



Model-Free Data-Driven Computing

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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*

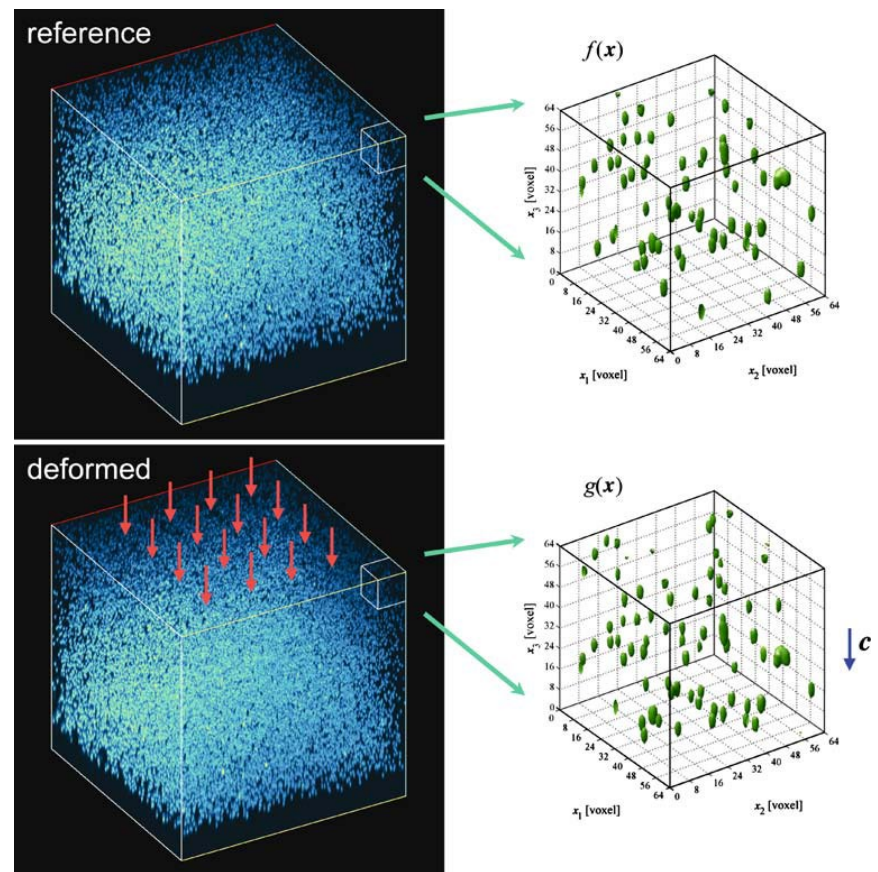
The new data-rich world of mechanics...

- 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

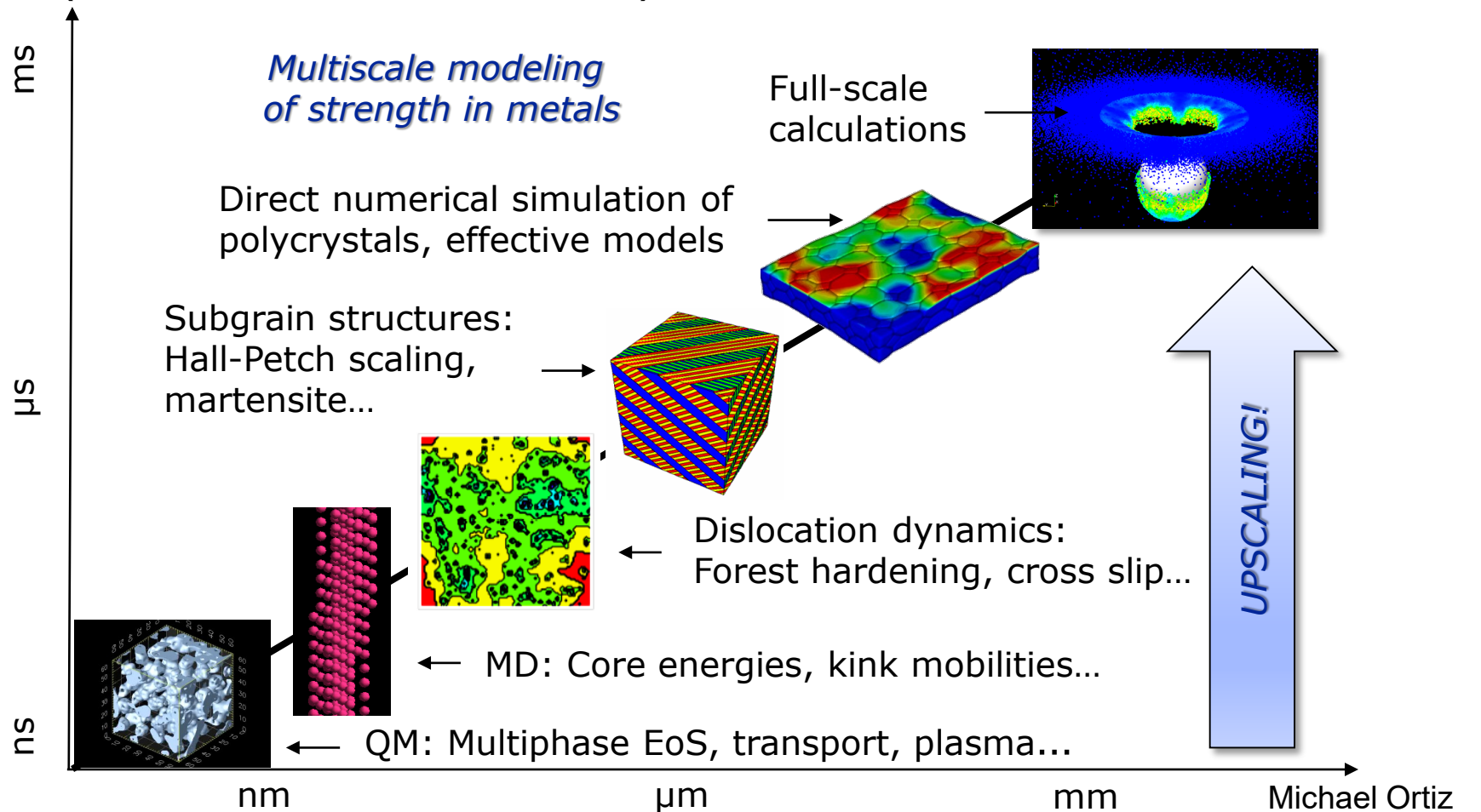
(DVC): Two confocal volume images of an agarose gel with randomly dispersed fluorescent particles before and after mechanical loading. The full displacement vector field is measured using 3D volume correlation methods.

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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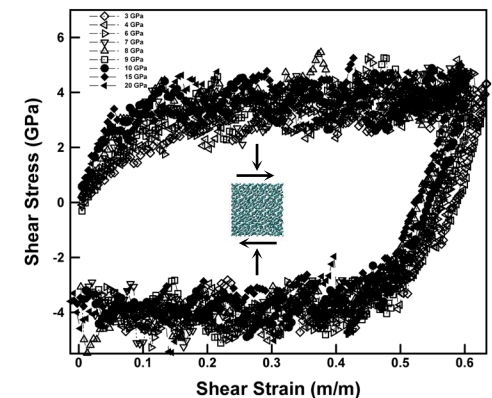
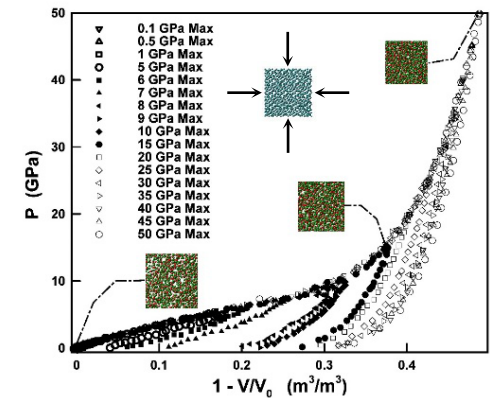
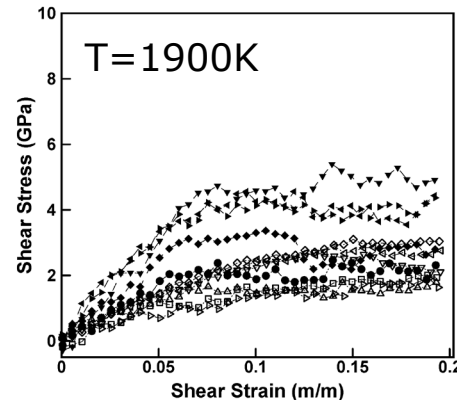
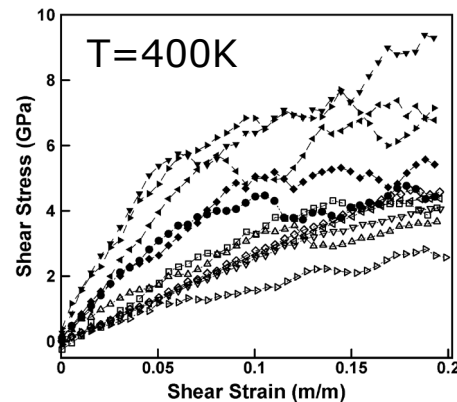
The new data-rich world of EM...

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Amorphous SiO_2 glass:

LAMMPS MD calculations of amorphous silica glass under *pressure-shear* loading over a range of *temperatures* and *strain rates*. RVEs are quenched from the melt, then analyzed using the BKS potential with Ewald summation.

Schill, W., Heyden, S., Conti, S.
& MO, *JMPS*, **113** (2018) 105-125.
Schill, W., Mendez, J.P., Stainier, L.
& MO, *JMPS*, **140** (2020) 103940.

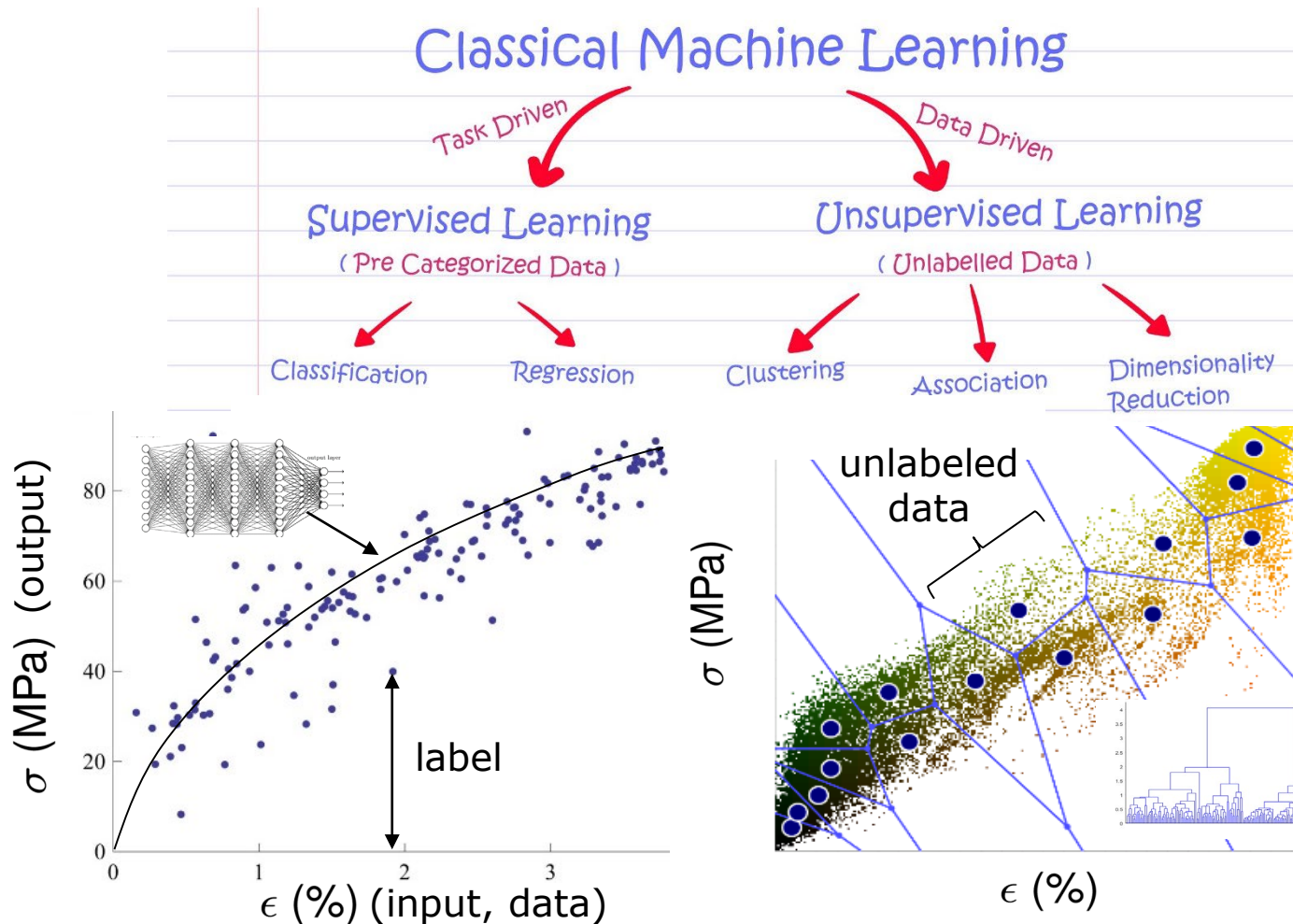


Data-Driven computational mechanics

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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)...



The model-free Data-Driven paradigm

Definition (Data-Driven Problem)

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

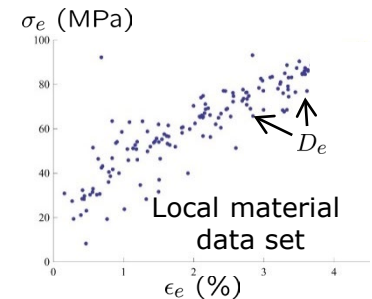
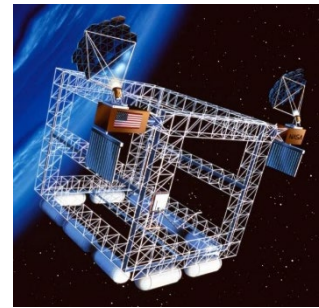
- i) $D = \{\text{material data}\} \subset Z$,
- ii) $E = \{\text{field equations}\} \subset Z$,

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



Example (Structural mechanics)

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



• Discussion:

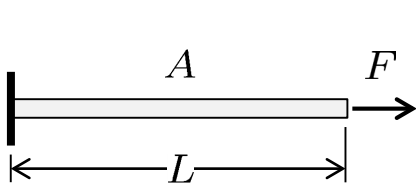
- Phase space Z determined by **field equations**
- **Fundamental data** (model-independent) = Points in phase space
- **No material modeling**, no loss of information, no biasing of the data
- DD problem **generalizes** and subsumes classical field-theoretical problems



• 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



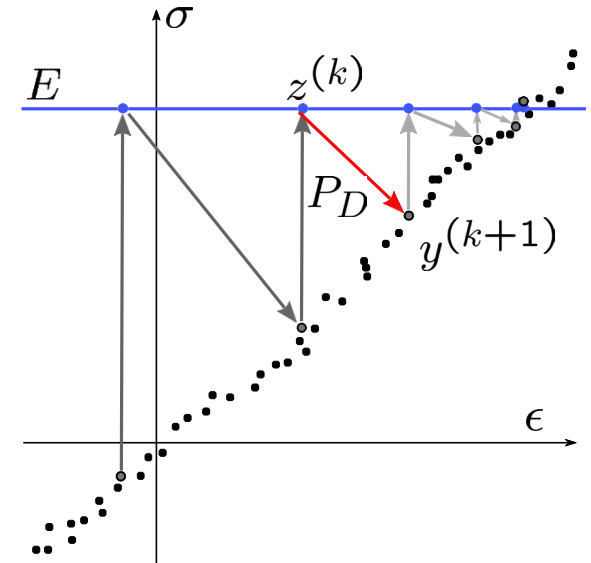
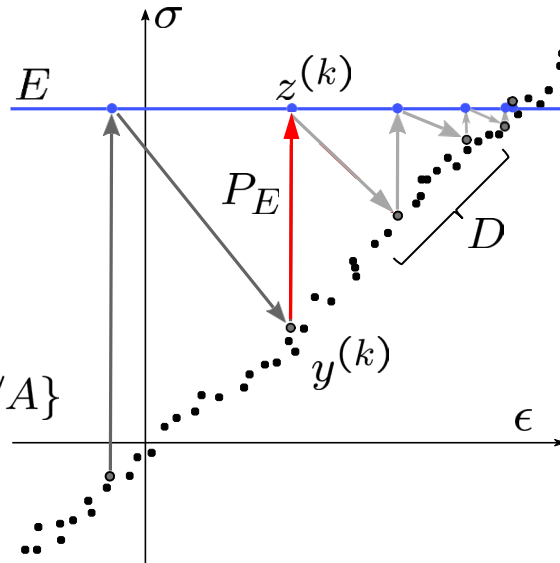
Example (Bar/dead load)

- Admissible subspace:

$$E = \{z := (\epsilon, \sigma) : \sigma = F/A\}$$

- Data set in $Z := \mathbb{R} \times \mathbb{R}$:

$$D = \{y := (\epsilon', \sigma') \in Z\}$$



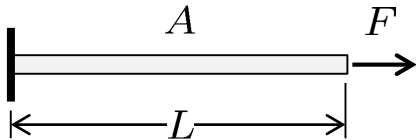
- Projection to E** (inner minimization at fixed (ϵ', σ')): i) Enforce compatibility directly by writing $\epsilon = Bu$; ii) Enforce equilibrium through a Lagrange multiplier v ,

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

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



Solvers: Fixed-point iteration



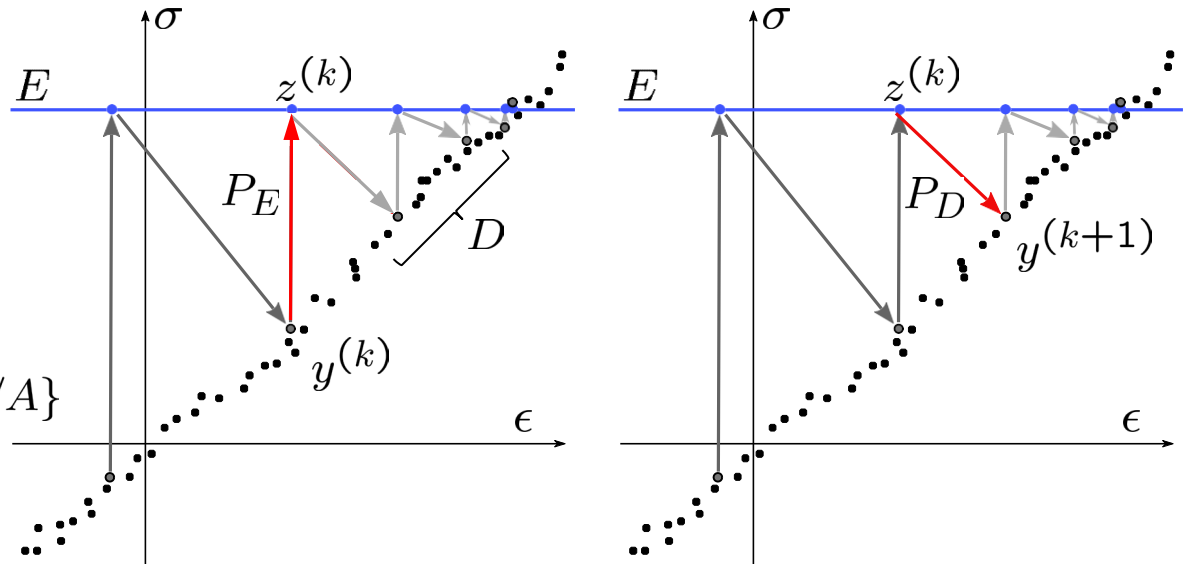
Example (Bar/dead load)

- Admissible subspace:

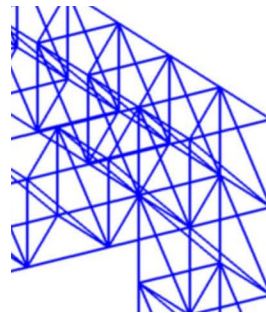
$$E = \{z := (\epsilon, \sigma) : \sigma = F/A\}$$

- Data set in $Z := \mathbb{R} \times \mathbb{R}$:

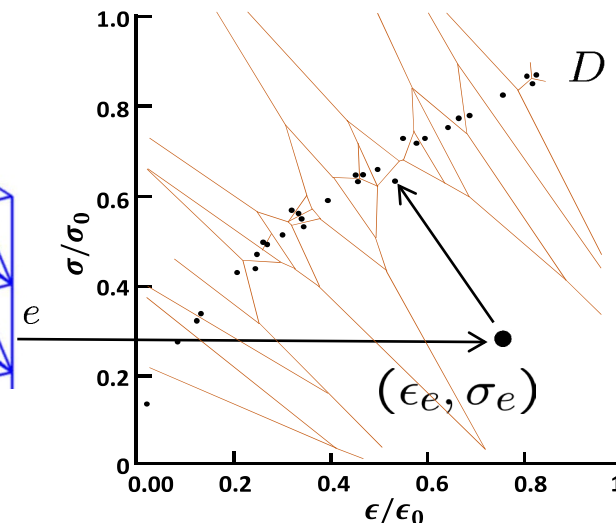
$$D = \{y := (\epsilon', \sigma') \in Z\}$$



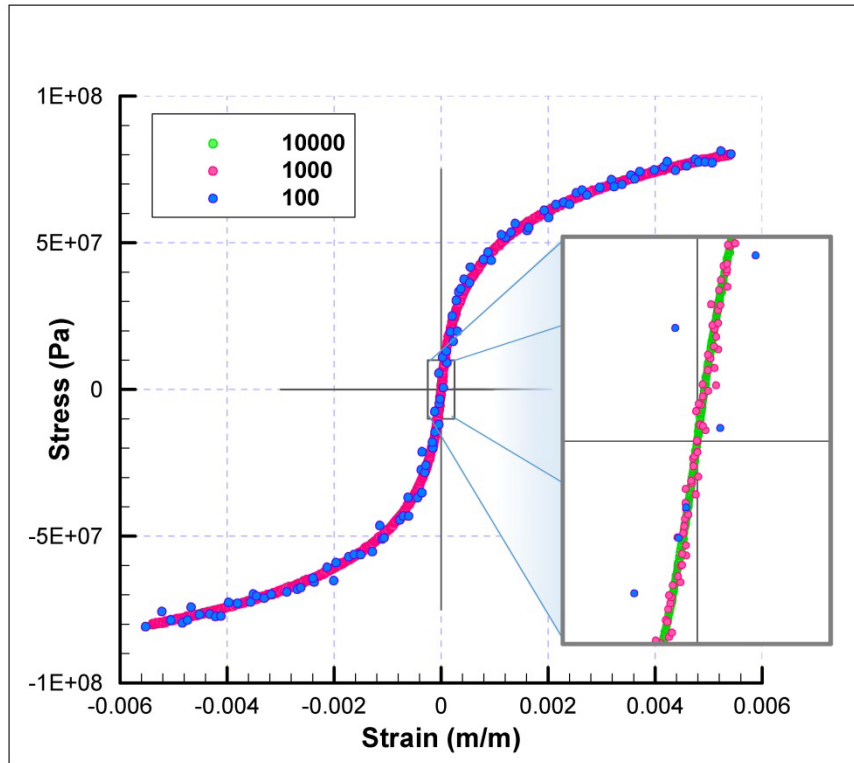
- Outer minimization: Projection onto (closest point in the) material data set D
- Fast searching algorithm
- Requires data structures
- 'Learning' structure of D
- Set-oriented (lossless) ML!



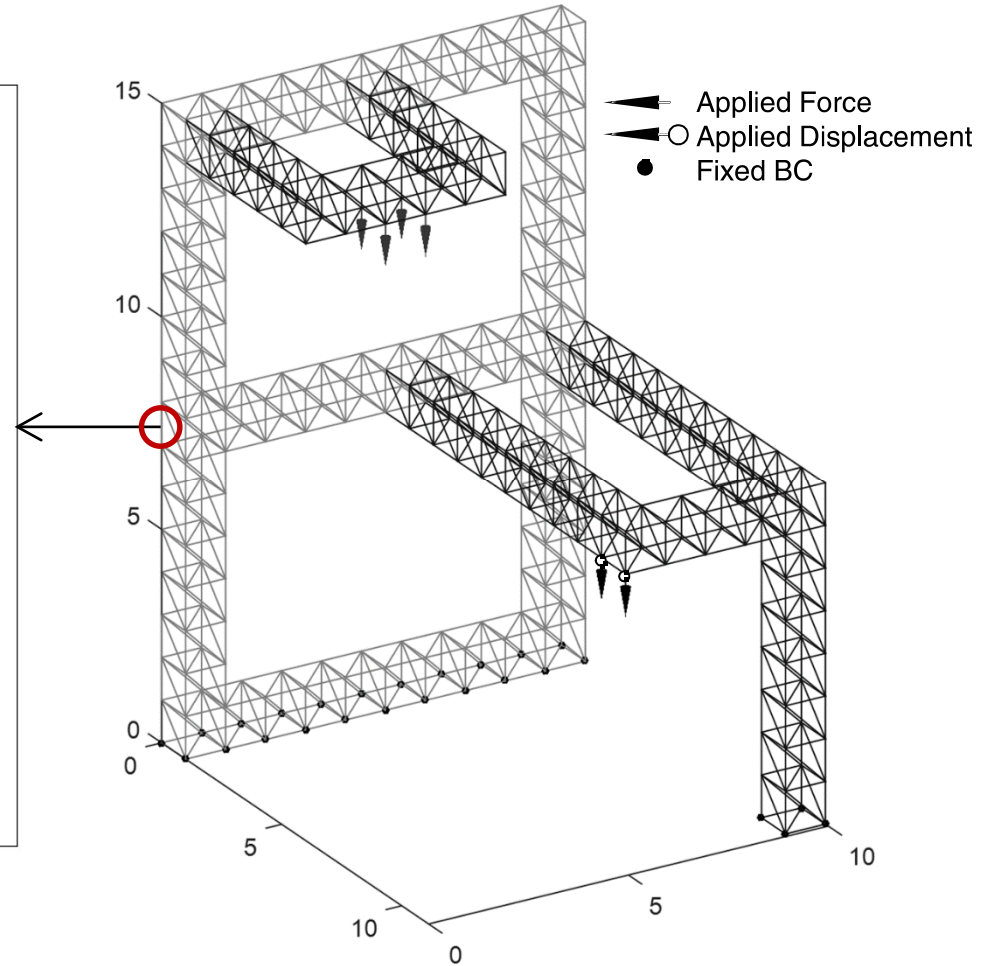
*Unsupervised
machine learning!*



Convergence with respect to the data

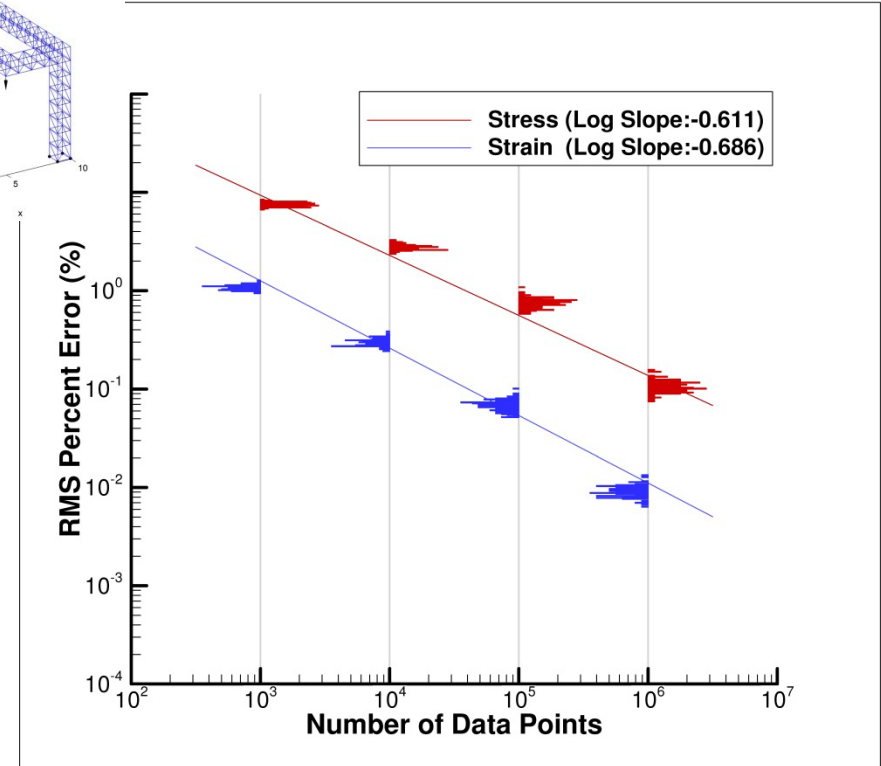
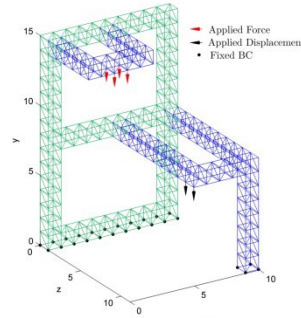
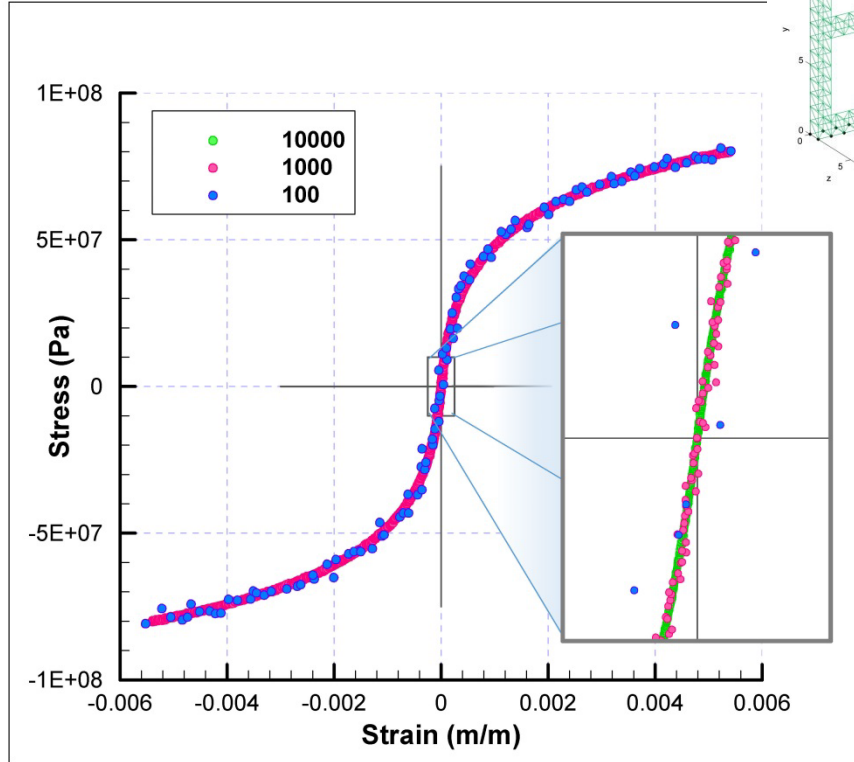


Sequence of
uniformly converging data sets
(increasing number of points,
decreasing scatter)



3D truss structure

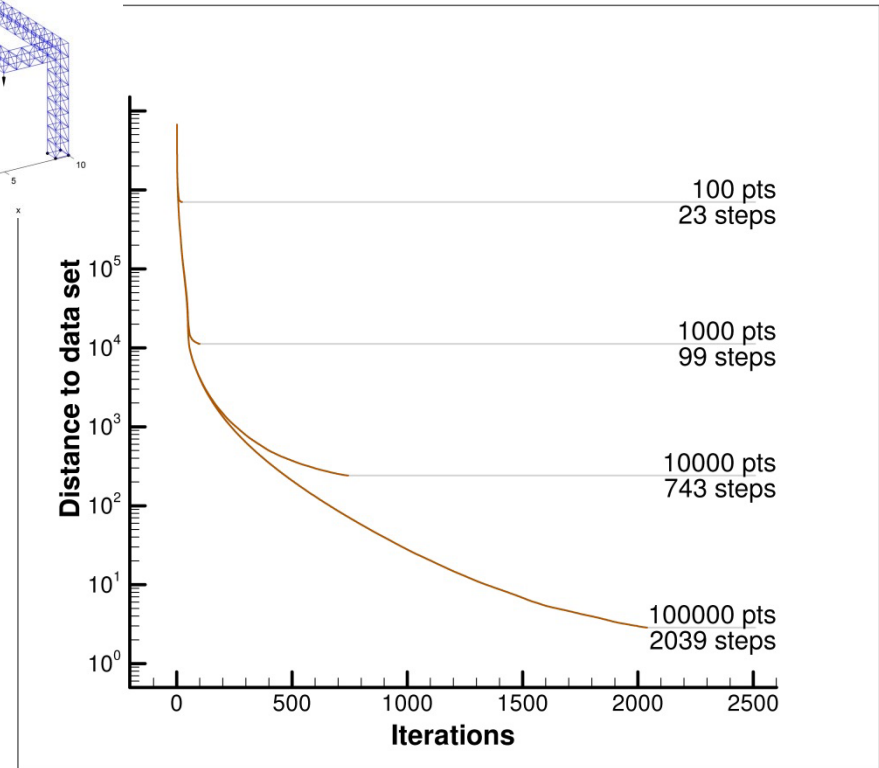
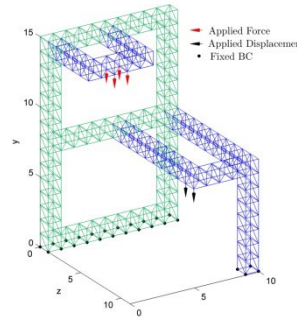
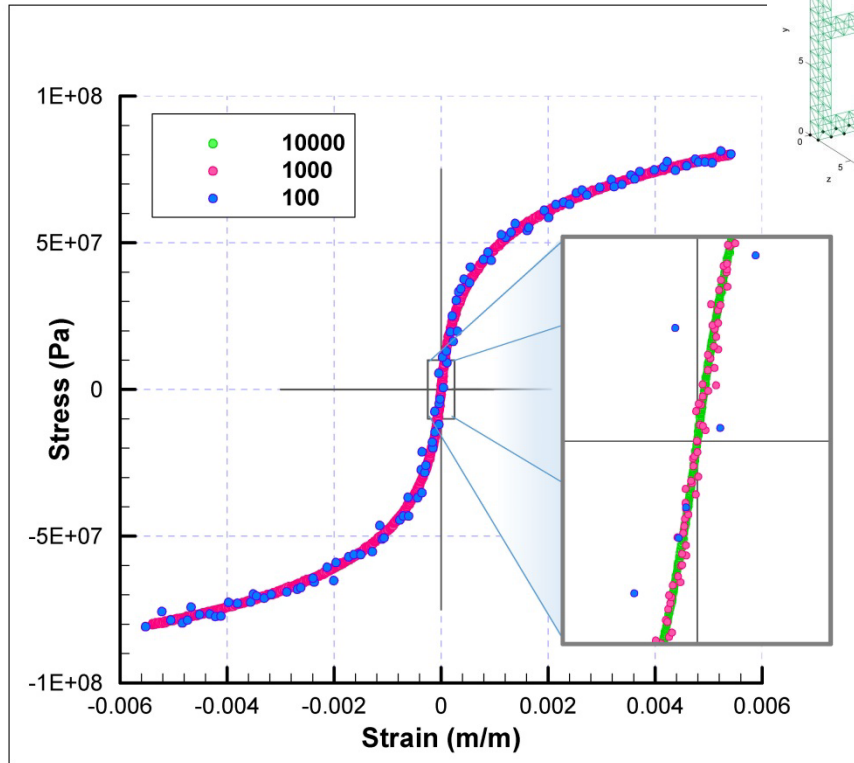
Convergence with respect to the data



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)

Convergence of fixed-point iteration

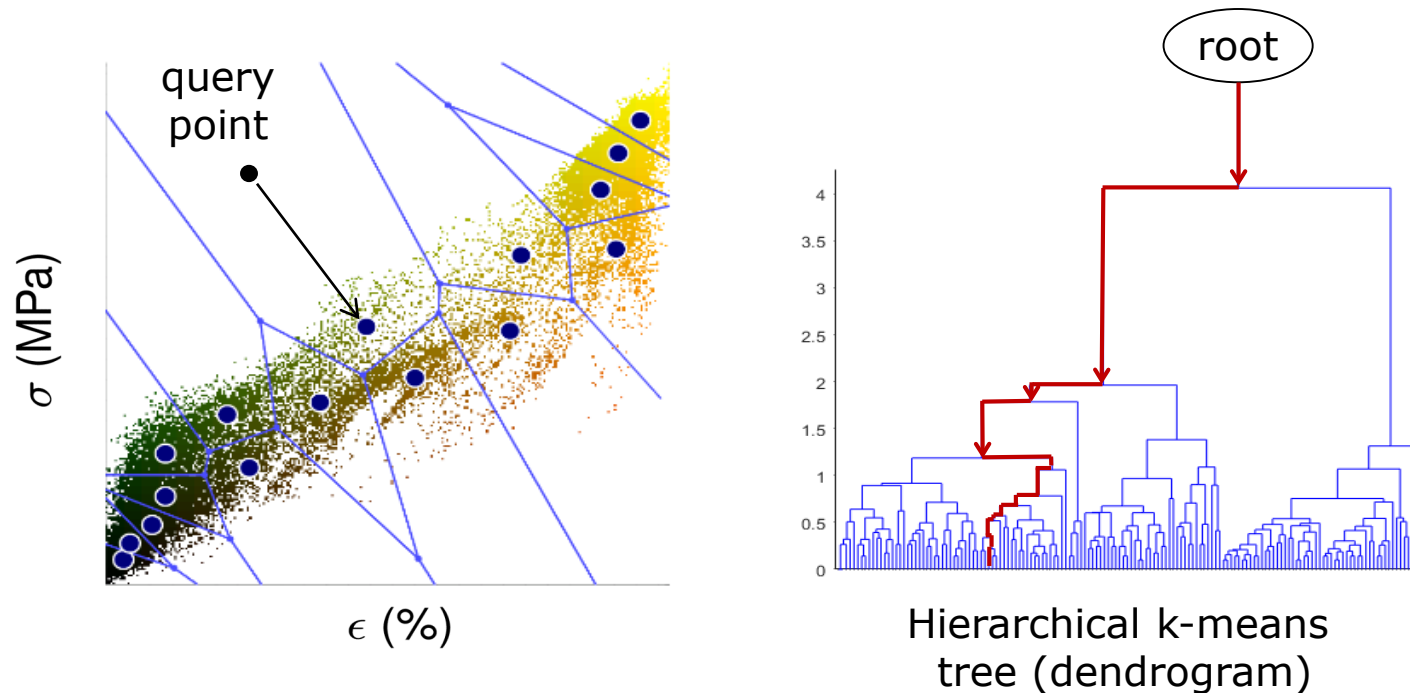


Sequence of
uniformly converging data sets
(increasing number of points,
decreasing scatter)

Convergence of fixed-point solver:

Each iteration requires two back-
substitutions for standard linear
systems and one material data
search/member

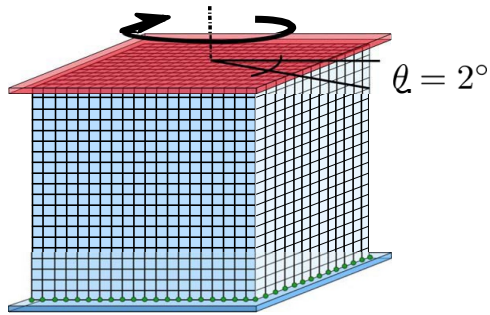
Navigating big material data sets (fast)



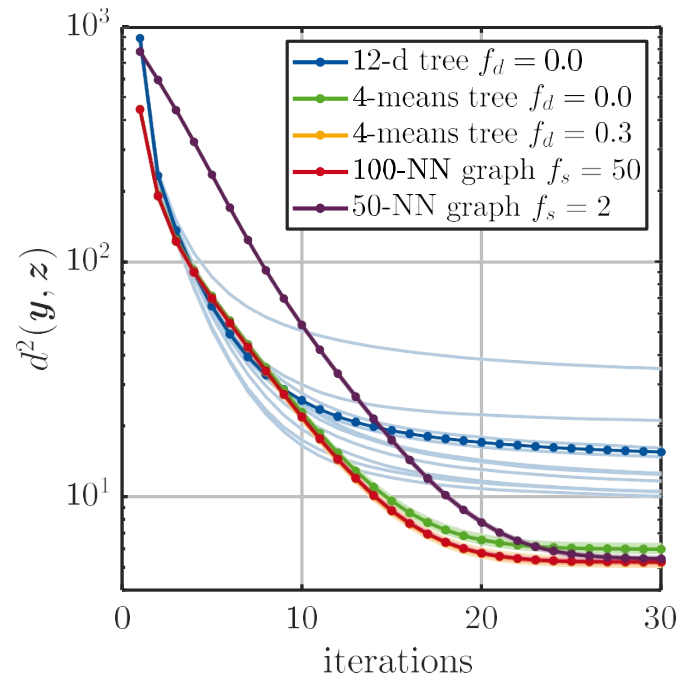
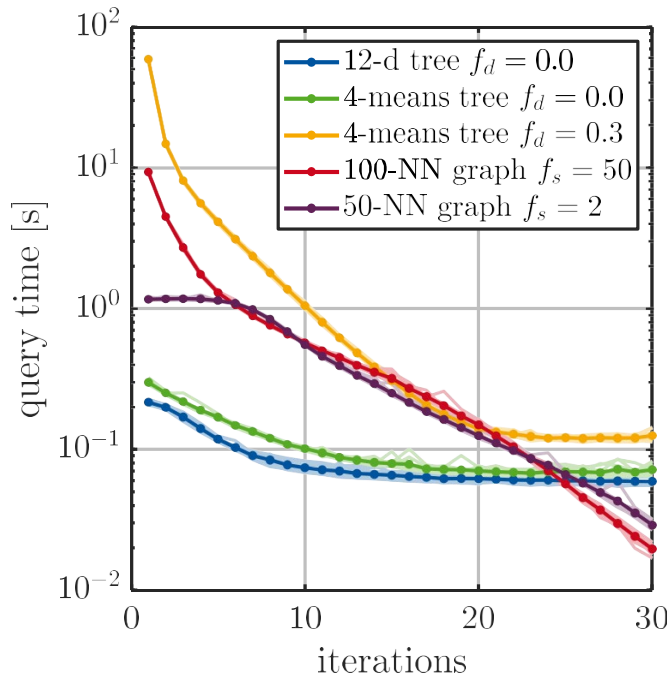
- Material data sets can be very large, cannot do naïve linear lookups!
- *k-means clustering* aims to partition n points into k clusters in which each point belongs to the cluster with the *nearest mean* (centroid).
- k -means clustering can be applied *recursively* to define a *k-means tree*
- *Queries*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

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Benchmark problem: Torsion of cube

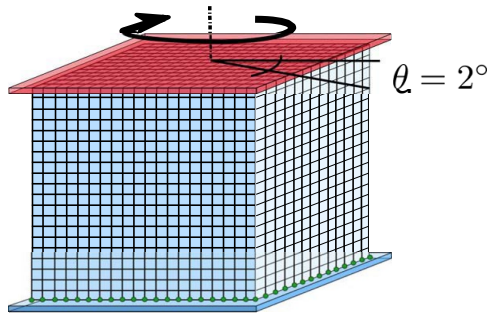


- DD nonlinear-elastic cube
- $20 \times 20 \times 20 = 8000$ elements
- 64,000 material (Gauss) points
- *100 million material data points*

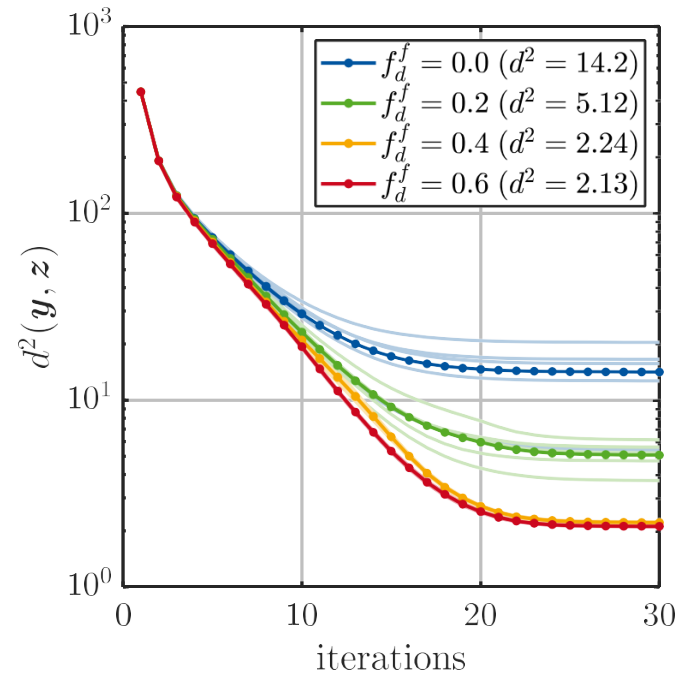
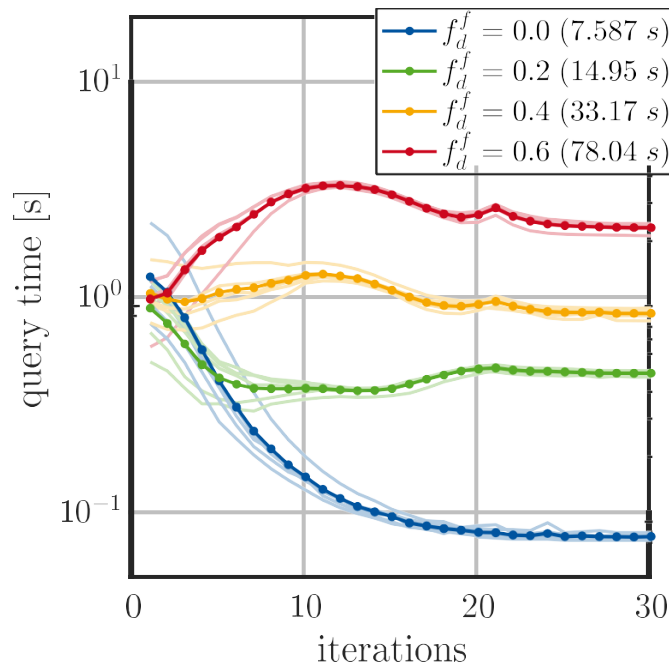


Comparison of search algorithms:
kd-tree, k-means and kNN graph algorithms

Benchmark problem: Torsion of cube

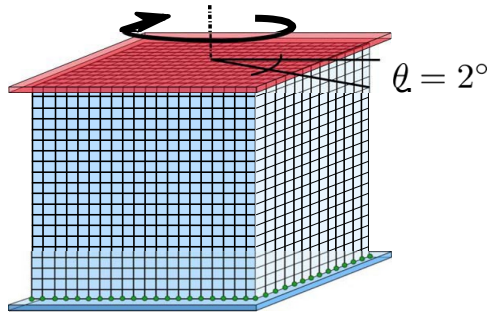


- DD nonlinear-elastic cube
- $20 \times 20 \times 20 = 8000$ elements
- 64,000 material (Gauss) points
- *1 billion material data points*

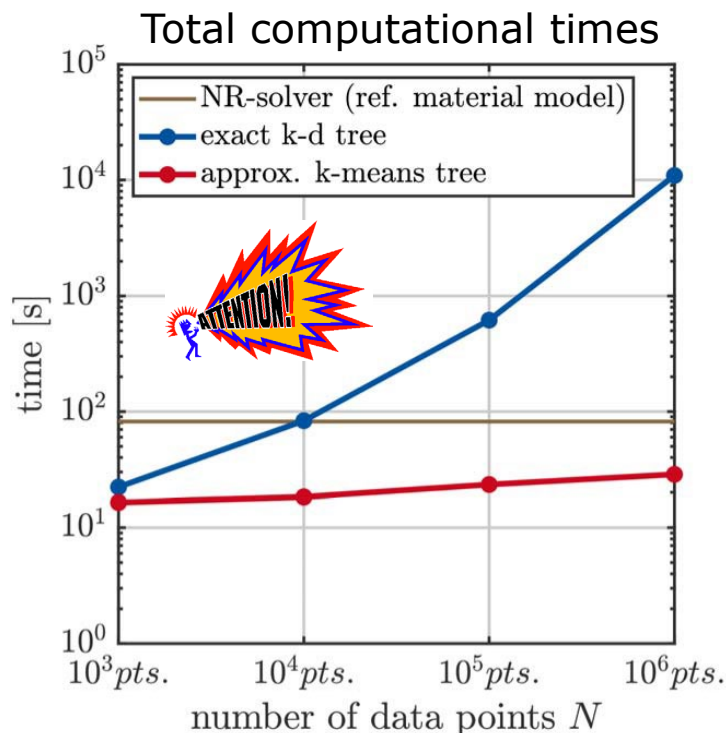


k-means with different degrees of backtracking.
search accuracy set to increase with DD iteration

Benchmark problem: Torsion of cube



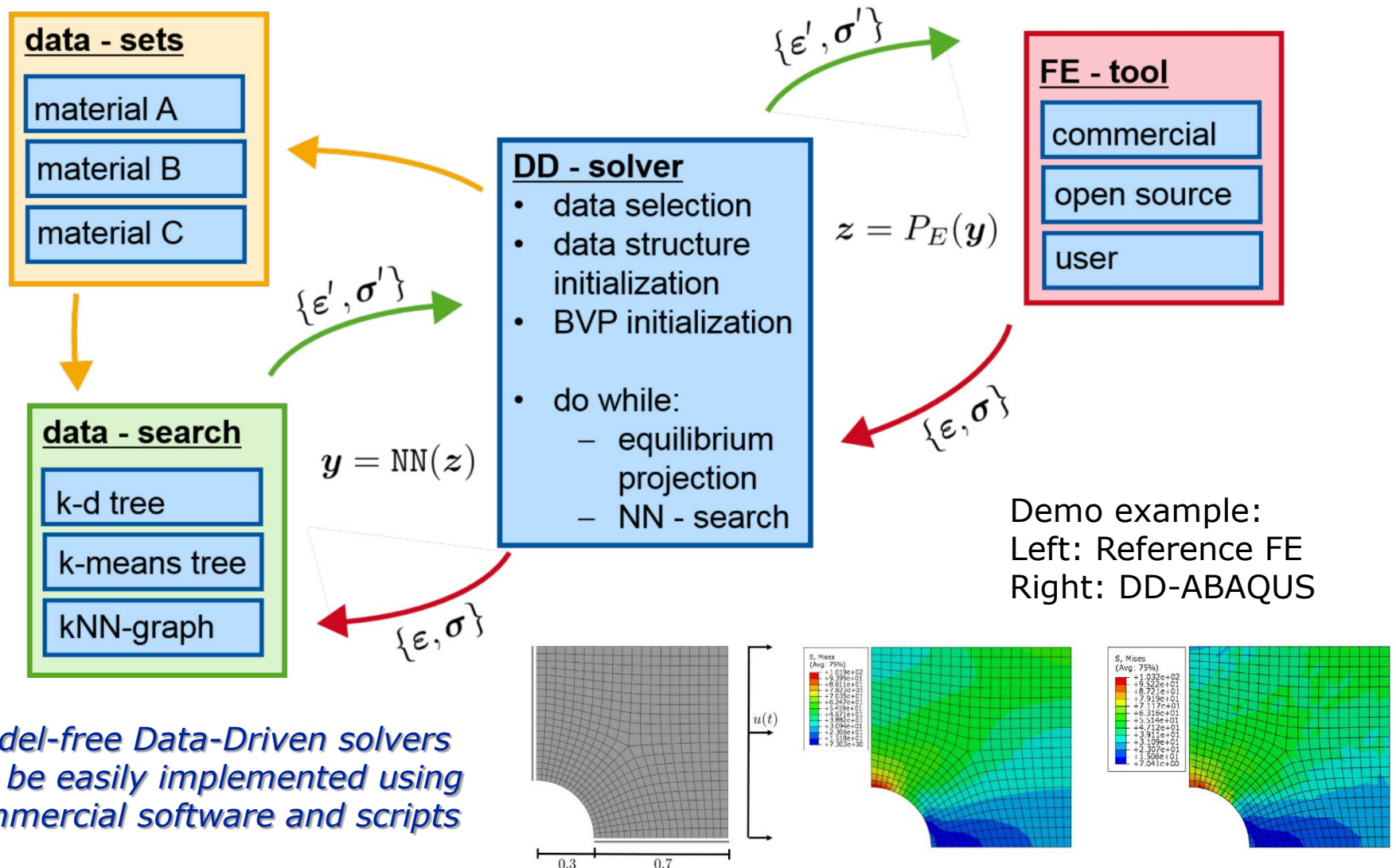
- DD nonlinear-elastic cube
- $20 \times 20 \times 20 = 8000$ elements
- 64,000 material (Gauss) points
- 10^3 - 10^6 material data points



- *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!*

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Implementation into commercial software

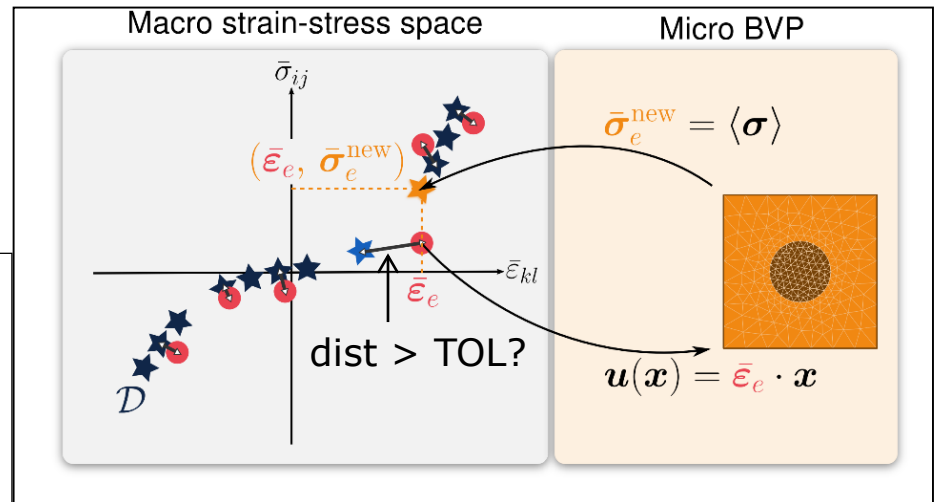
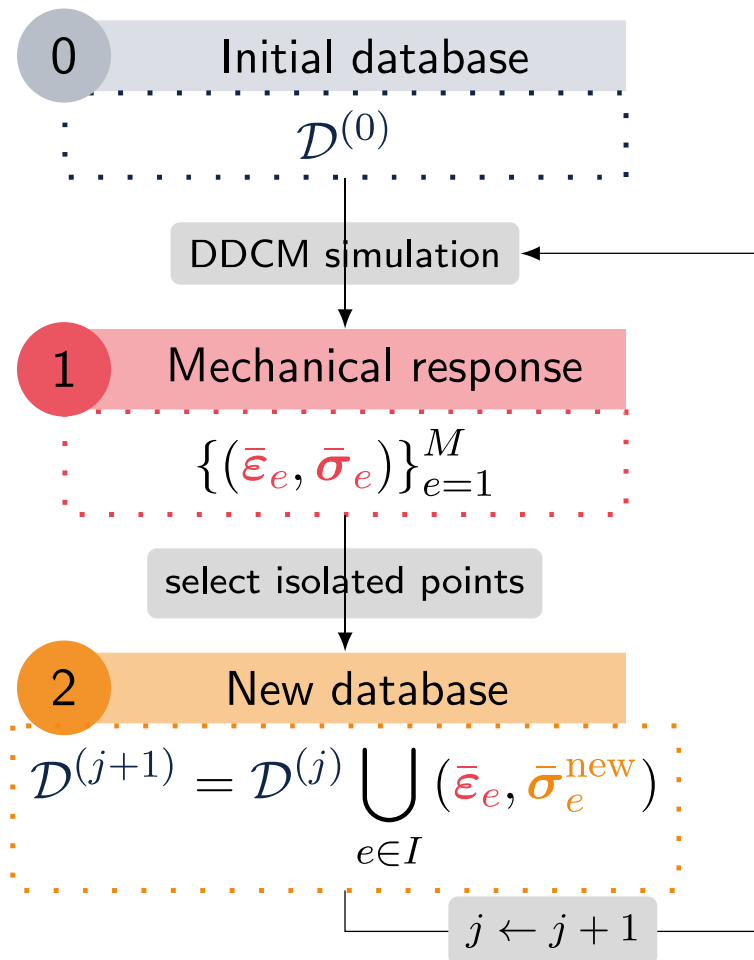


Model-free Data-Driven solvers can be easily implemented using commercial software and scripts

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*?
- Where do the data come from? *Data acquisition!*

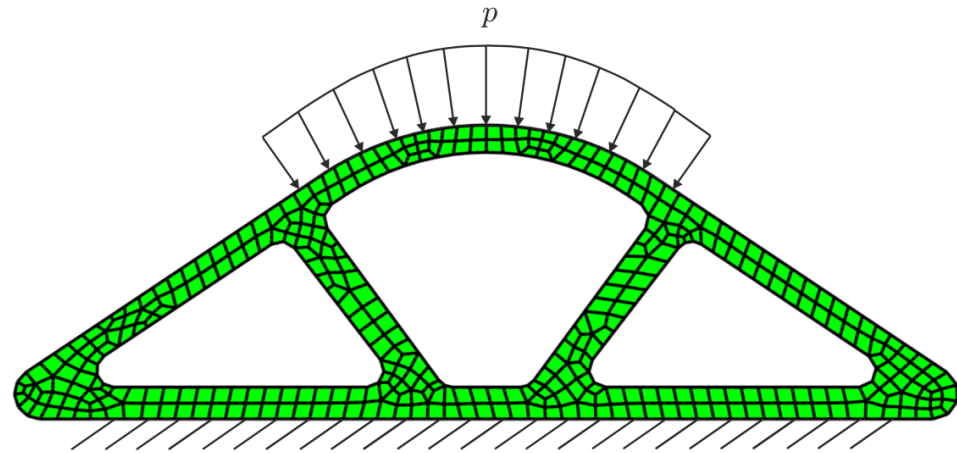
RVE data acquisition – Adaptive Learning



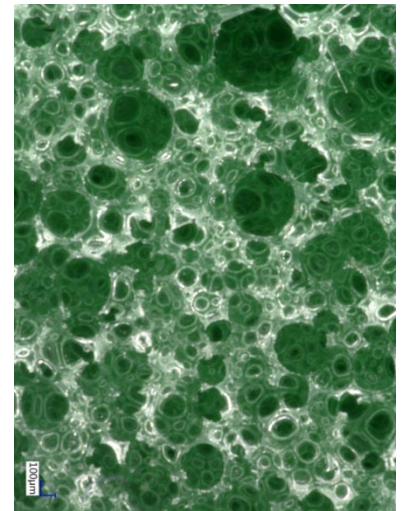
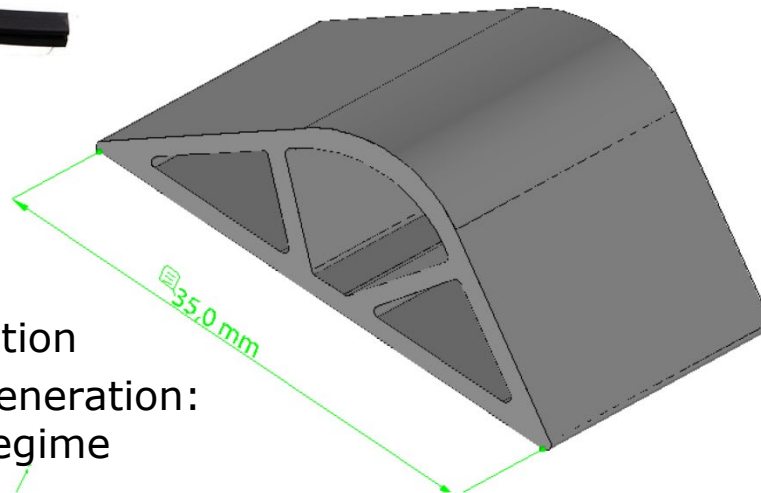
- *Generate new data from RVE when local state $\text{dist}(z_e, D) > TOL$!*
- Areas of *poor coverage* in the material data set are detected by DD solver, filled in *on-the-fly* as needed
- Material data set adapted to solution (*goal-oriented adaptive learning*)
- *Concurrent multiscale analysis* with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

Adaptive Learning – Elasticity

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



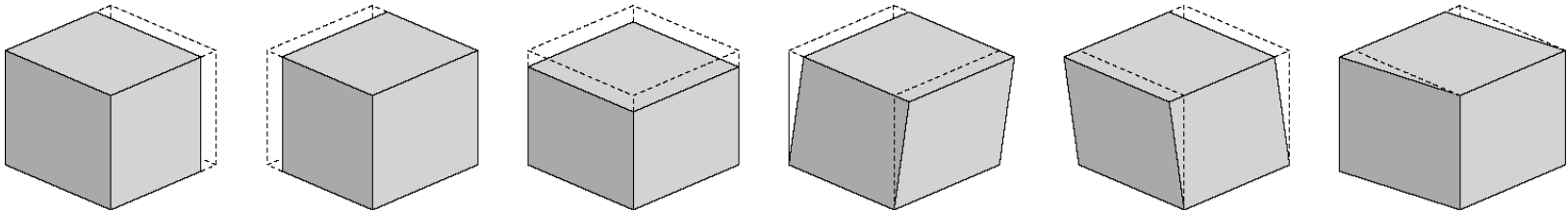
- Open-cell foam
- Isotropic material
- 3D analysis/simulation
- Microscopic data generation: linear/non-linear regime



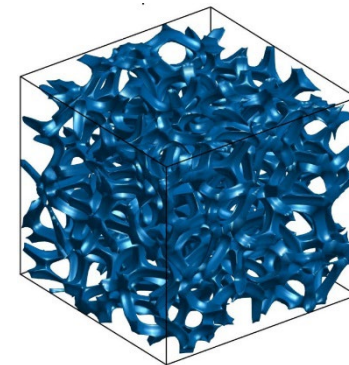
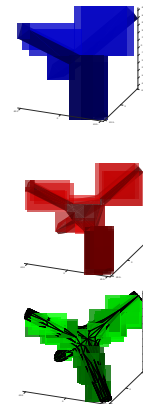
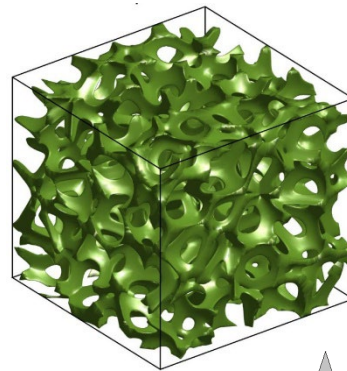
microstructure

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)

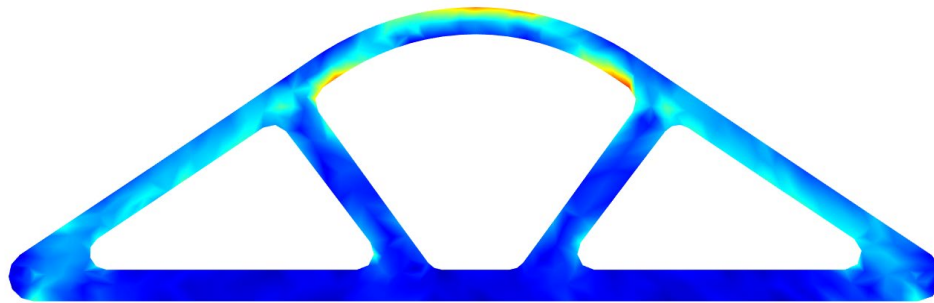


- 3D open-cell foam RVEs:

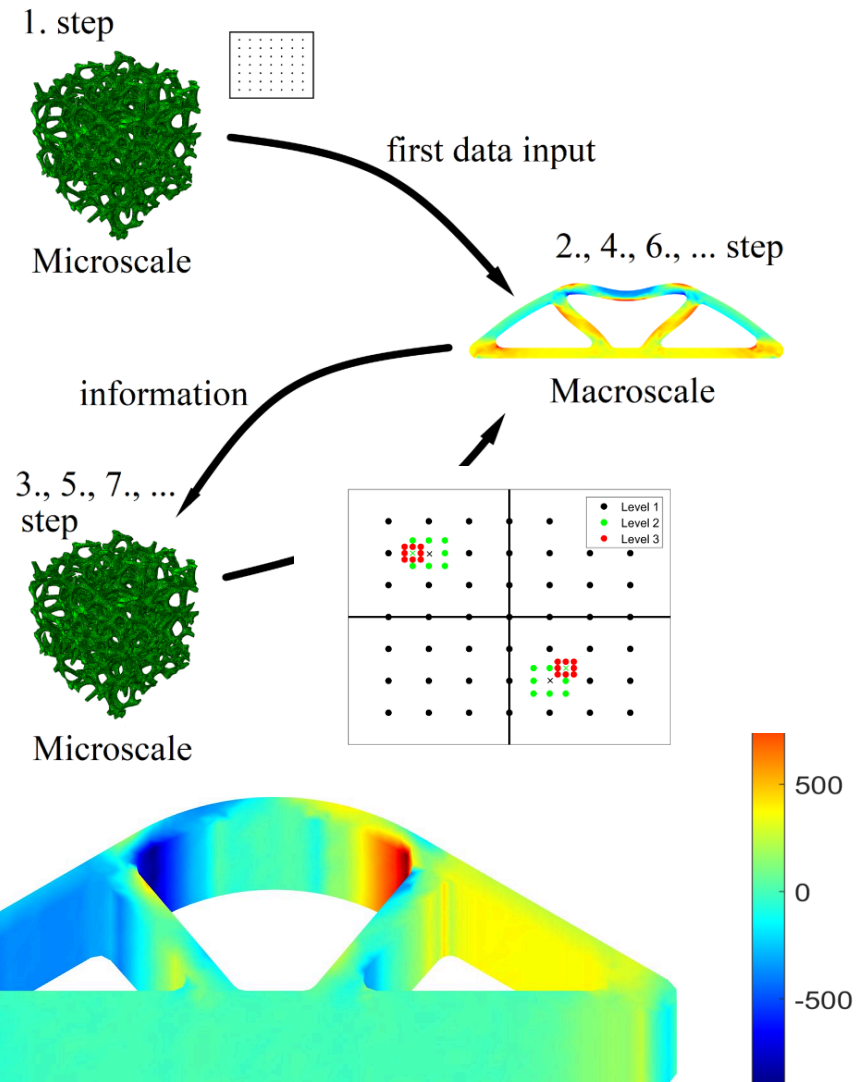
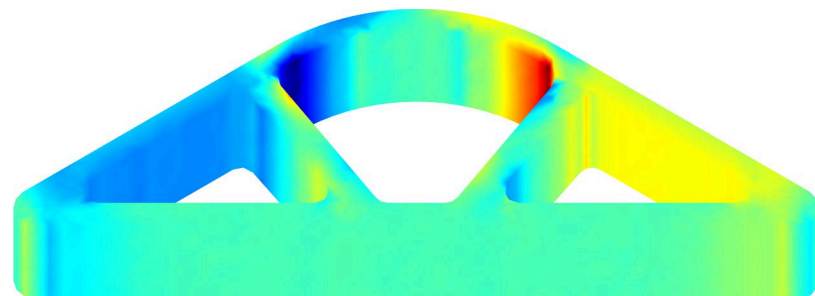
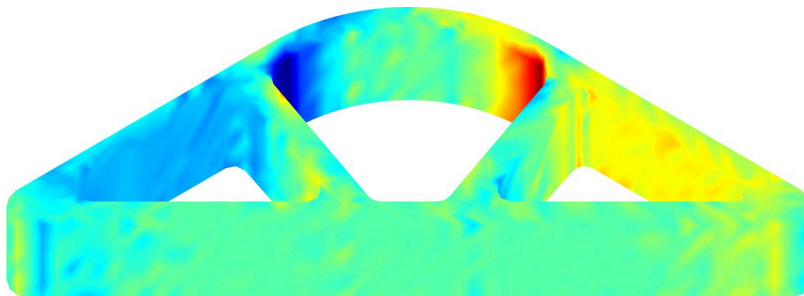


Adaptive Learning – Elasticity

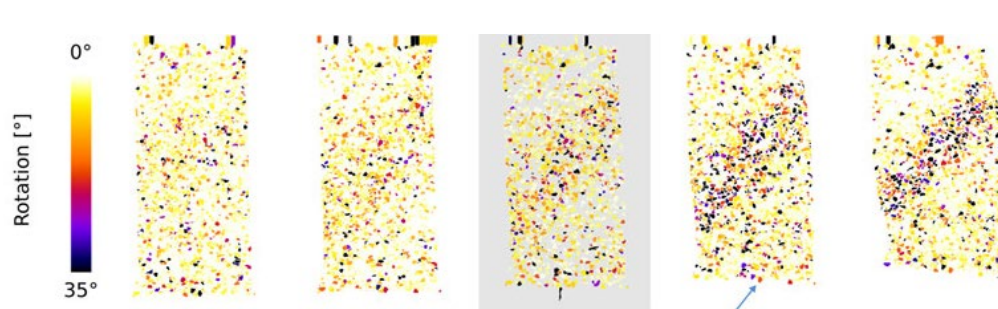
- Cauchy stress distribution (vertical)
- Start with a coarse level of data
- Identify data points of interest
- Do additional RVE calculations
- Redo computation at finer level till TOL



- Shear stress at level 1 and level 4



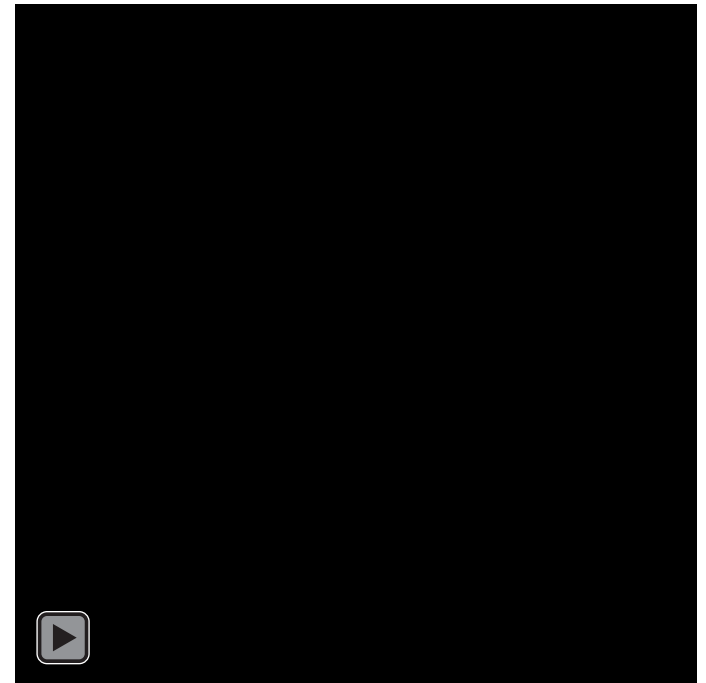
Adaptive Learning – Plasticity



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.

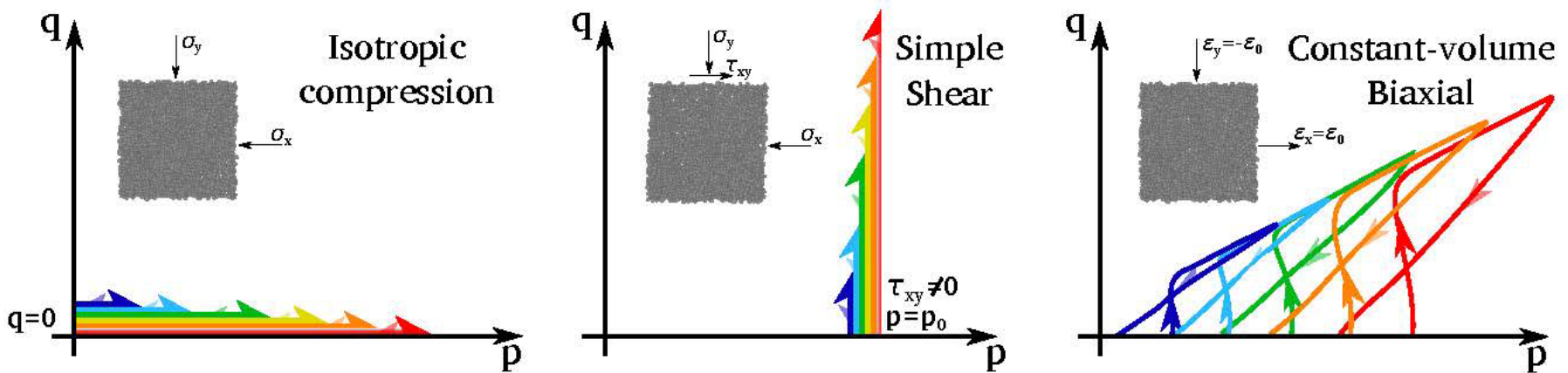
RVE
generation



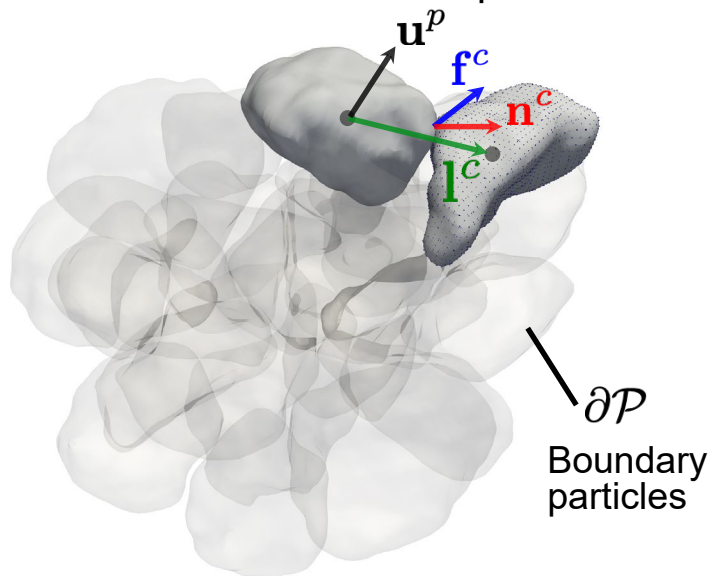
Kawamoto, R., Andò, E., Viggiani, G., Andrade,
J.E., *JMPS*, **91** (2016) 1-13.

K. Karapiperis, L. Stainier, M. Ortiz, J.E. Andrade, *JMPS*, (2020) 104239. Michael Ortiz
Oxford 11/07/22

Adaptive Learning – Plasticity

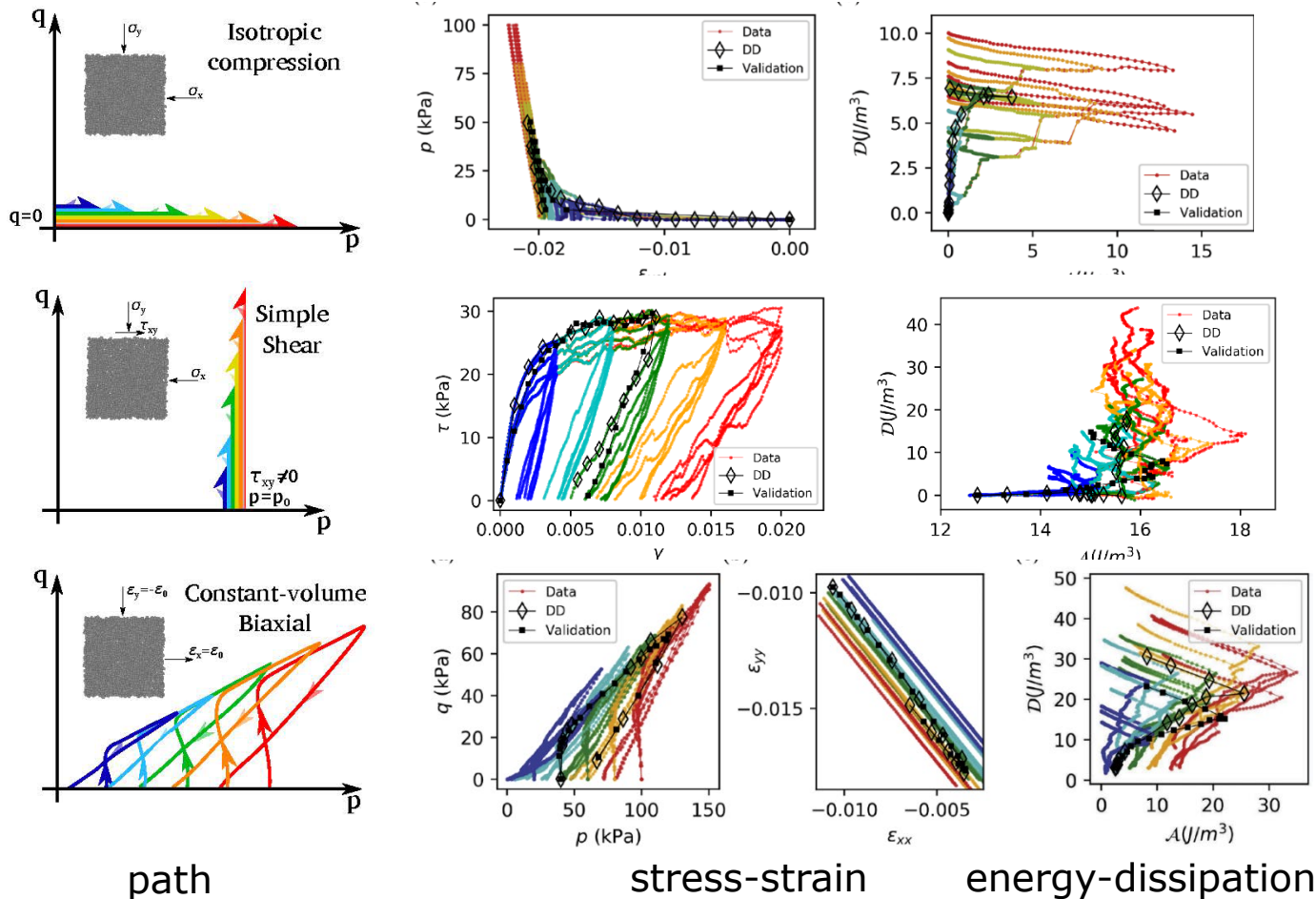


Selected paths for building the material data repository



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

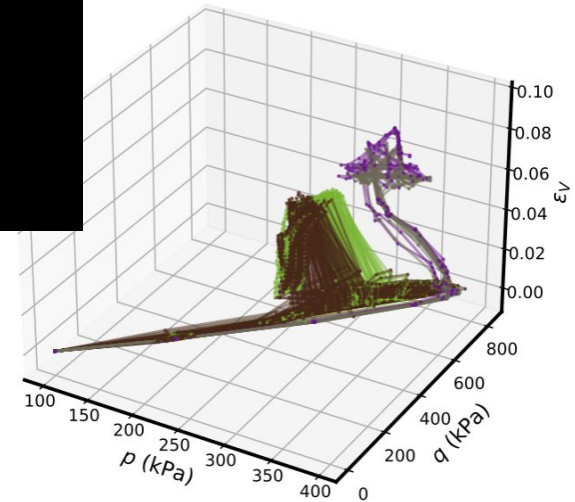
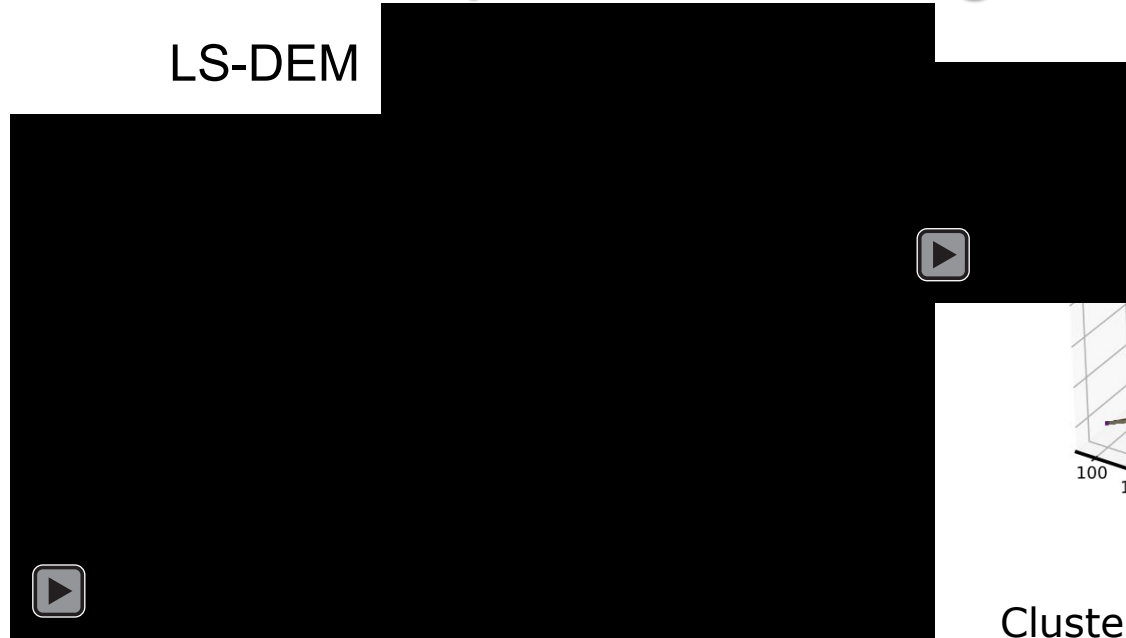
Adaptive Learning – Plasticity



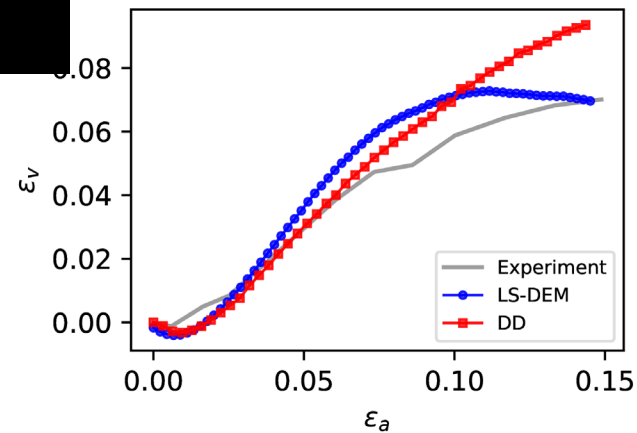
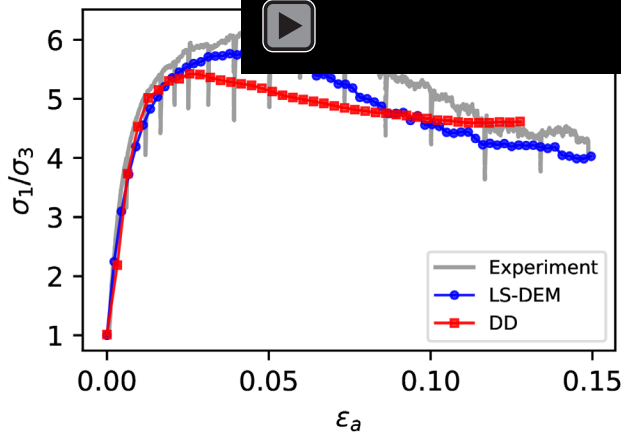
Compilation of path data for Hatsun angular sand
computed from RVEs using LS-DEM

Adaptive Learning – Plasticity

LS-DEM

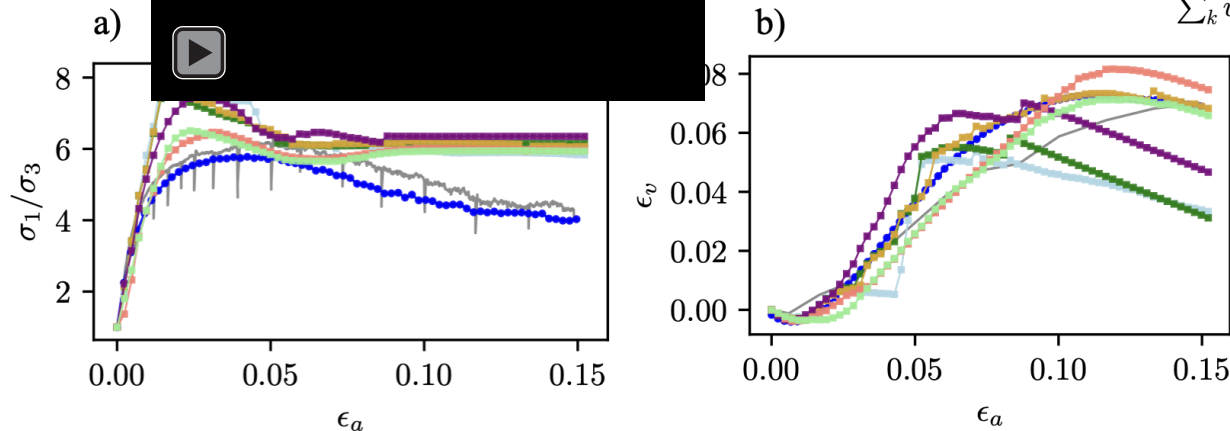
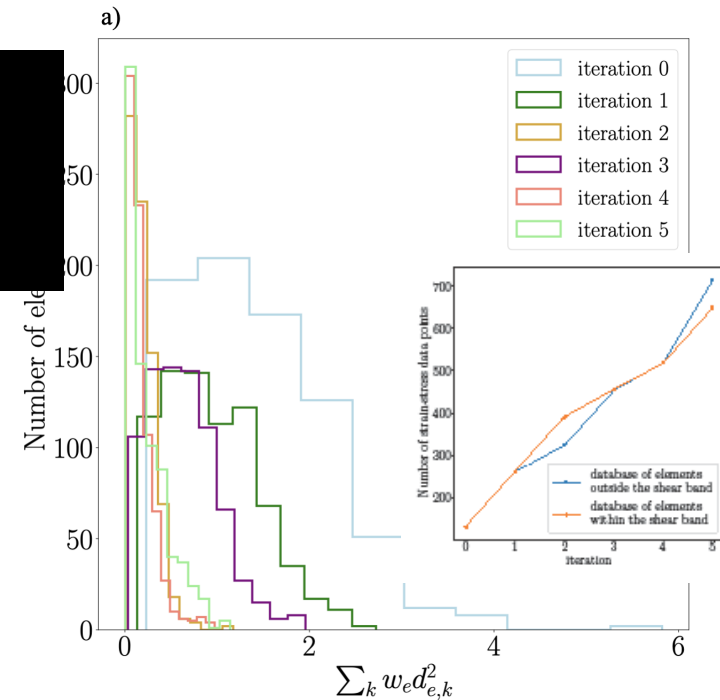
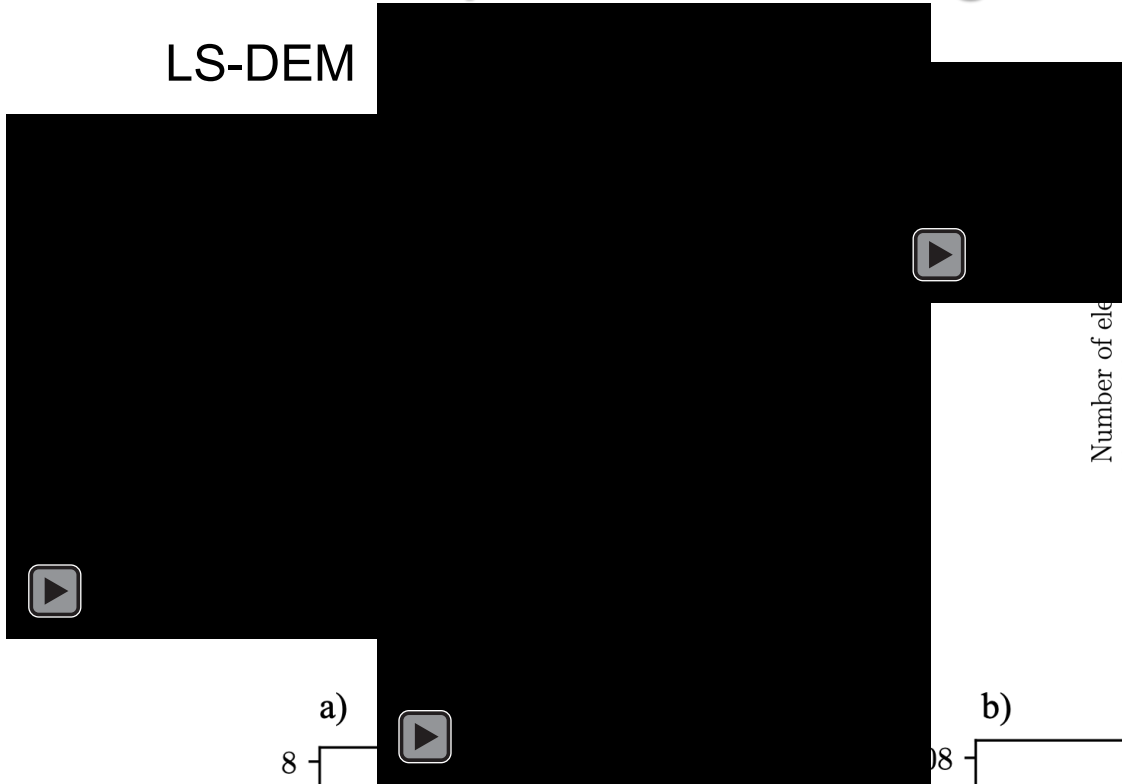


Clustering of mechanical paths
traversed in the initial DD simulation



Adaptive Learning – Plasticity

LS-DEM



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

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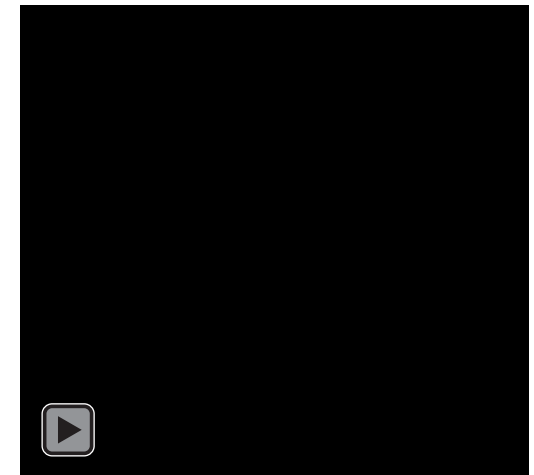
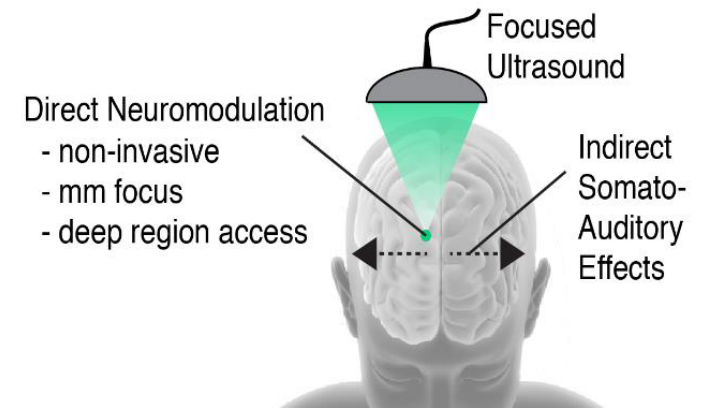
Concurrent (on-the-fly) data acquisition: Towards DD patient-specific UNM

- *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)

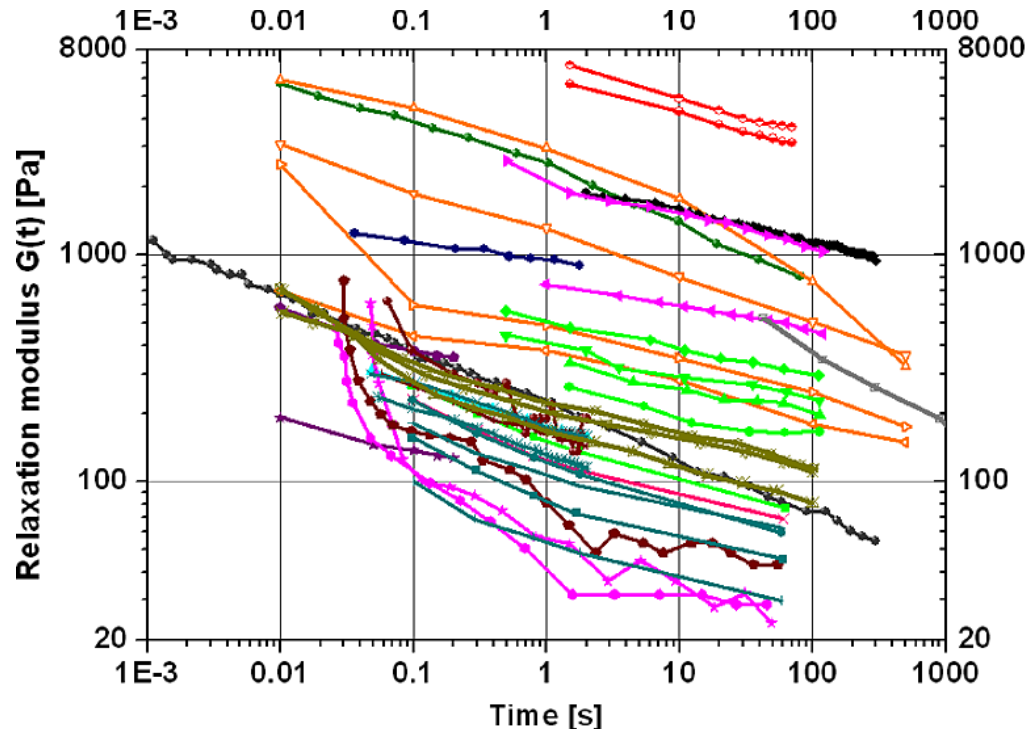


3D FE simulation of
Pressure waves under
Transcranial LIFUS (100 kHz).

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Towards DD patient-specific UNM

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



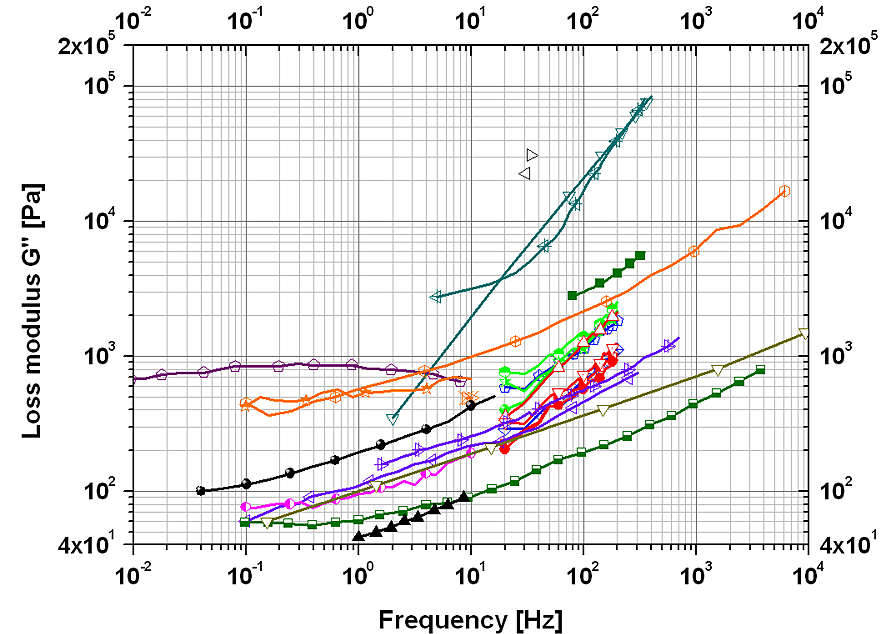
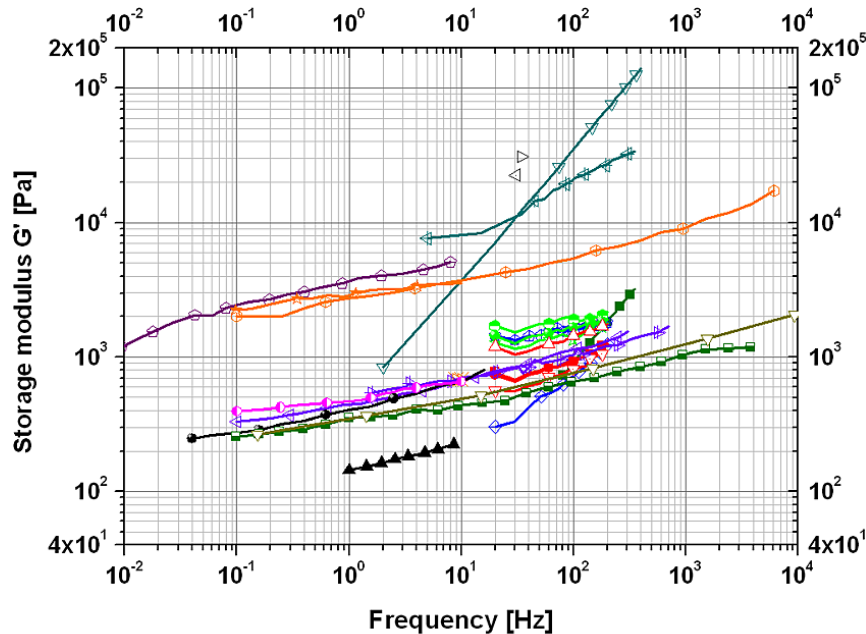
In vitro relaxation modulus versus time from literature survey.
Curves were obtained from either compression or shear
quasi-static experiments.

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



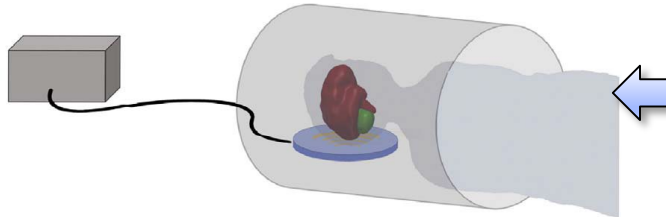
Storage and loss moduli of brain tissue compiled from literature survey of *in vitro* dynamic frequency sweep tests in shear.

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.

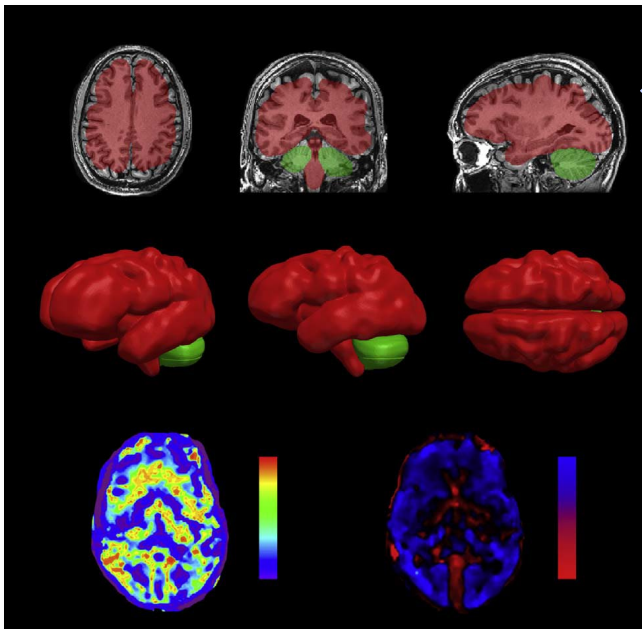
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Towards DD patient-specific UNM

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

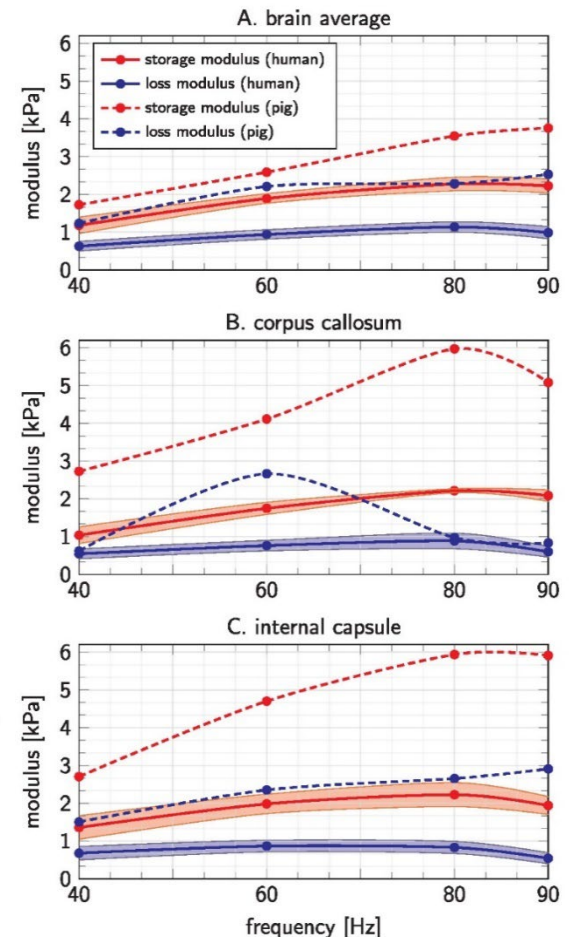


Human subjects scanned in the supine position



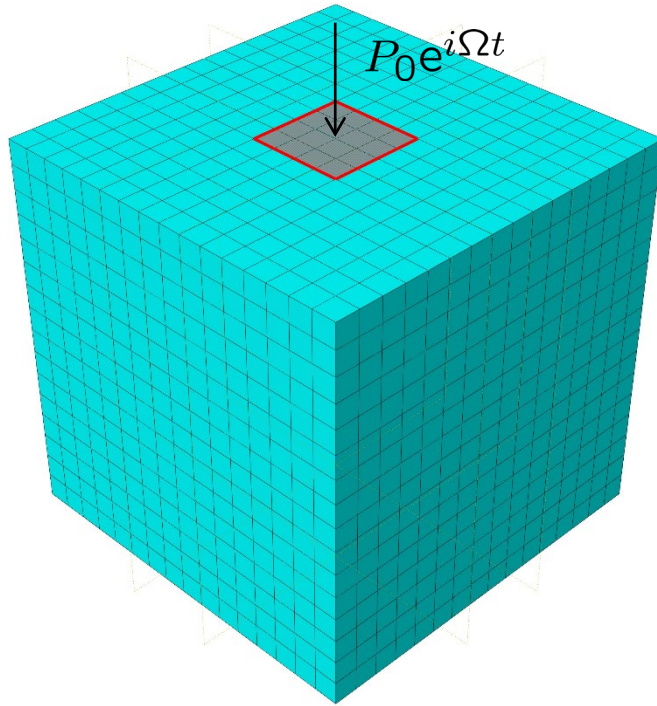
Structural scan, reconstruction map of storage and loss moduli

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

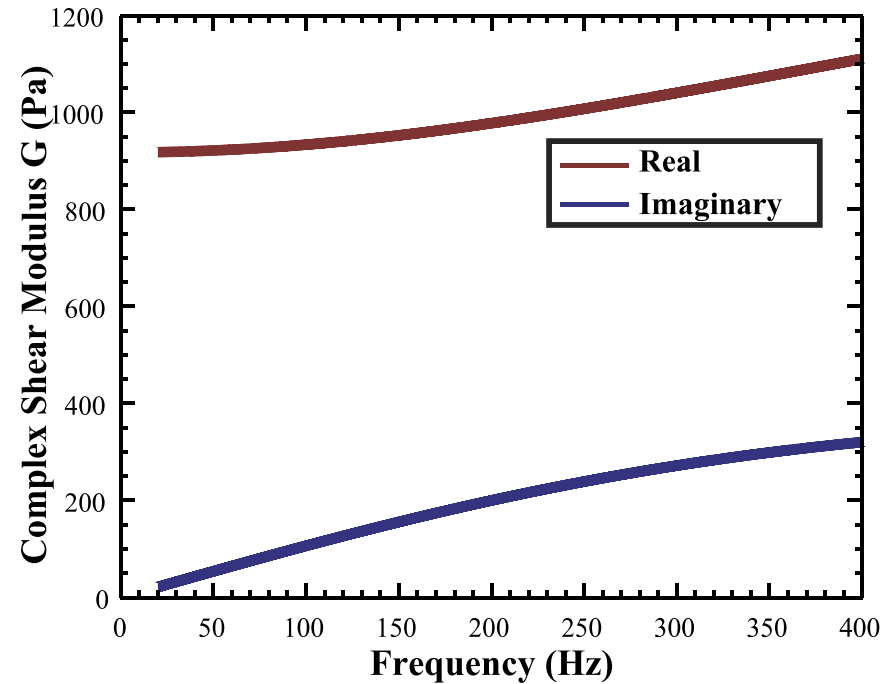


Model-free Data-Driven viscoelasticity

- 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



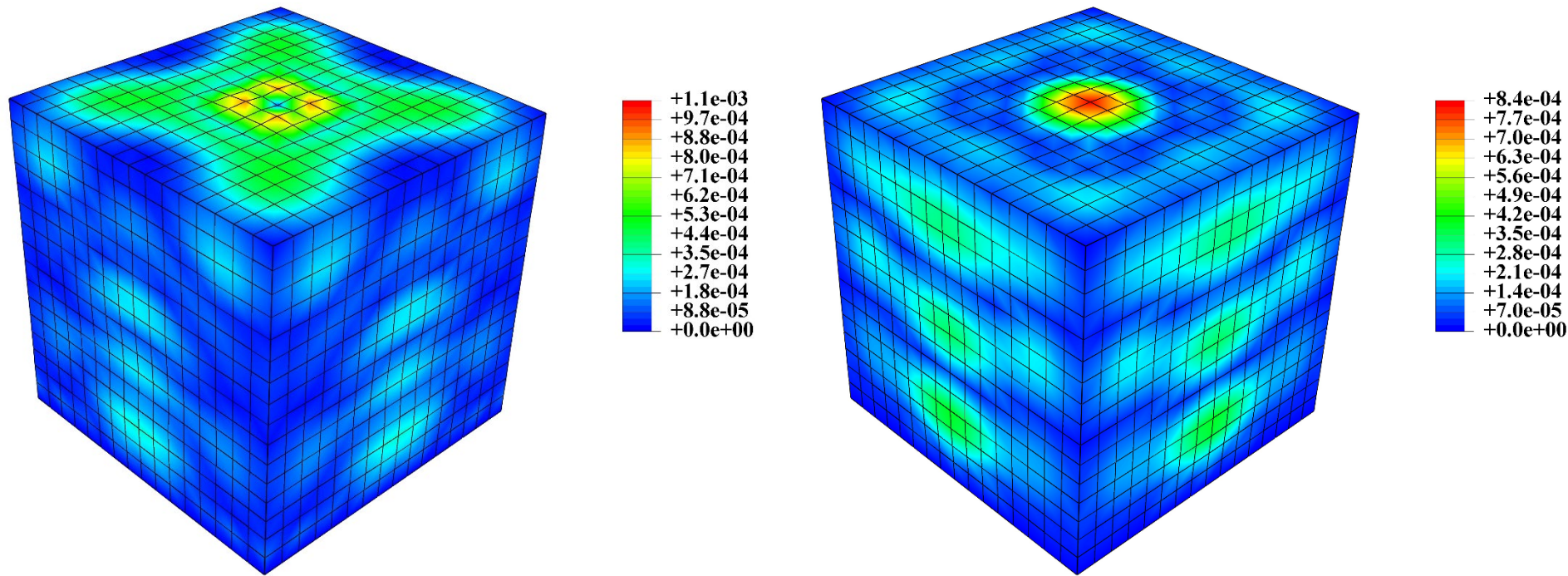
Complex moduli of agarose gel measured using dynamic shear testing (DST) and magnetic resonance elastography (MRE).

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

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Model-free Data-Driven viscoelasticity

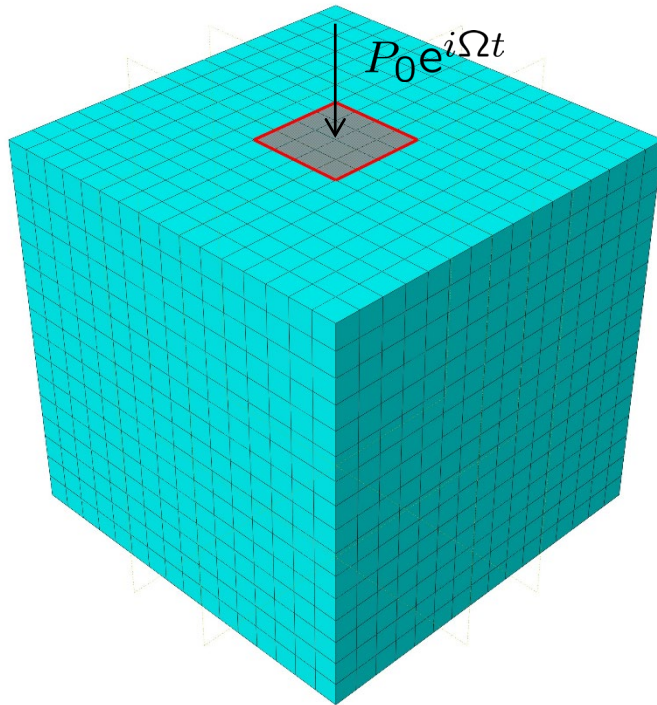
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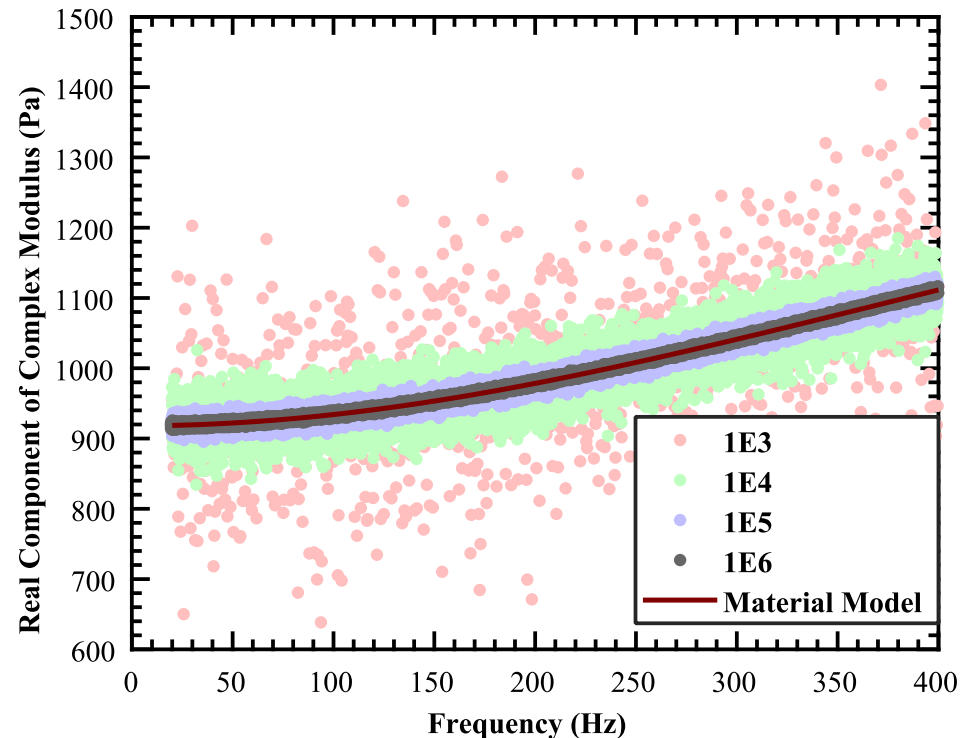
Insonated agarose gel block.
Displacements for applied frequency $\Omega = 1000$ Hz.
a) Real component. b) Imaginary component.

Model-free Data-Driven viscoelasticity

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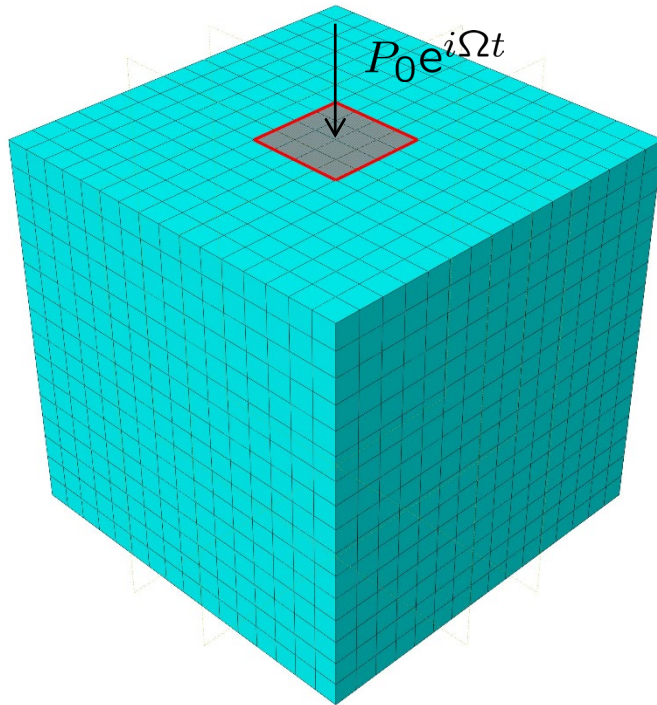
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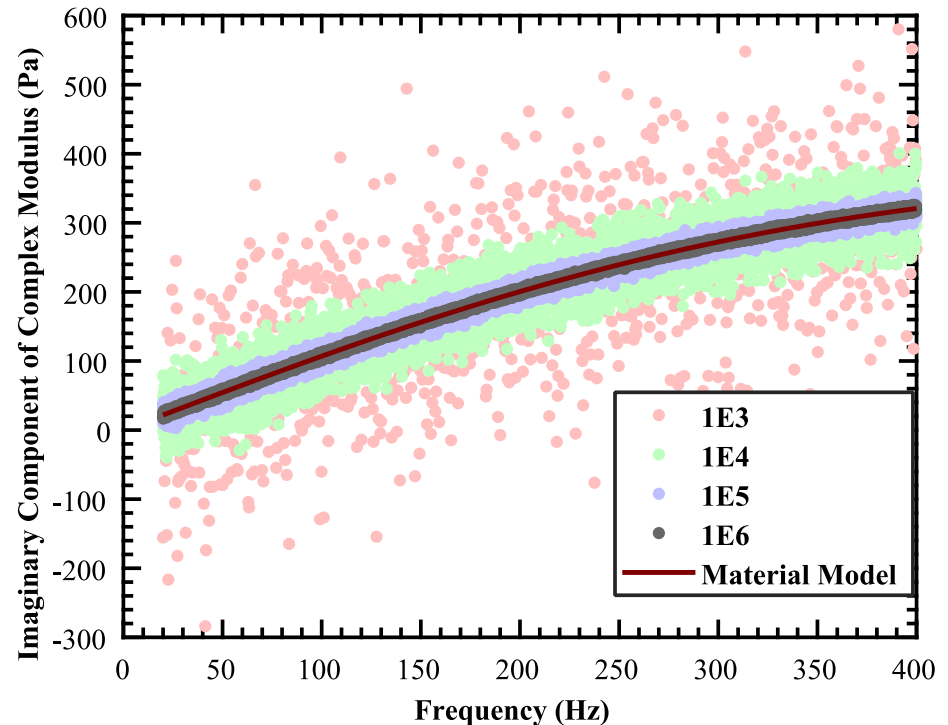
Data of sizes 10^3 , 10^4 , 10^5 and 10^6 used in the DD calculations. Real component of complex modulus.

Model-free Data-Driven viscoelasticity

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



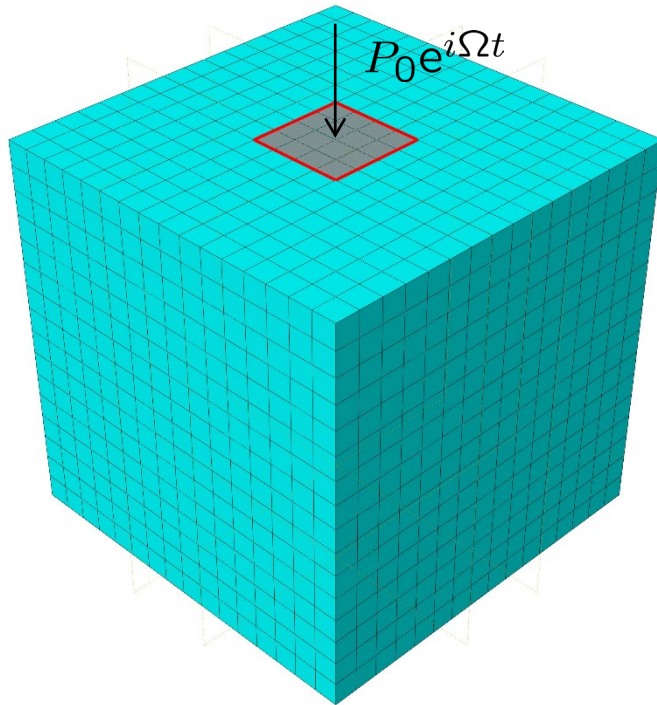
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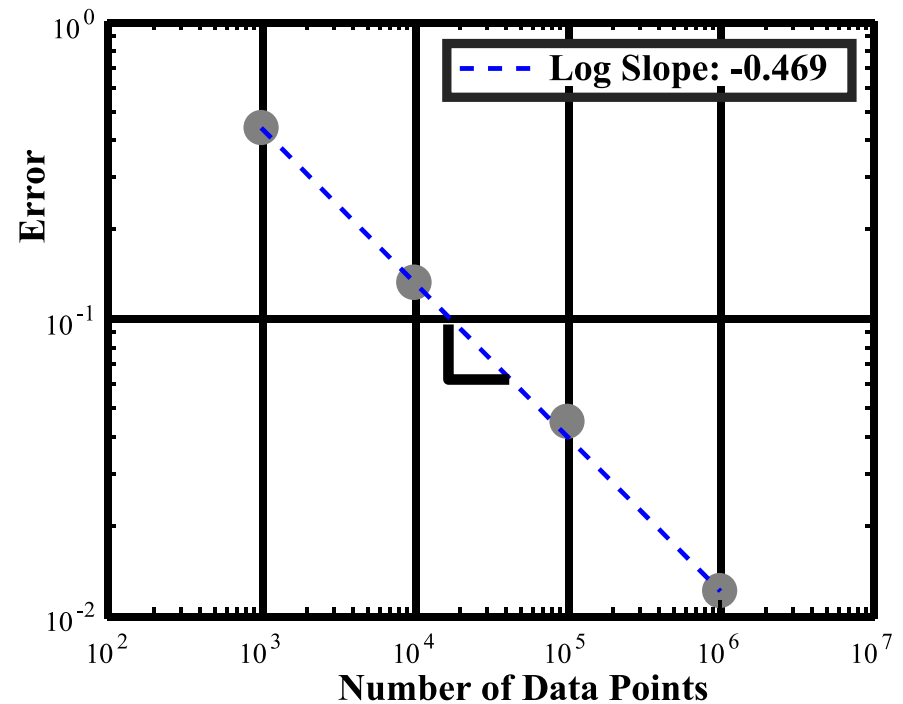
Data of sizes 10^3 , 10^4 , 10^5 and 10^6 used in the DD calculations. Imaginary component of complex modulus.

Model-free Data-Driven viscoelasticity

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

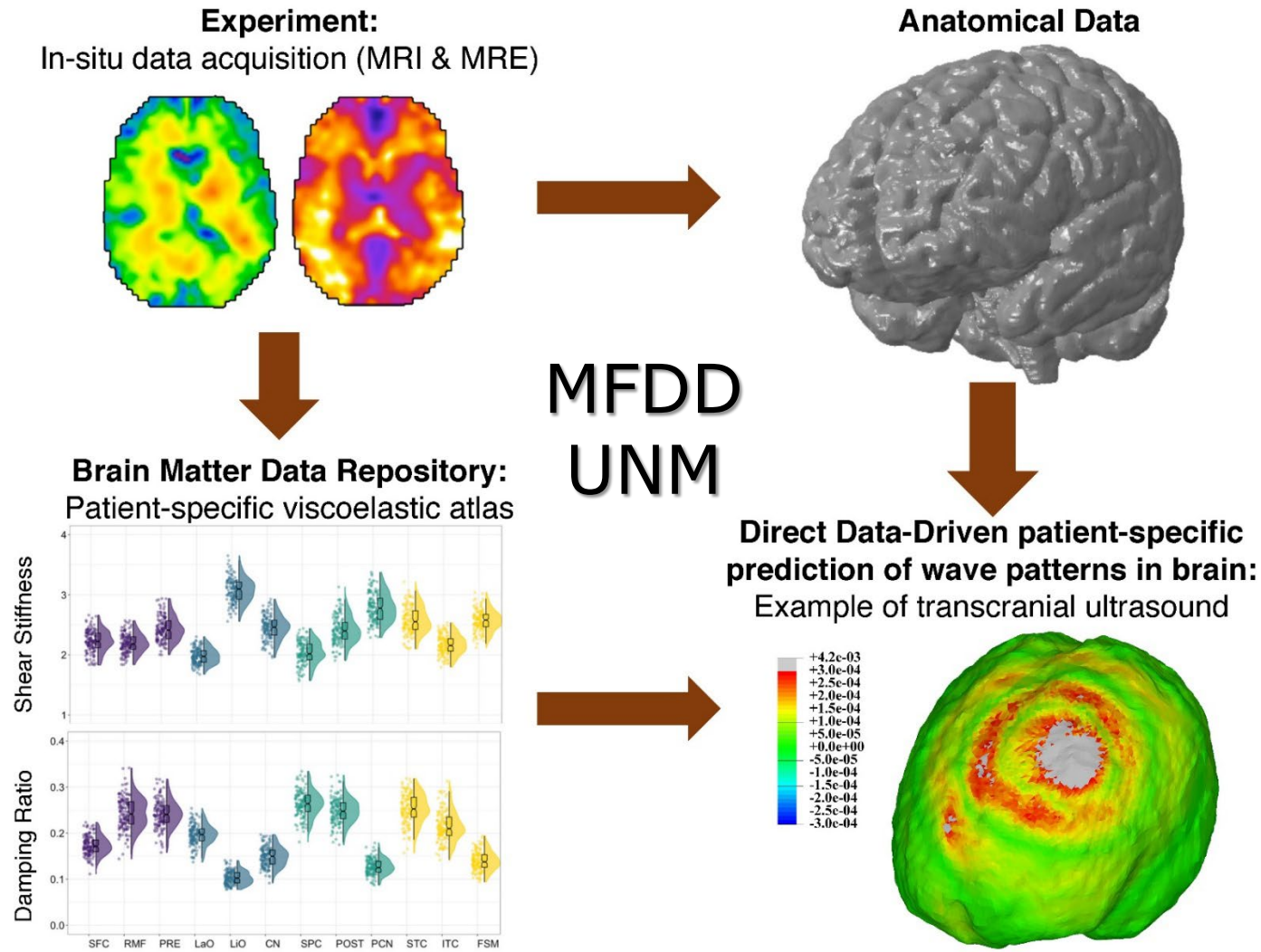


Finite-element discretization of agarose gel block into hex-elements. The square on the top surface marks area of application of harmonic pressure



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

Towards DD patient-specific UNM



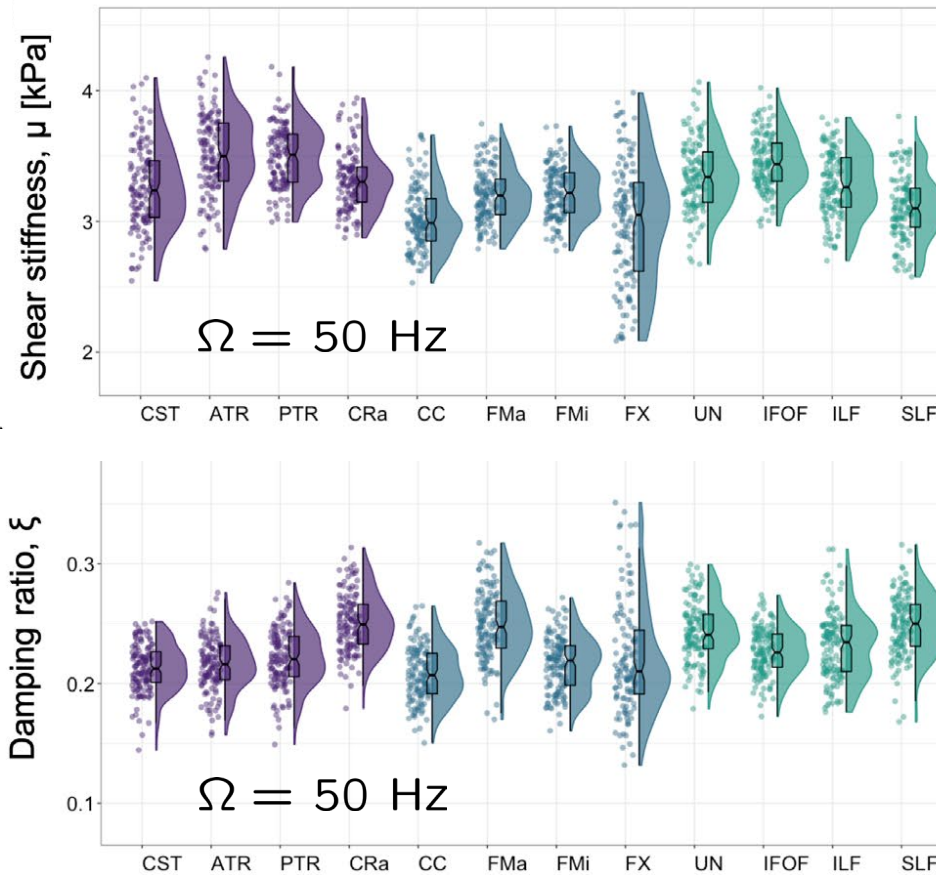
L.V. Hiscox *et al.*, *Hum Brain Mapp.*, 2020;**41**:5282–5300

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

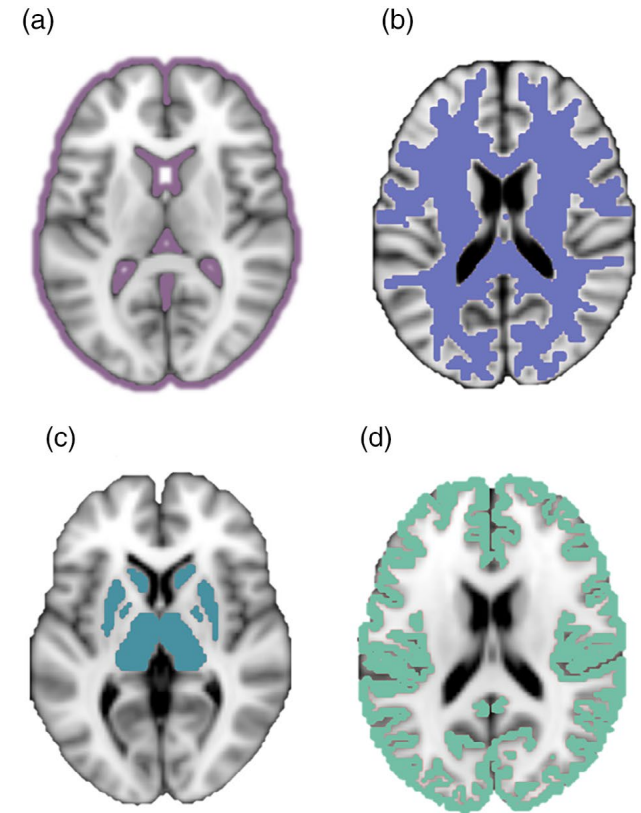
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- MRE is based on the magnetic resonance imaging of shear wave propagation.

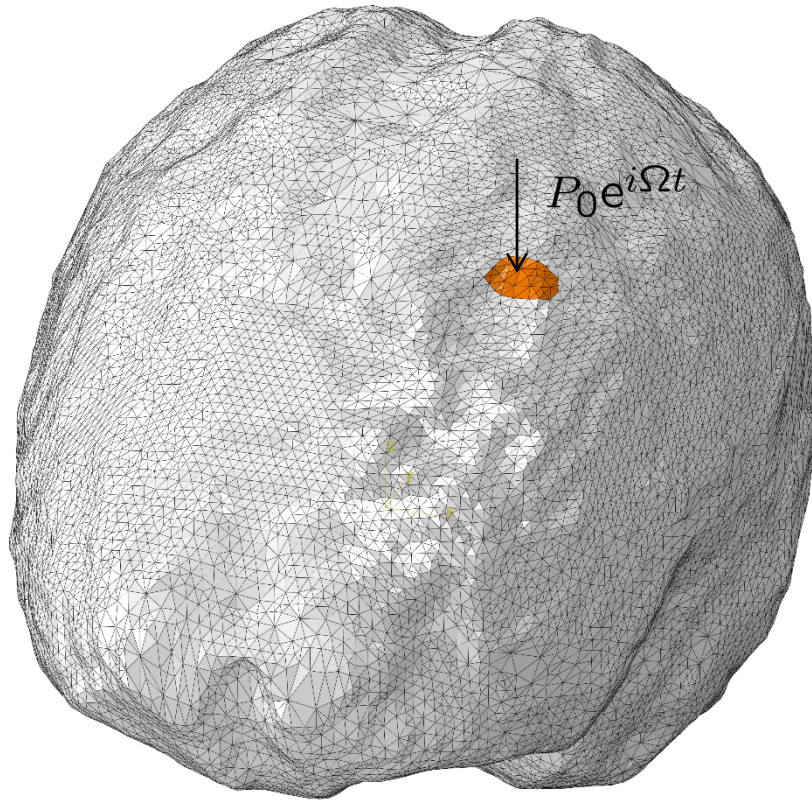


MRE viscoelastic data atlas at 12 regions of interest (Desikan–Killiany–Tourville cortical labelling protocol).

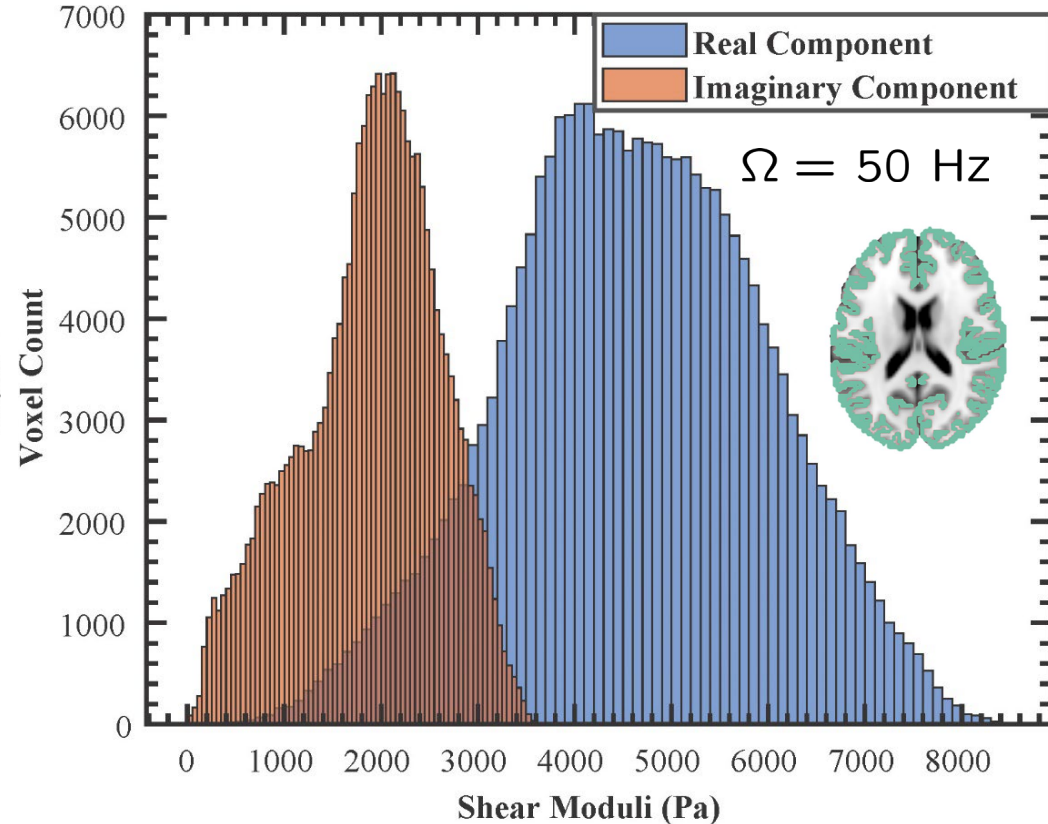


MRE data for (a) the entire brain (b) white matter (c) subcortical gray matter (d) cerebral cortex.

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.

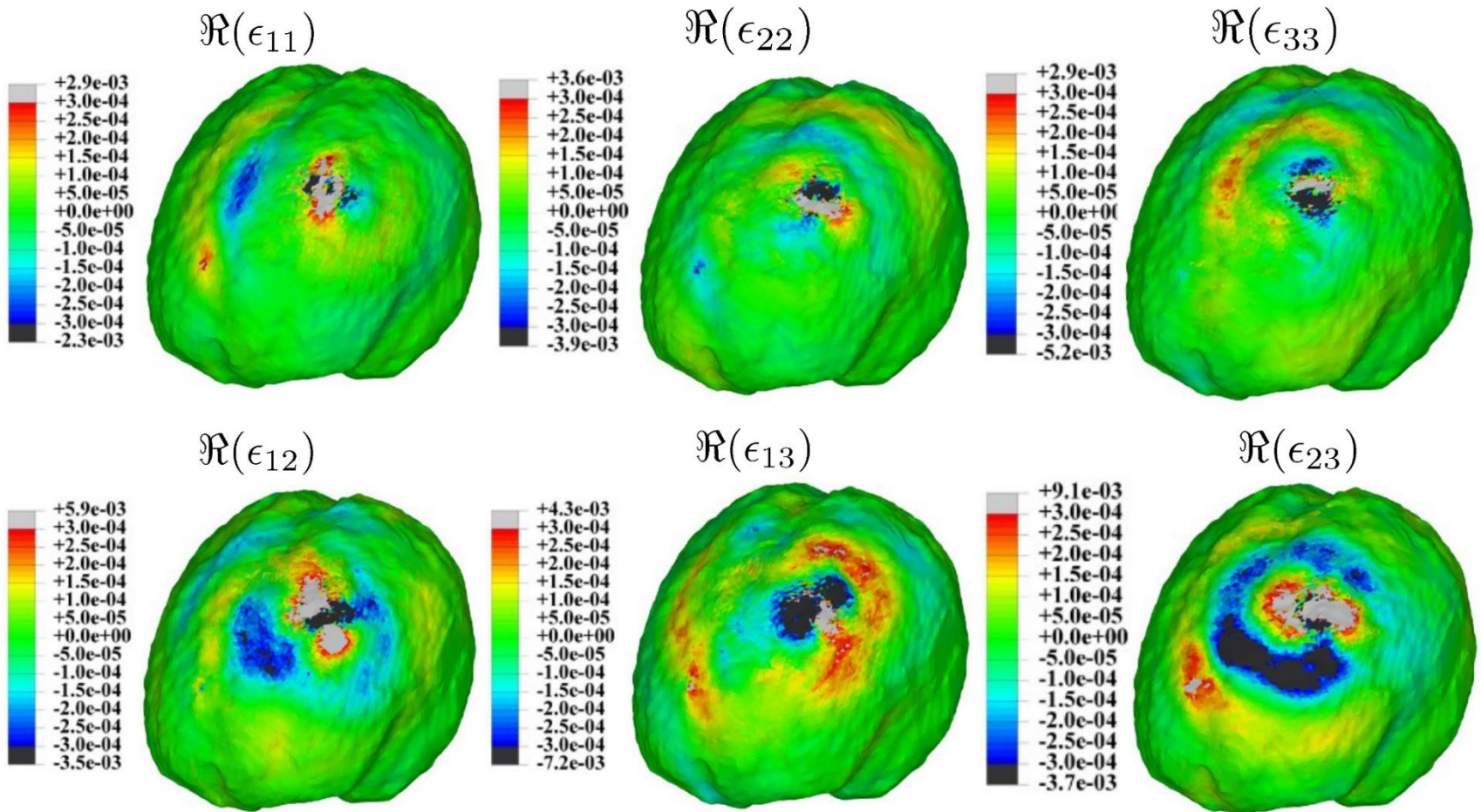


Histogram of complex moduli from in vivo MRE data. The finite-element model is co-registered to the MRE data.

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

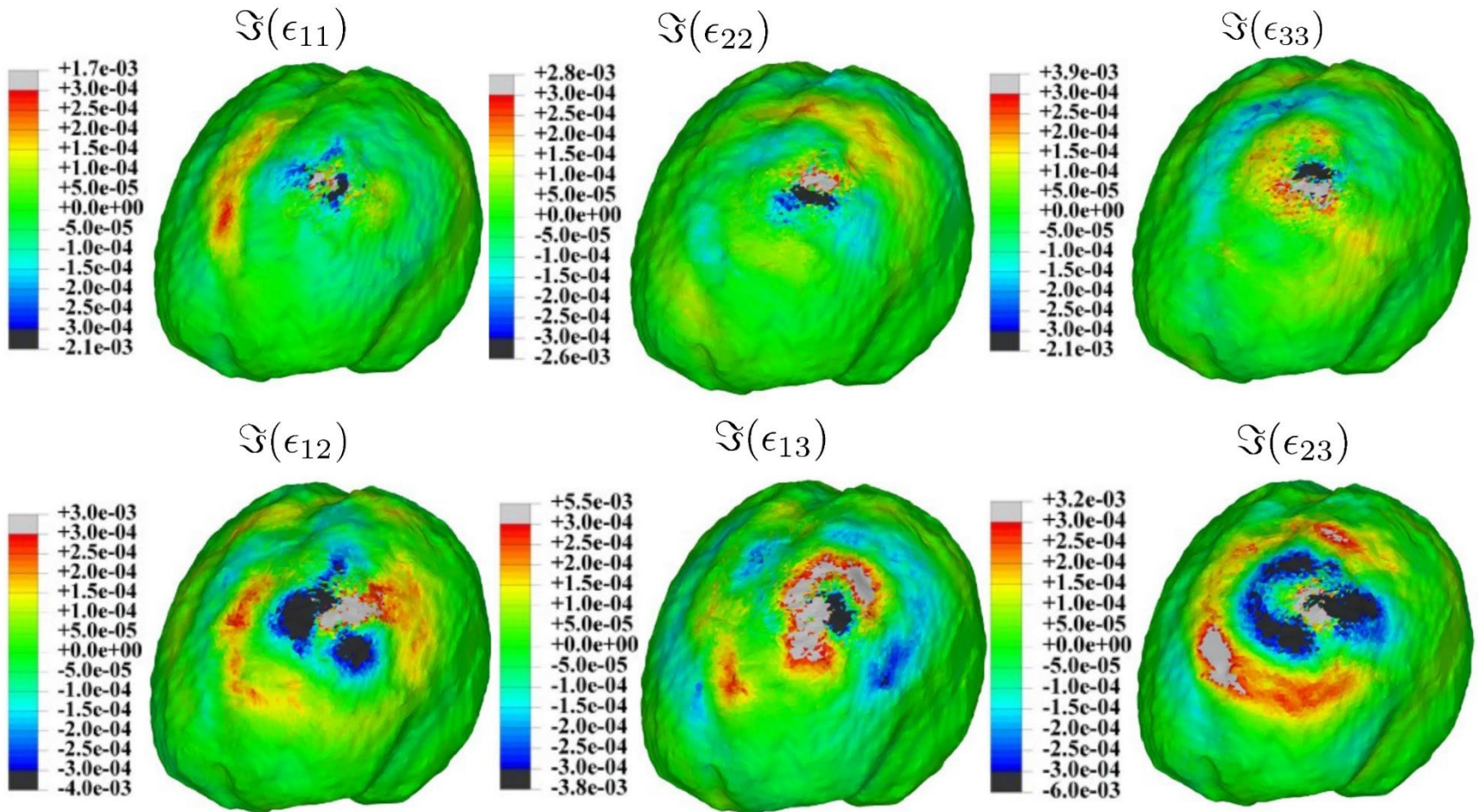
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Towards DD patient-specific UNM



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

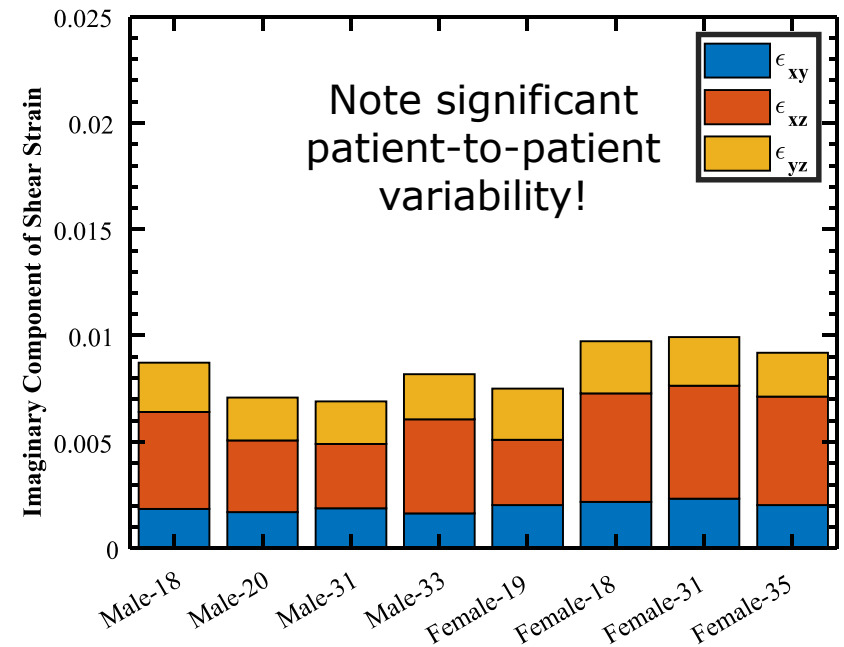
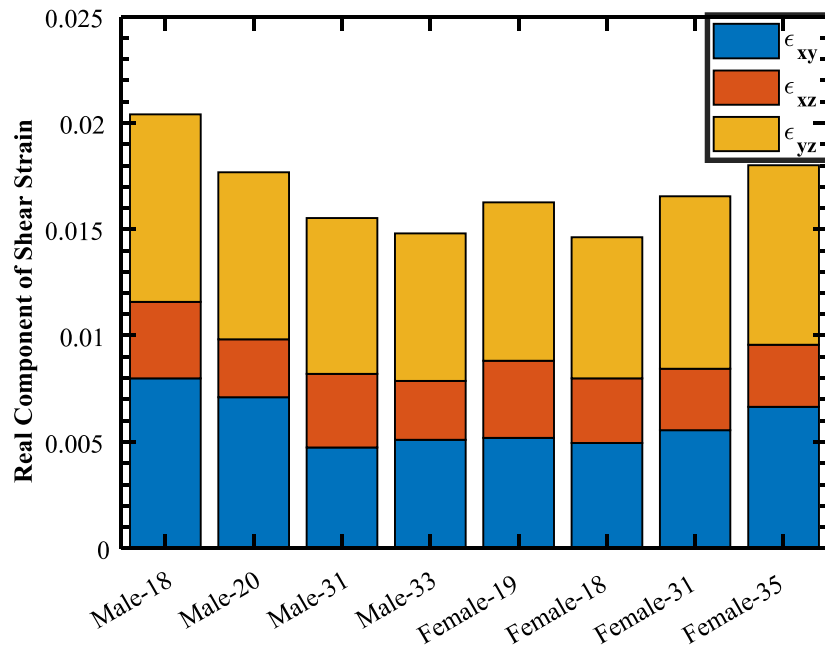
Towards DD patient-specific UNM



Model-free Data-Driven simulation of transcranial harmonic stimulation
on a region on the frontal lobe of the brain at $\Omega = 50$ Hz.

Imaginary part of the strain field components at steady state.

Towards DD patient-specific UNM



Model-free Data-Driven simulation of transcranial harmonic stimulation on a region on the frontal lobe of brain at $\Omega = 50$ 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!

Concluding remarks

Thank you!