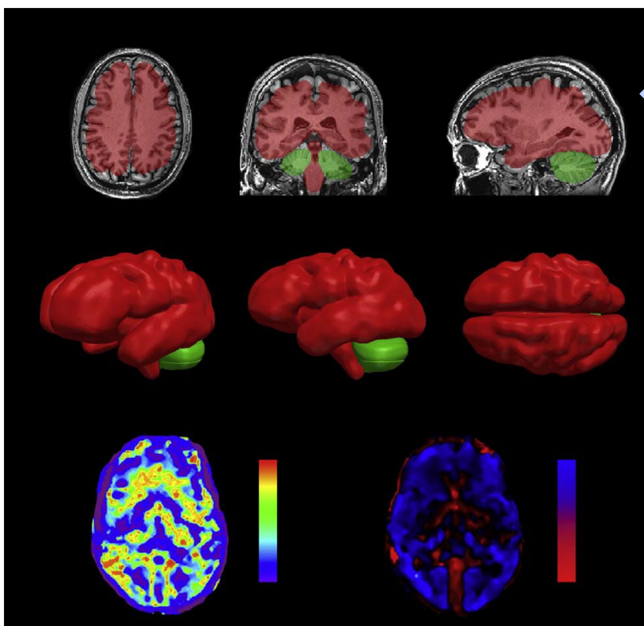
Chatelin, S., Constantinesco, A., Willinger, R., "Fifty years of brain tissue mechanical testing: from in vitro to in vivo investigations." *Biorheology*. 2010;**47**(5-6):255-76.

Towards DD patient-specific UNM

- Data can be acquired *in vivo* through Magnetic Resonance Elastography (EMR).
- MRE is based on the magnetic resonance imaging of shear wave propagation.

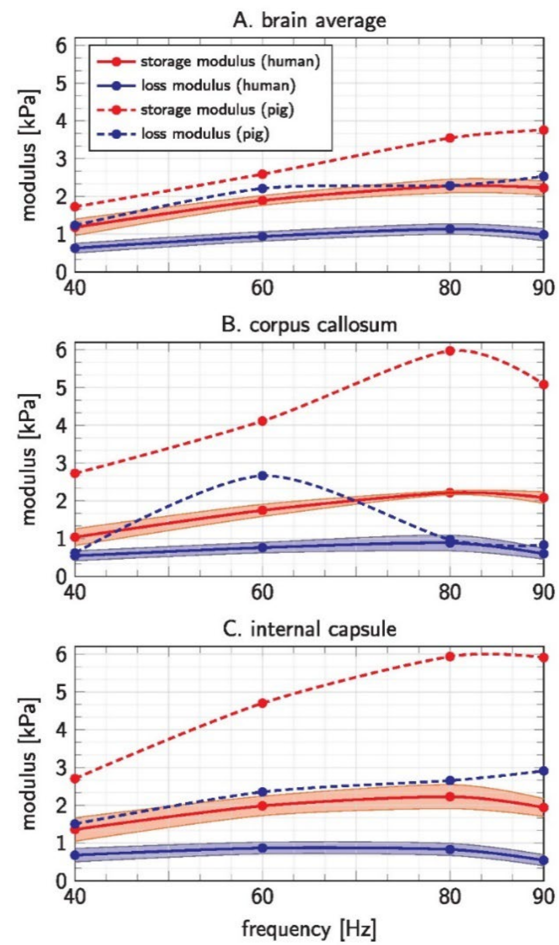


Human subjects scanned in the supine position



Structural scan, reconstruction map of storage and loss moduli

Region-specific storage and loss moduli for human and porcine brains as functions of driving frequency



J. Weickenmeier, M. Kurt, E. Ozkaya, M. Wintermark, K.B. Pauly, E. Kuhl, *J. Mech. Behav. Biomed. Mater.*, **77** (2018) 702-710.

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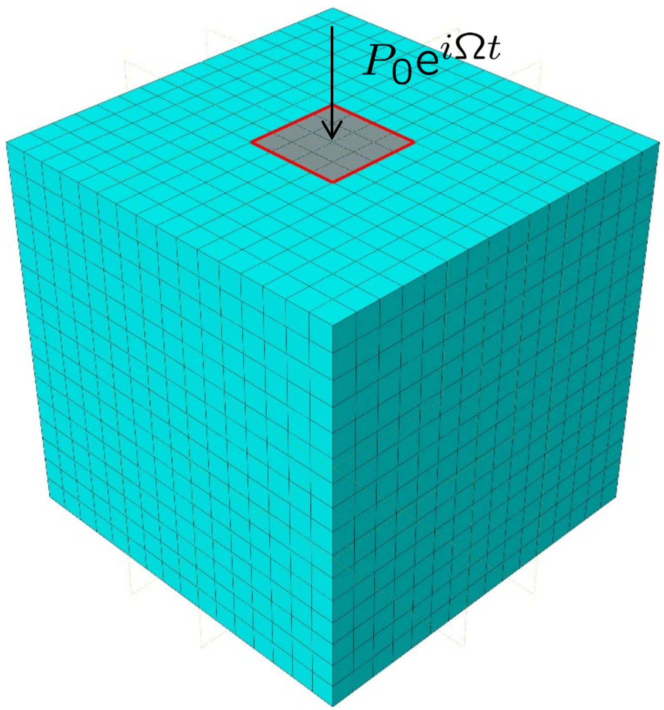
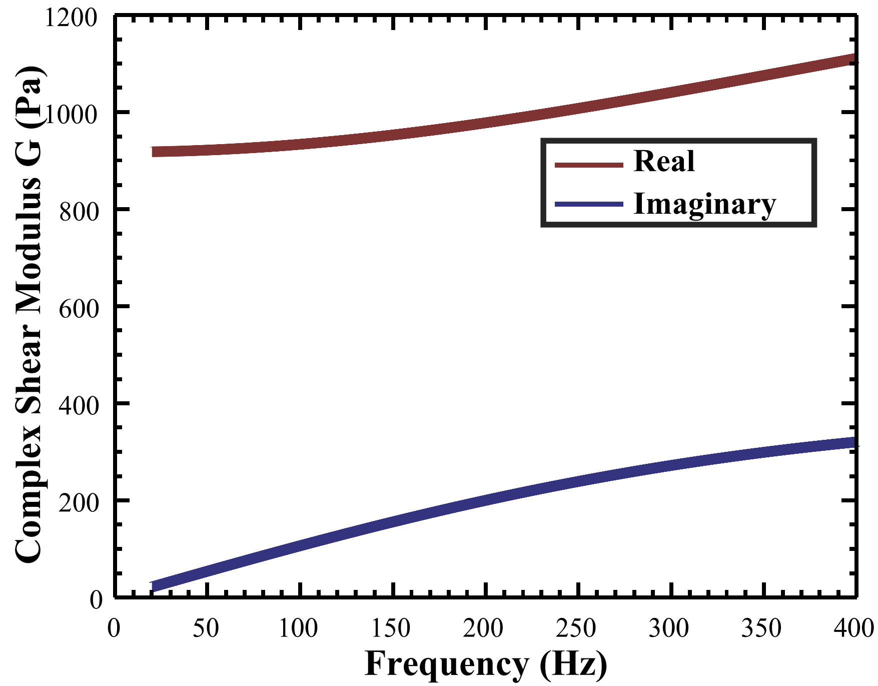
Model-free Data-Driven viscoelasticity

- Test of convergence: *Insonated agarose gel block*.



Finite-element discretization of agarose gel block into hex-elements. The square on the top surface marks area of application of harmonic pressure



Complex moduli of agarose gel measured using dynamic shear testing (DST) and magnetic resonance elastography (MRE).

R. J. Okamoto, E. H. Clayton and P. V. Bayly, Physics in Medicine & Biology 56 (19) (2011) 6379.

H. Salahshoor and M. Ortiz, arXiv 2205.06674v1, May 13, 2022.

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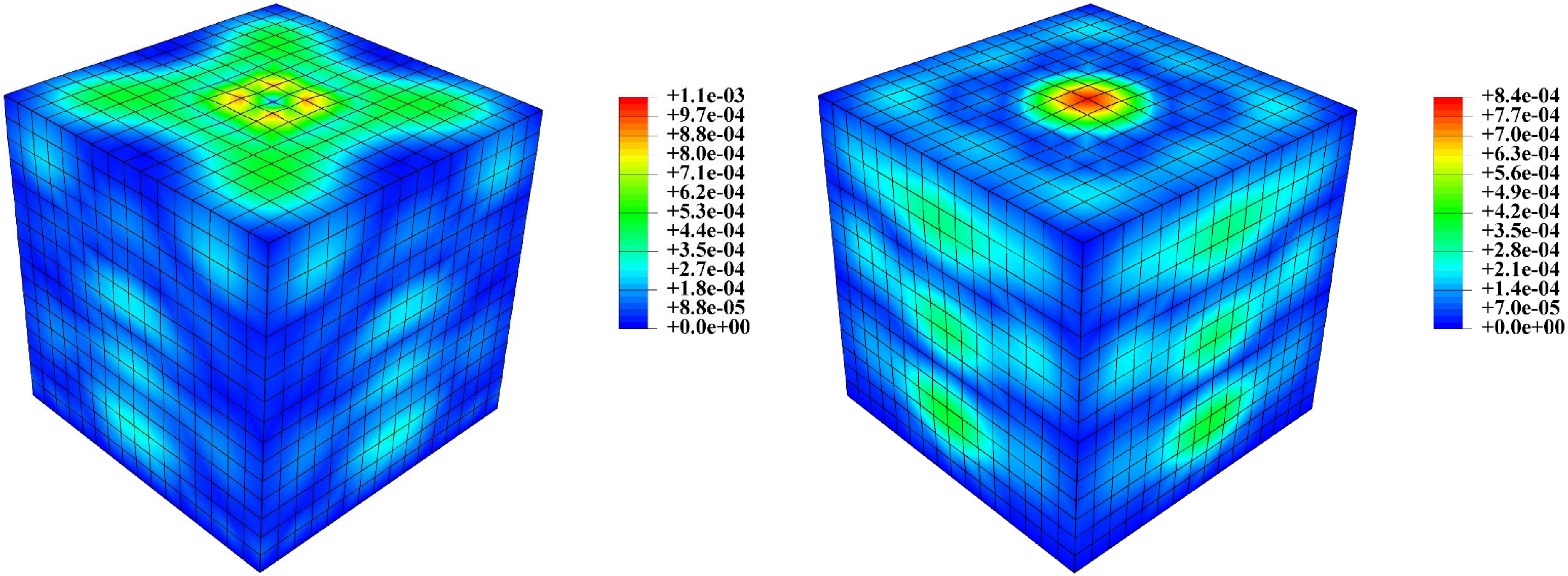

Insonated agarose gel block.
Displacements for applied frequency Ω = 1000 Hz.
a) Real component. b) Imaginary component.

H. Salahshoor and M. Ortiz, arXiv 2205.06674v1, May 13, 2022.

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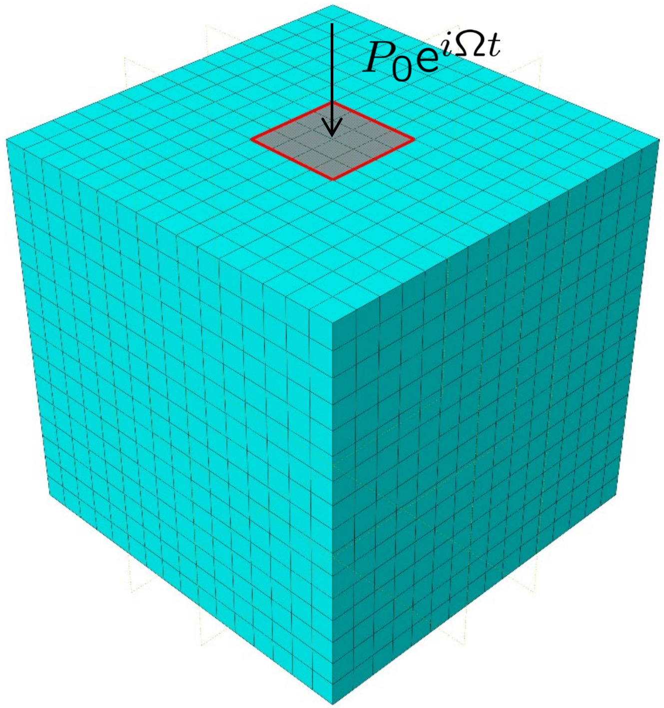

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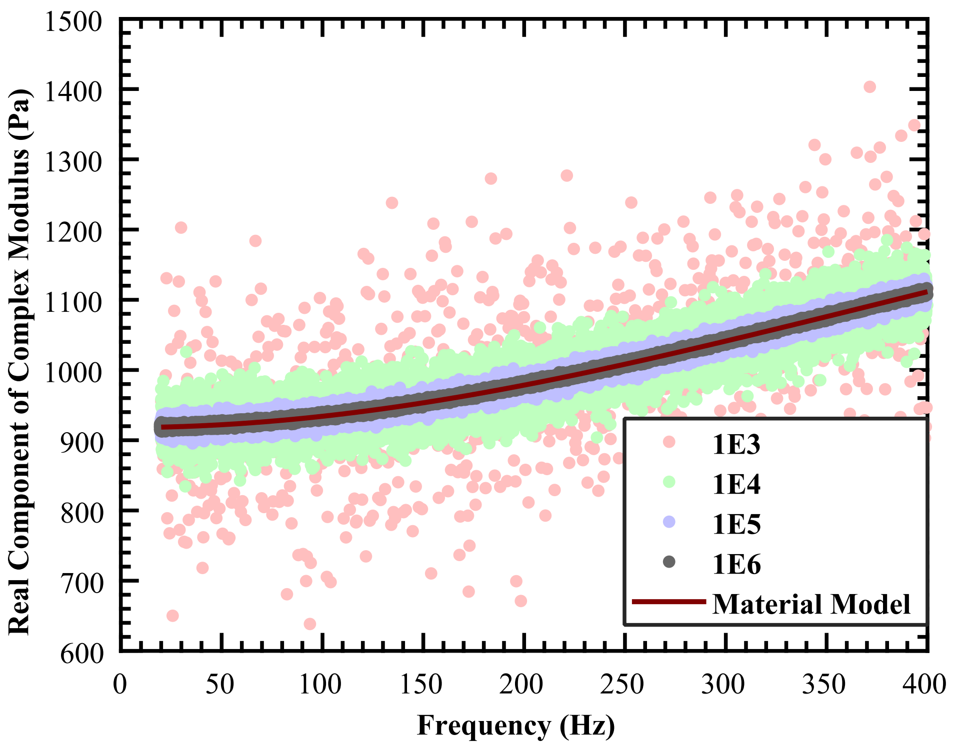

Data of sizes 10^3, 10^4, 10^5 and 10^6 used in the DD calculations. Real component of complex modulus.

H. Salahshoor and M. Ortiz, arXiv 2205.06674v1, May 13, 2022.

Model-free Data-Driven viscoelasticity

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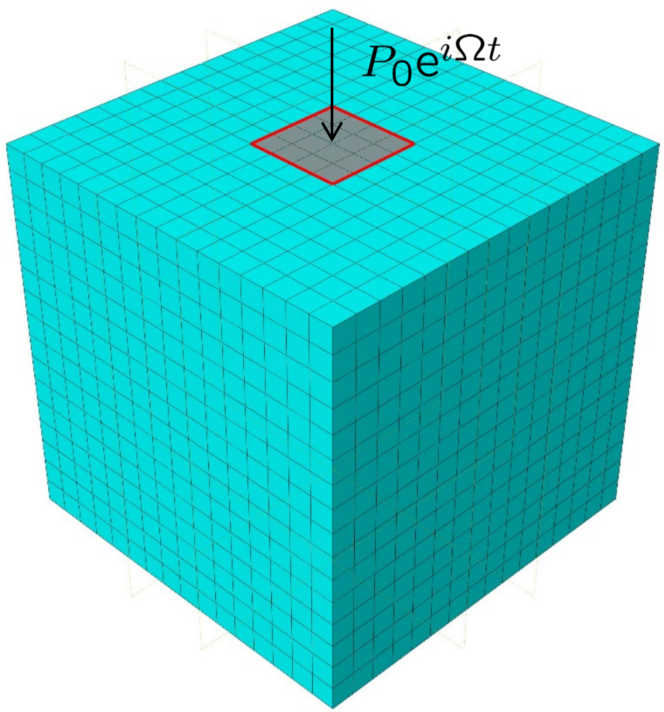

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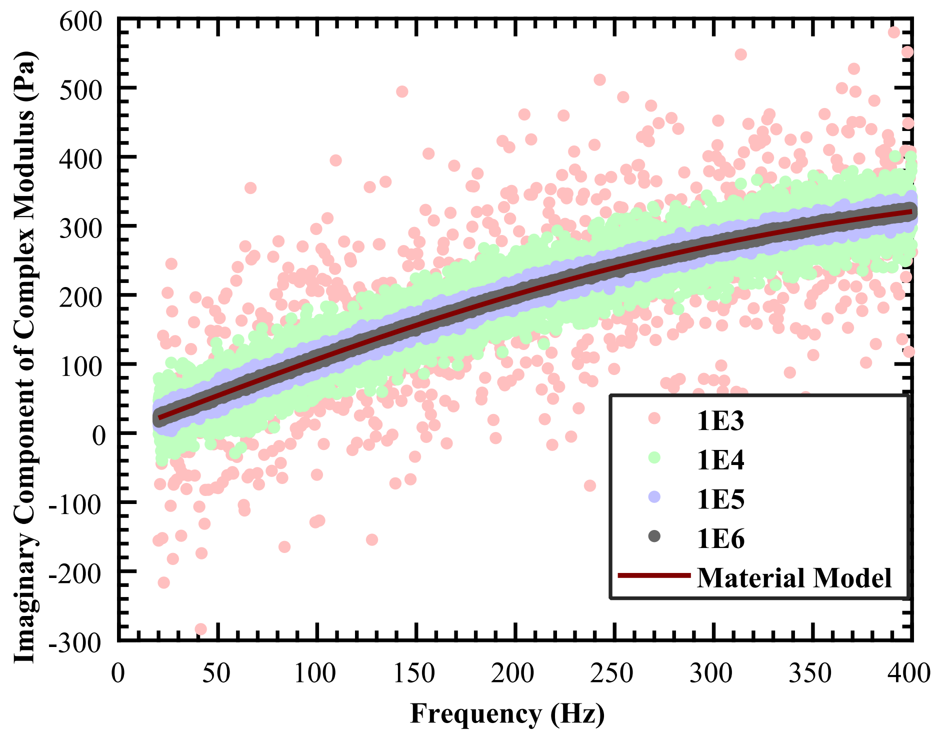

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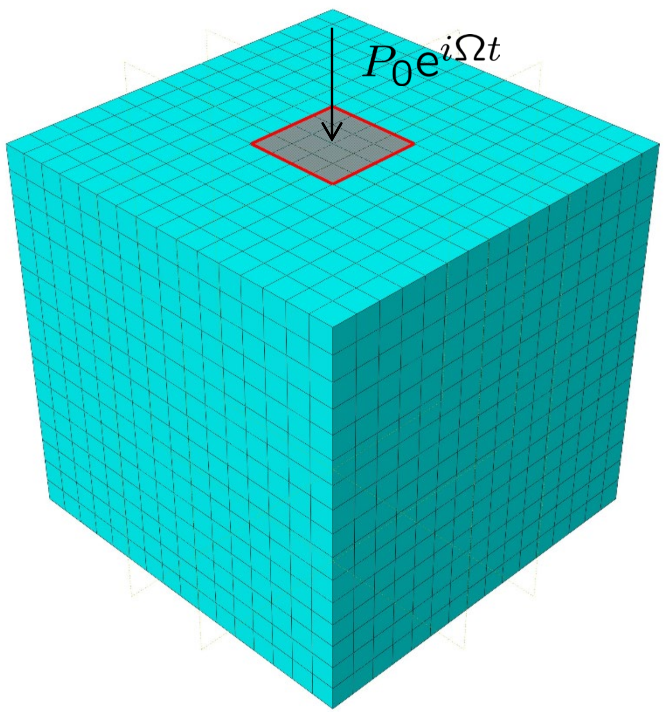

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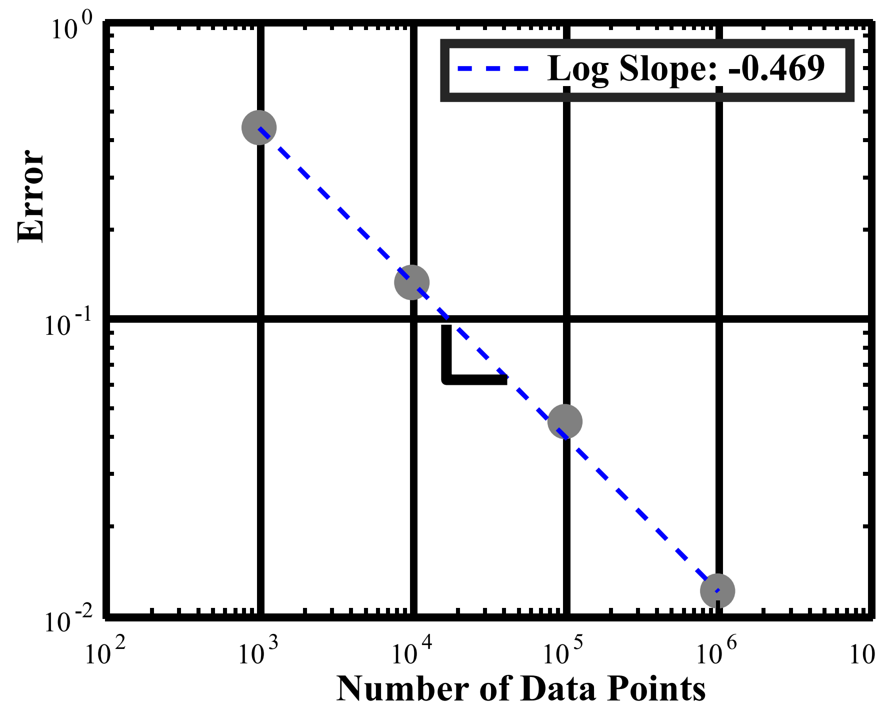
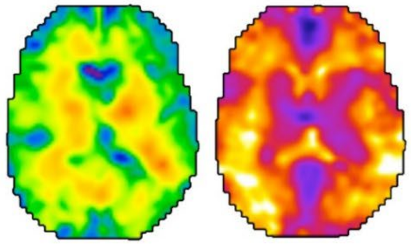


Normalized flat-norm convergence error as a function of the number of data points, showing a clear trend towards convergence.

H. Salahshoor and M. Ortiz, arXiv 2205.06674v1, May 13, 2022.

Towards DD patient-specific UNM

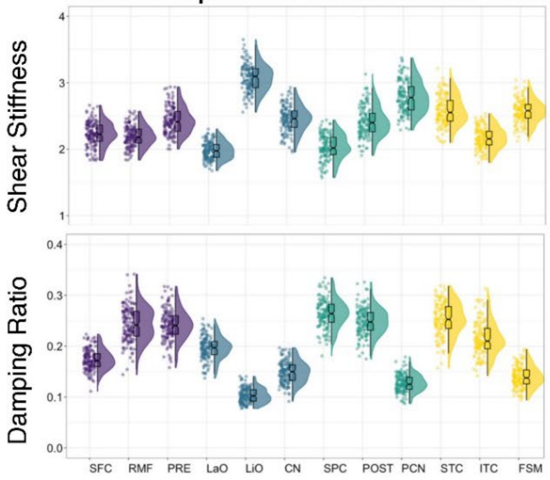
Experiment:
In-situ data acquisition (MRI & MRE)



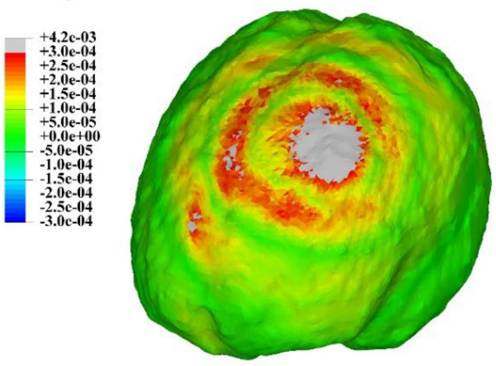
Anatomical Data

MFDD
UNM

Brain Matter Data Repository:
Patient-specific viscoelastic atlas



Direct Data-Driven patient-specific prediction of wave patterns in brain:
Example of transcranial ultrasound



L.V. Hiscox *et al.*, *Hum Brain Mapp.*, 2020;**41**:5282–5300

H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

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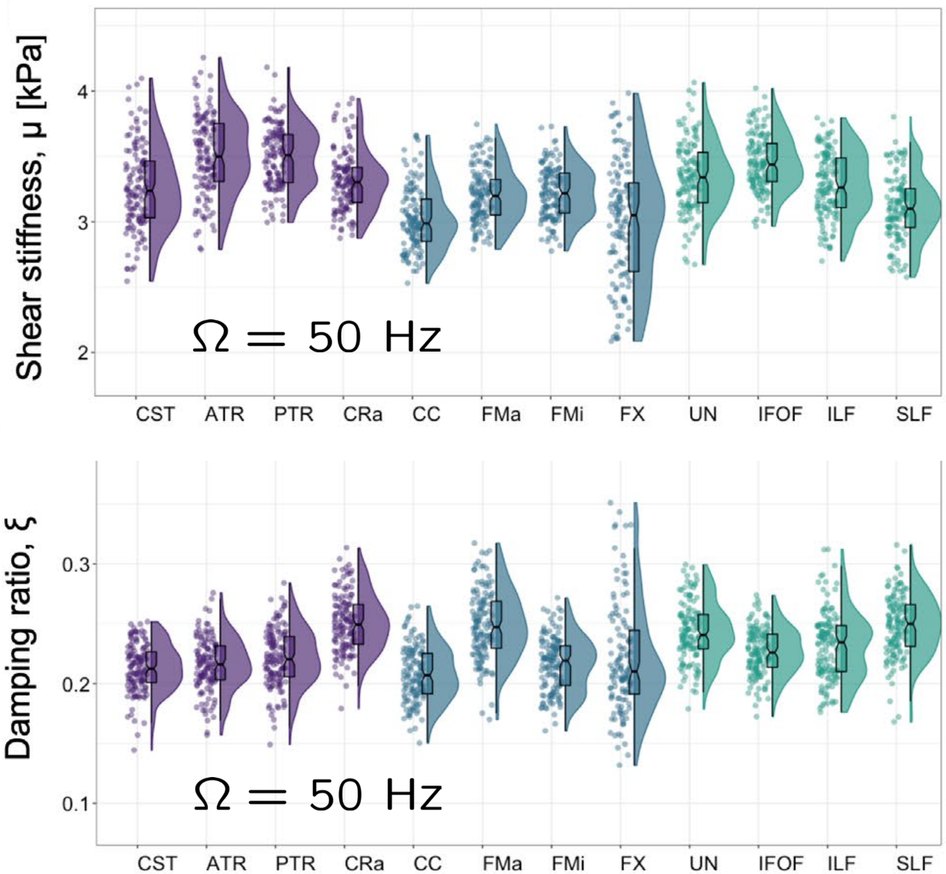
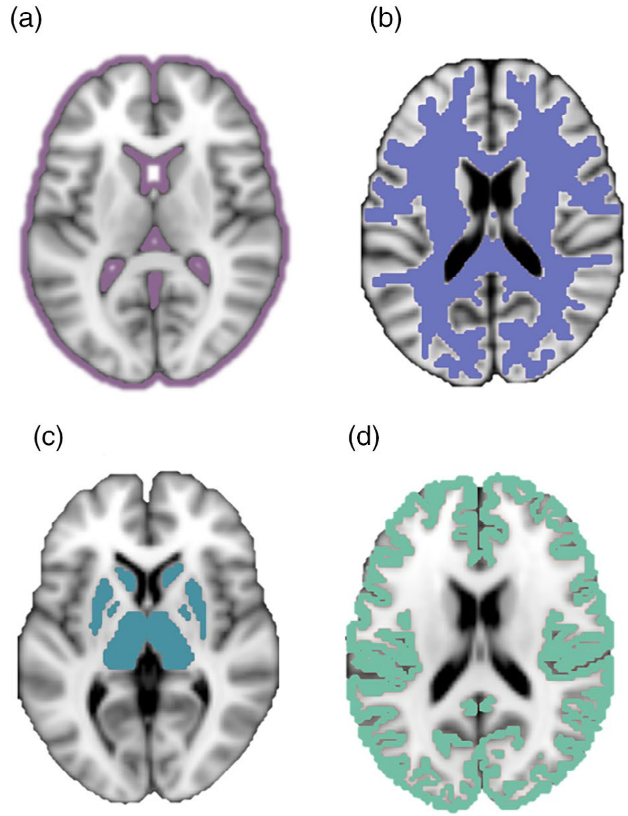


MRE viscoelastic data atlas at 12 regions of interest (Desikan–Killiany–Tourville cortical labelling protocol).



MRE data for (a) the entire brain (b) white matter (c) subcortical gray matter (d) cerebral cortex.

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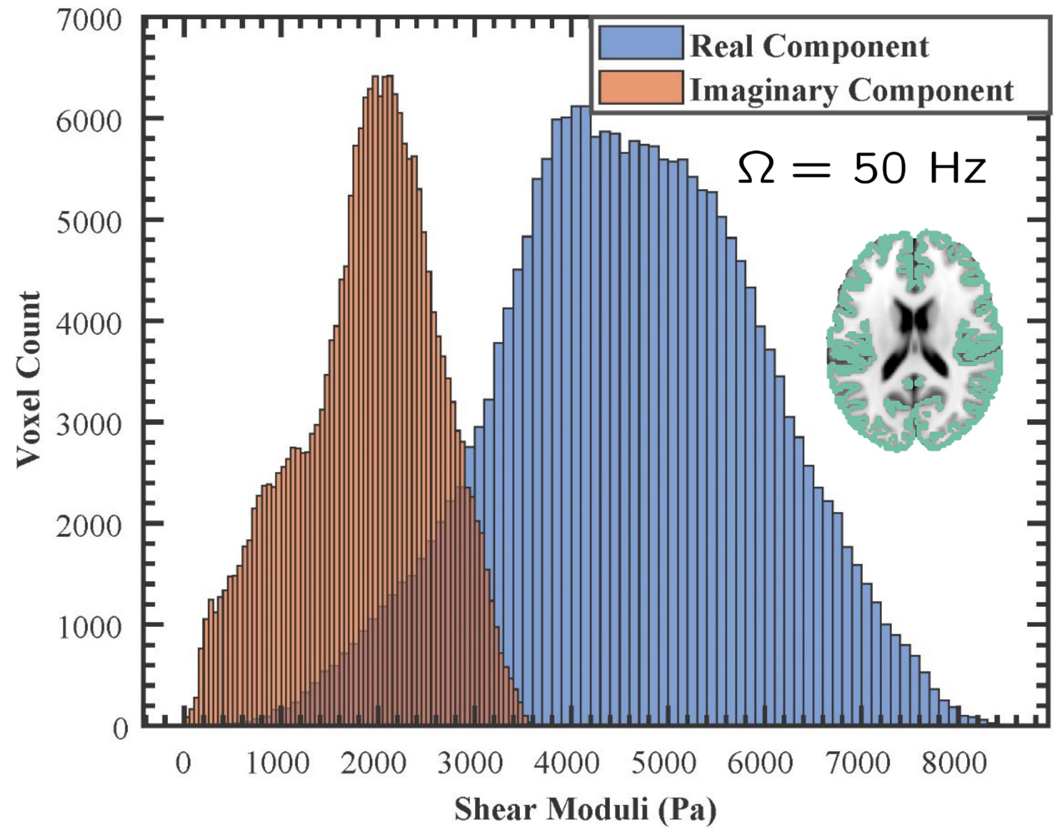
H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

Towards DD patient-specific UNM

Finite element model of human brain reconstructed from MRI data, 0.2 million tetrahedral elements. Transcranial stimulation is modeled by subjecting the highlighted region to harmonic pressure as a traction boundary condition.

H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.



Histogram of complex moduli from in vivo MRE data. The finite-element model is co-registered to the MRE data.

L.V. Hiscox *et al.*, *Hum Brain Mapp.*, 2020;**41**:5282–5300

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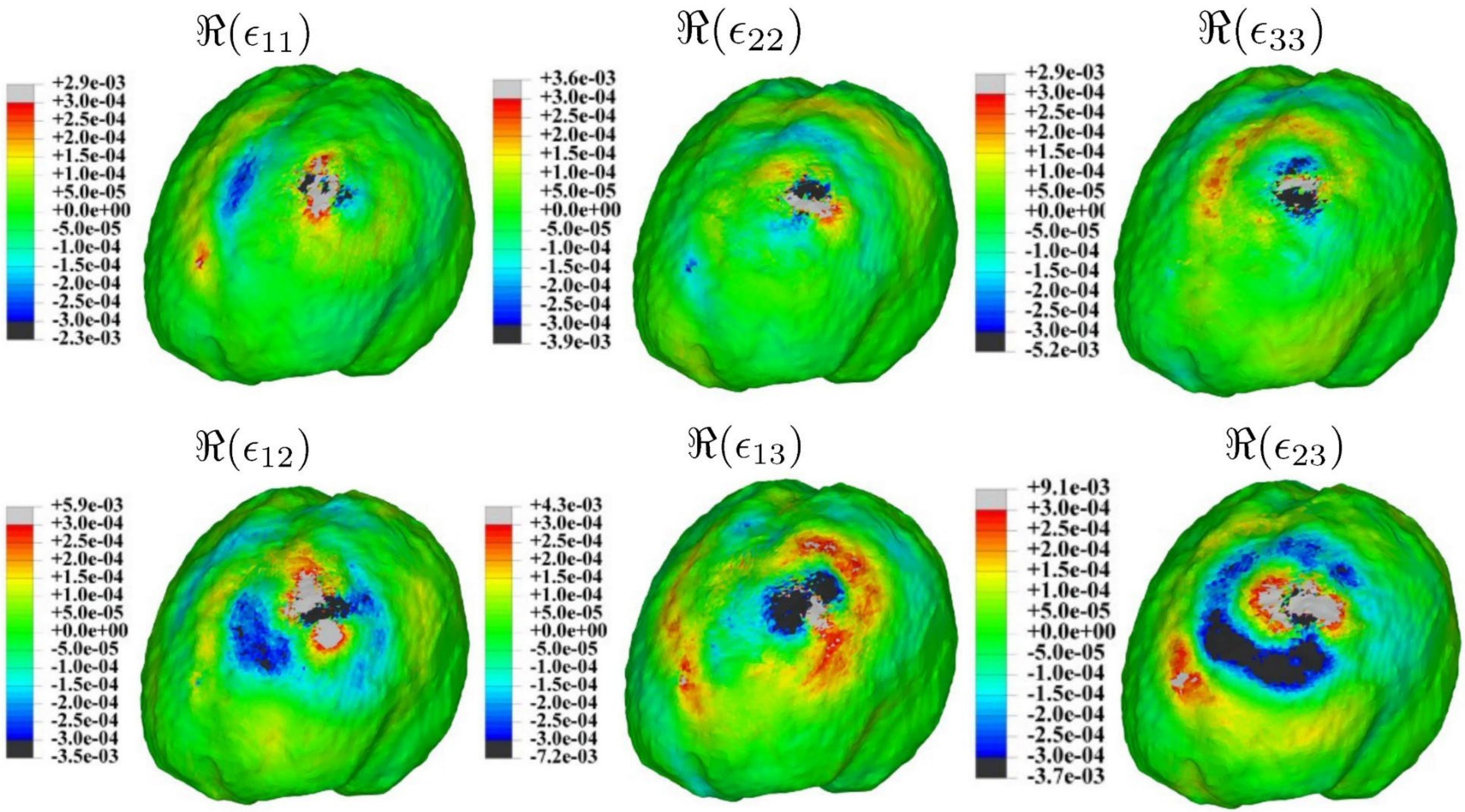
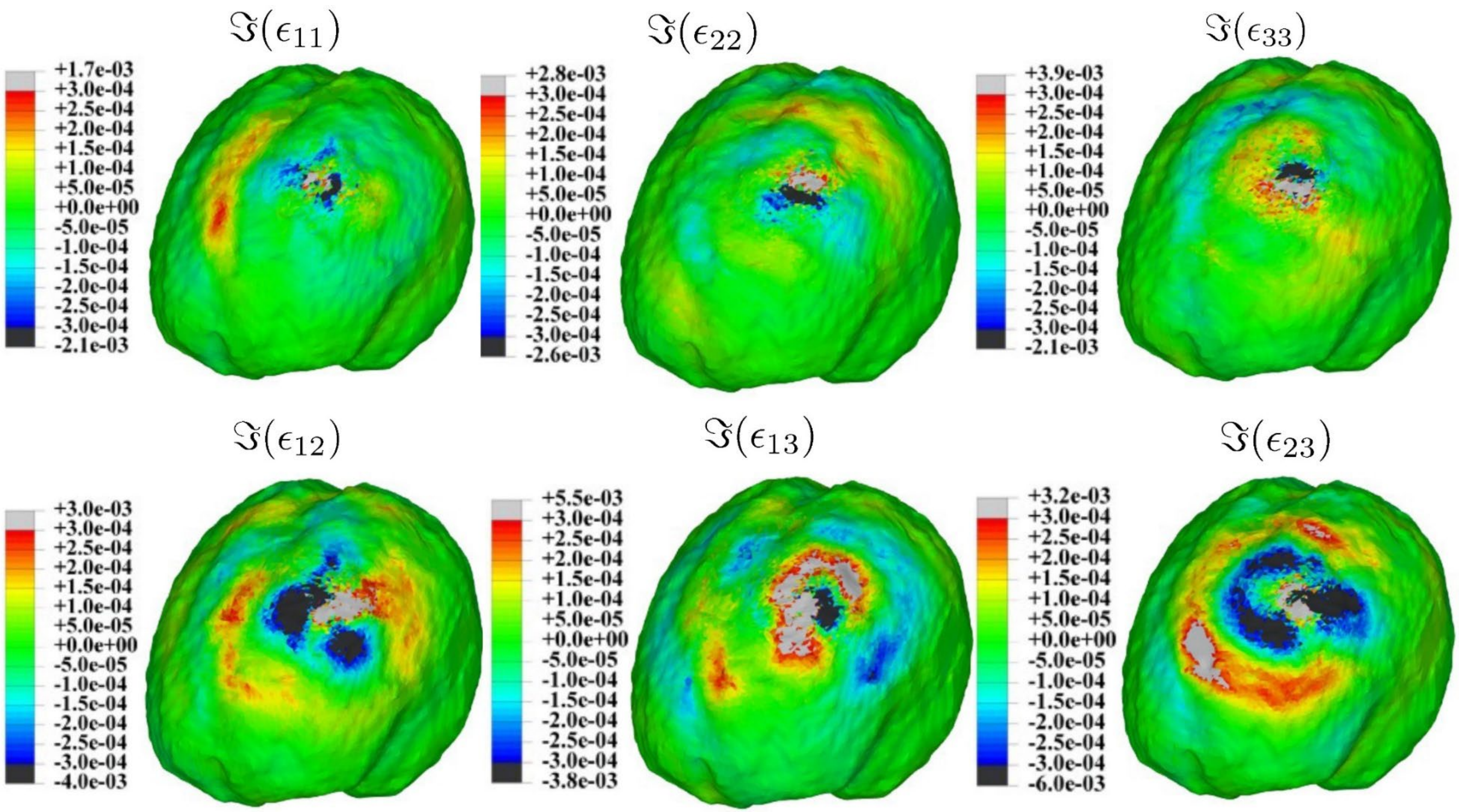
Towards DD patient-specific UNM



Model-free Data-Driven simulation of transcranial harmonic stimulation
on a region on the frontal lobe of the brain at Ω = 50 Hz.
Real part of the strain field components at steady state.

H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

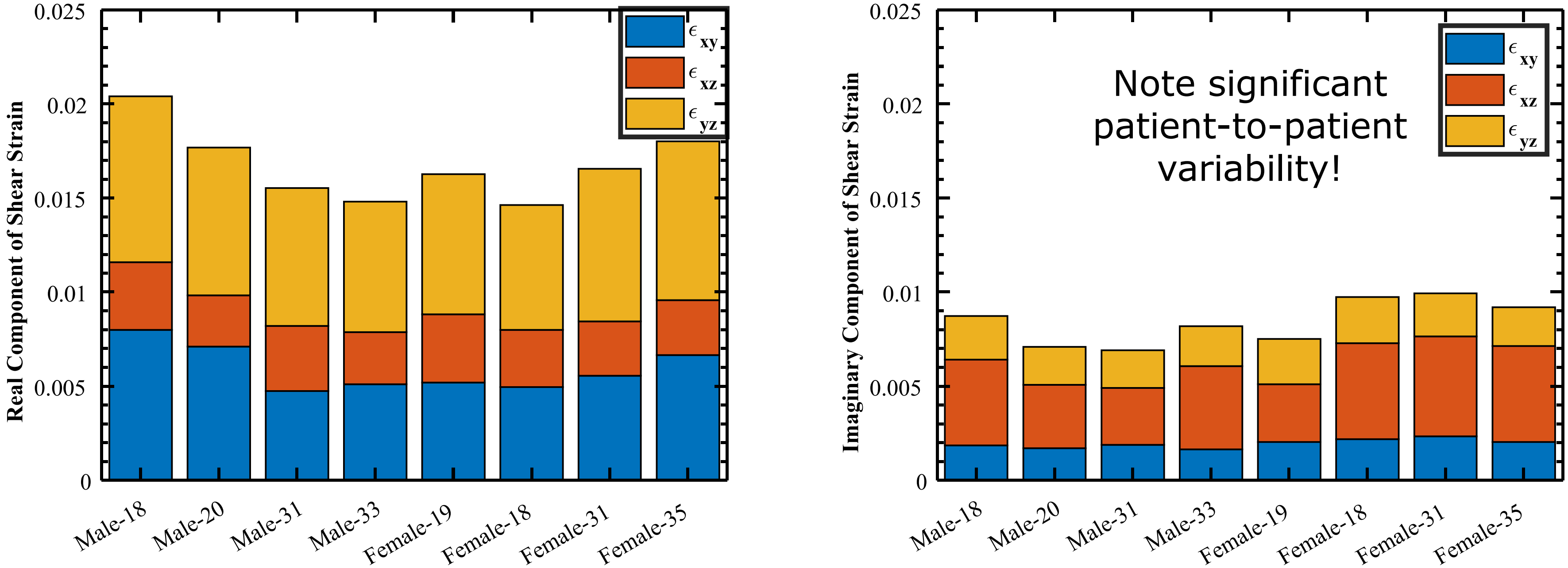
Towards DD patient-specific UNM



Model-free Data-Driven simulation of transcranial harmonic stimulation on a region on the frontal lobe of the brain at Ω = 50 Hz. Imaginary part of the strain field components at steady state.

H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

Towards DD patient-specific UNM



Model-free Data-Driven simulation of transcranial harmonic stimulation on a region on the frontal lobe of brain at Ω = 50 Hz, for eight patient-specific MRE data sets. Real and imaginary maximum strain amplitudes at steady state.

- NB: Improvements to MRE required to extend the technology to the *ultrasound range*, currently under development.
- *Model-Free Data-Driven viscoelasticity* provides a path for the direct on-the-fly integration of *in vivo* patient-specific data into calculations supporting future UNM clinical applications!

H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

Concluding remarks

Thank you!