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Model-Free Data-Driven Computing

Michael Ortiz California Institute of Technology and Rheinische Friedrich-Wilhelms Universität Bonn

25th Engineering Mechanics Symposium Arnhem, the Netherlands October 25, 2022

To Warner Tjardus Koiter, in memoriam



Amsterdam, June 16, 1914 Delft, September 2, 1997

 Dedicated, grato animo, to the memory of Warner T. Koiter, eximious engineer and educator, for his pioneering contributions to linear and non-linear thin shell theory, plasticity, elasticity and applied mathematics

A Translation of THE STABILITY OF ELASTIC EQUILIBRIUM

By

WARNER TJARDUS KOITER

Sponsored by
Lockheed Missiles & Space Company
Sunnyvale, Calif.











Data Science, Big Data, Al... What's in it for us?



Why Data-Science now?

- New emerging paradigm: *Data-Driven Science*
- Fundamental premise: Unprecedented *abundance of material data*, be it *experimental* or from *multiscale analysis*

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



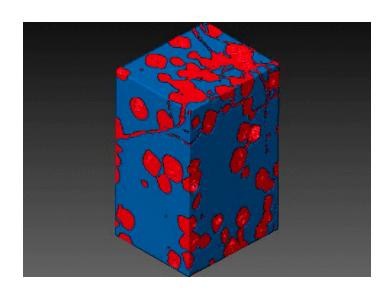


3D tomographic reconstruction of particles in battery electrode

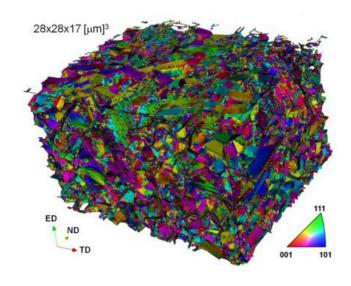
3D DIC-measured internal-strain full-field compressed PDMS sample

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

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Two-phase µCT analysis of Ti2AlC/Al composite¹



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

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

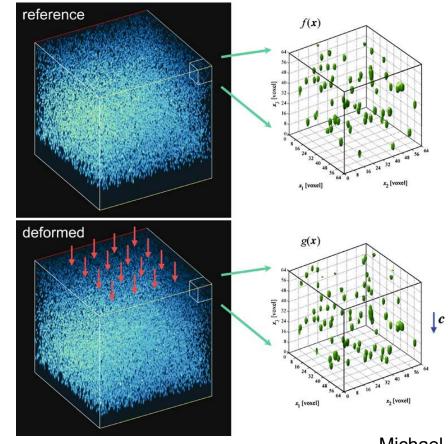
²Khorashadizadeh, *Adv Eng Mater*, **13** (2011) 237.

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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.



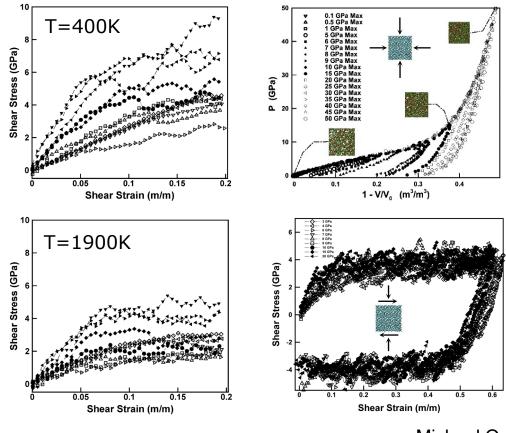
 Material data is currently plentiful due to dramatic advances in experimental science (DIC, EBSD, microscopy, tomography...) and multiscale analysis $(\mathsf{DFT} \to \mathsf{MD} \to \mathsf{DDD} \to \mathsf{SM} \to \mathsf{Hom})$ Multiscale modeling Full-scale of strength in metals calculations Direct numerical simulation of polycrystals, effective models Subgrain structures: Hall-Petch scaling, martensite... **JPSCALING** Dislocation dynamics: Forest hardening, cross slip... MD: Core energies, kink mobilities... ns QM: Multiphase EoS, transport, plasma... Michael Ortiz nm μm mm

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

Amorphous SiO₂ 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.



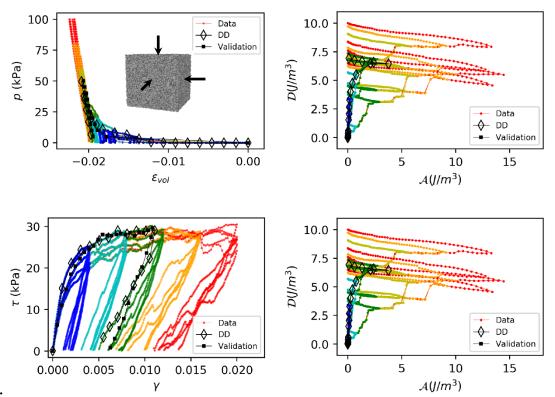
Michael Ortiz EC25 10/25/22

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

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.

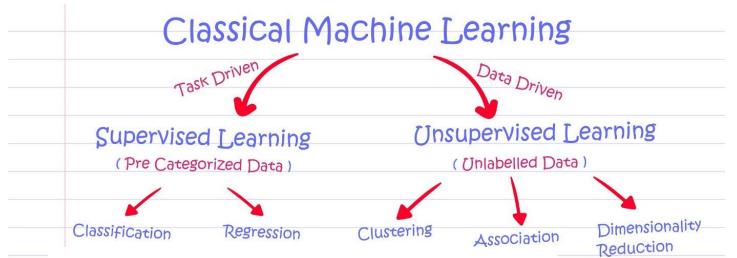
Karapiperis, K., Stainier, L., Ortiz, M. & Andrade, J.E., *JMPS*, **147** (2021) 104239.



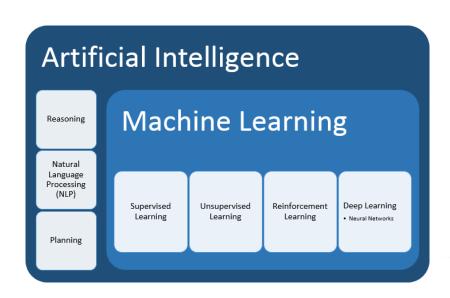
Why Data-Science now?

- New emerging paradigm: *Data-Driven Science*
- Underlying premise: Unprecedented abundance of material data, be it experimental or from multiscale analysis
- Challenge: Forge a *closer connection between data and predictions!*
- Fundamental dilemma: *To fit or not to fit* (that is the question)

Model-Based Data-Driven computing: Data \rightarrow Model \rightarrow Prediction Model-Free Data-Driven computing: Data \longrightarrow Prediction

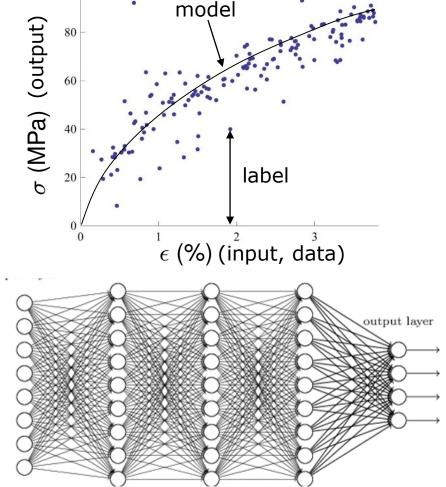


To fit or not to fit, that is the question



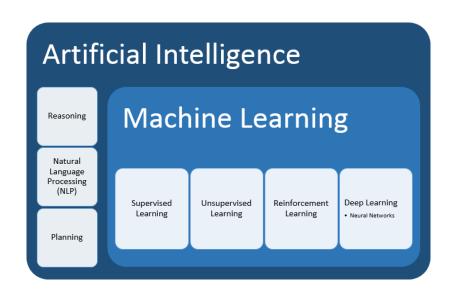
Supervised learning: Find (e.g., by regression) a function (e.g., deep Neural Network) from data containing both inputs and outputs (labels).

J. Hurwitz & D. Kirsch, *Machine Learning*, John Wiley & Sons, 2018.



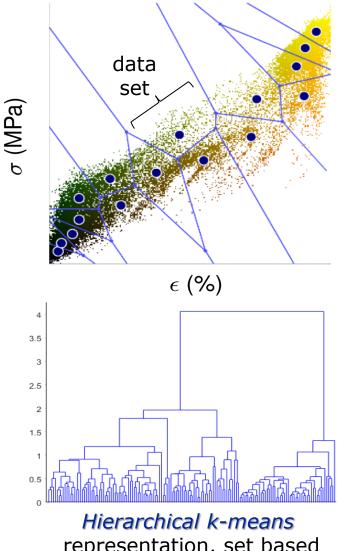
Deep Neural Network representation, regression

To fit or not to fit, that is the question



Unsupervised learning: Find structure in unlabeled data sets (grouping, clustering, density, *data mining*), make predictions directly from data structures.

J. Hurwitz & D. Kirsch, *Machine Learning*, John Wiley & Sons, 2018.



representation, set based

Supervised machine learning, pros and cons

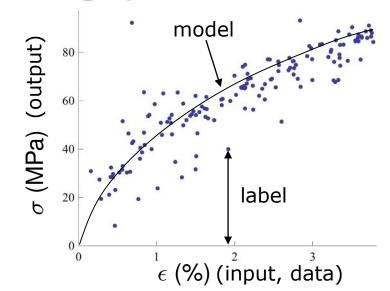
• Advantages:

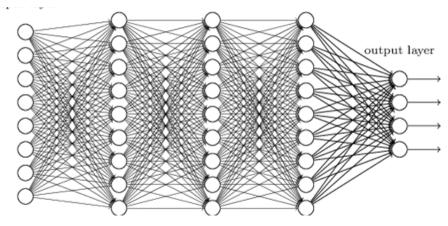


- Universal approximation theorem for C⁰ functions
- Powerful for regression of data in high dimensions
- Availability of versatile tools in the public domain
- Easy to integrate into FEM

• Disadvantages:

- Loss of information with respect to data set
- Modelling error, bias (e.g., choice of network topology)
- Poor error estimation, control of convergence wrt data
- Poor extrapolation properties
- Poor physical interpretability
- Enormous number of hidden parameters, costly training
- Slower than classical analytical material laws





Deep Neural Network representation, regression

Unsupervised machine learning, pros and cons

• Advantages:



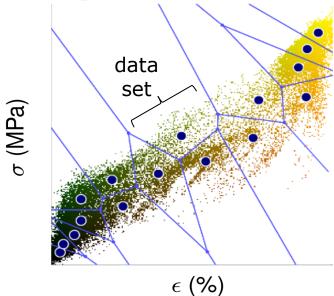
- Lossless: The data, all the data, nothing but the data
- No modeling error, bias
- No prior ansaetze, modeling
- Powerful error estimates, convergence wrt to data
- Standardization of solvers, material data repositories
- Concurrent data generation, multiscale analysis, RVEs
- Faster than conventional solvers (e.g., Newton-Raphson)

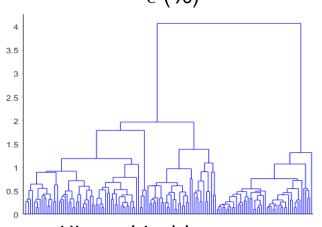
Disadvantages:



- Specialized solvers for FEM (software interfaces, scripting)
- Fast data searching algorithms, efficient data structures







Hierarchical k-means representation, set based











- Phase space, $Z = \{(\epsilon, \sigma)\}.$
- Note (ϵ, σ) work-conjugate
- ullet Dimension of Z is even
- Compatibility: $\epsilon = u/L$
- Equilibrium: $\sigma A = k(u_0 u)$
- Eliminate u: $\sigma A = k(u_0 \epsilon L)$

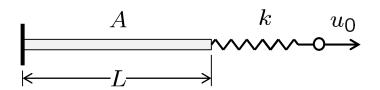
Definition (Constraint set)

The constraint set is the affine subspace of Z containing all admissible states (ϵ, σ) satisfying compatibility and equilibrium:

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

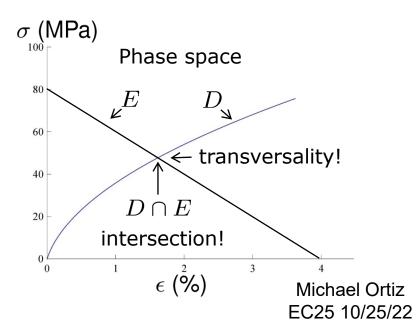
Definition (Material data set)

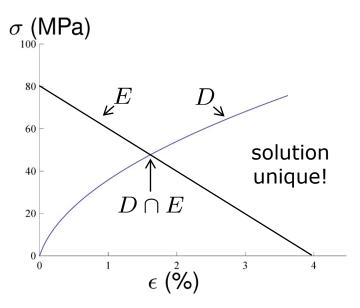
The material data set D is the subset of Z containing all the observed states (ϵ, σ) .

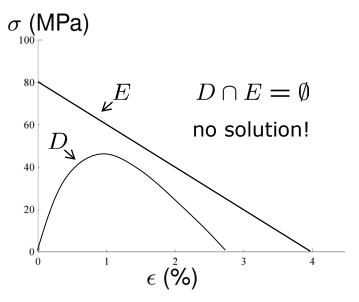


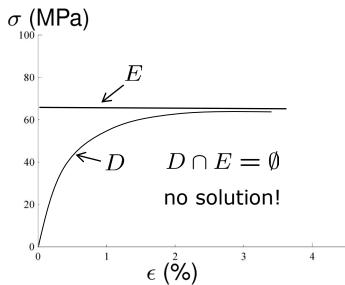
Definition (Classical solution)

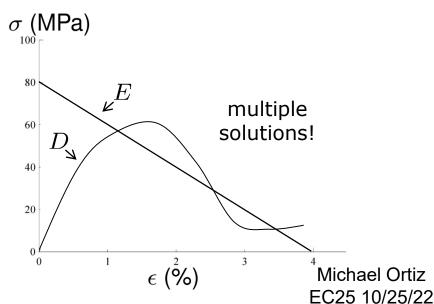
The classical solution is the intersection $D \cap E$, i. e., the set of all material states that are admissible.











- ullet Suppose that D= point set
- ullet Then, $D \cap E = \emptyset$
- No classical solutions! Must extend the concept of solution, classical approach is too rigid

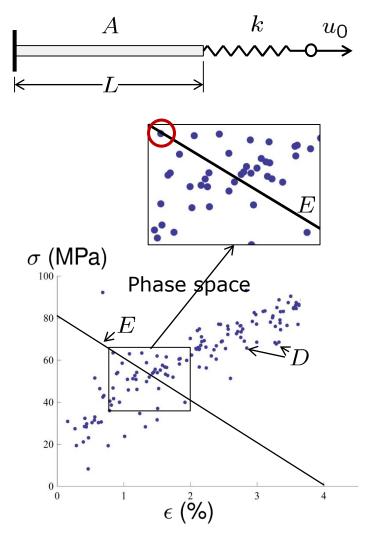
Definition (Data-Driven solution)

An admissible state $z \in E$ is a Data-Driven solution if it minimizes the distance to the material data set D,

$$dist(z, D) \to min!, \quad z \in E$$

- Recall: $dist^{2}(z, D) = \min_{y \in D} ||y z||^{2}$
- Data-Driven problem:

$$\min_{z \in E} \min_{y \in D} \left\| y - z \right\|^2 = \min_{y \in D} \min_{z \in E} \left\| y - z \right\|^2$$



ullet Find material state $y\in D$ and admissible state $z\in E$ closest to each other.

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

• 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)
- Extensions to geometrically-nonlinear problems? (e.g., finite elasticity)
- Well-posedness of Data-Driven problems? Convergence with respect to data?
- Solvers? Computational performance? Scaling?





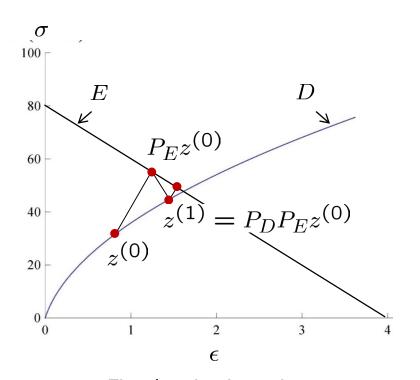




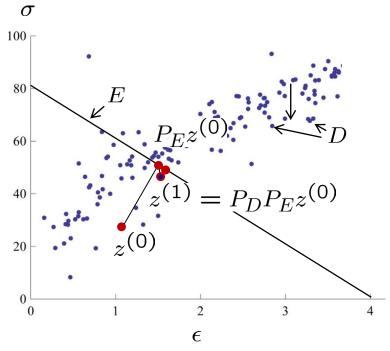


- Find: $\operatorname{argmin}\{\operatorname{dist}(z,D),\ z\in E\}$
- Solver: $z^{(k)} = P_D \circ P_E z^{(k-1)}$
 - $P_D :=$ closest-point projection onto D.
 - $P_E := \text{closest-point projection onto } E$.

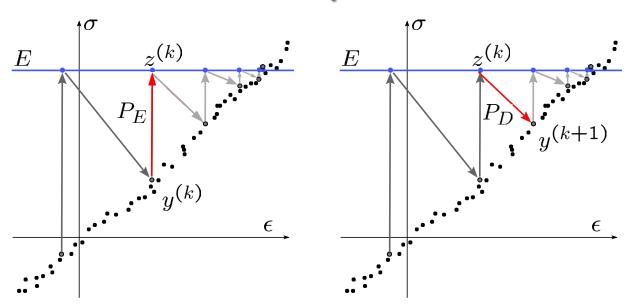
- Implementation?
- Convergence?



Fixed-point iteration, manifold data set D



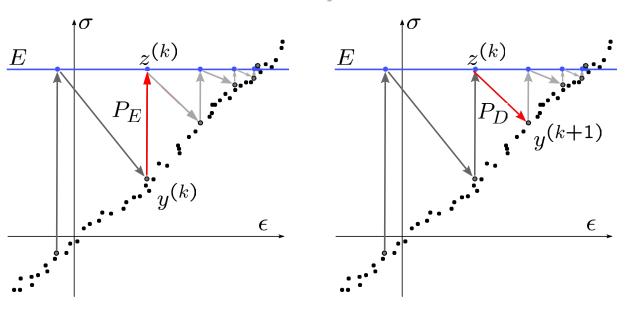
Fixed-point iteration, point data set D



• 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,

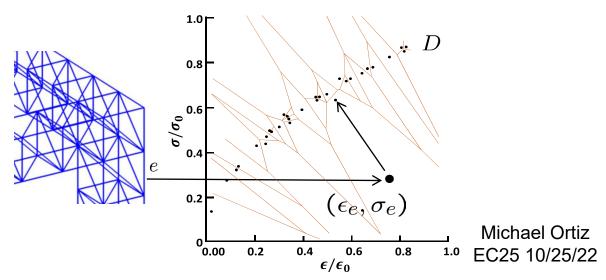
$$\delta \Big(\| (Bu - \epsilon', \sigma - \sigma') \|^2 - (B^T W \sigma - f) \cdot v \Big) = 0$$

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

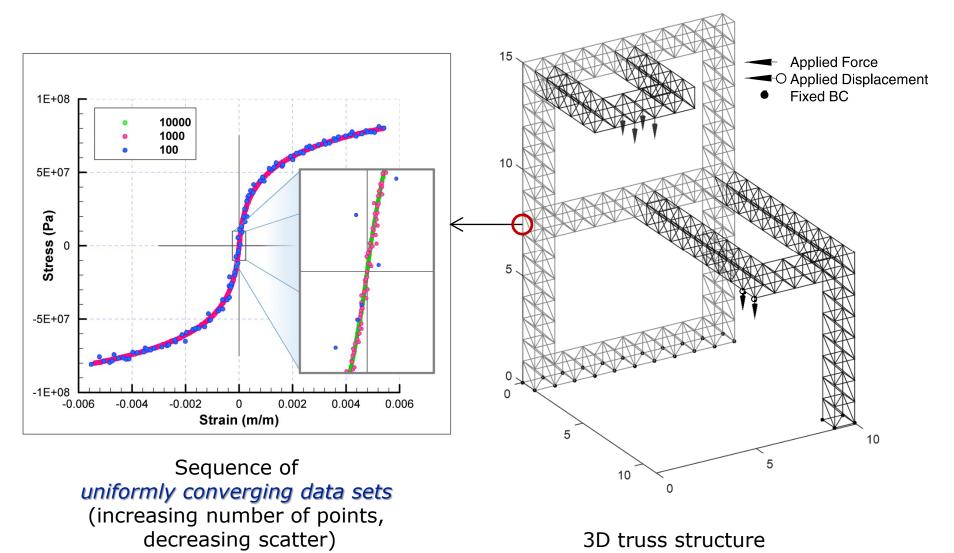


- ullet Outer minimization: Projection onto (closest point in the) material data set D
- Fast searching algorithm
- Requires data structures
- ullet 'Learning' structure of D
- Set-oriented (lossless) ML!

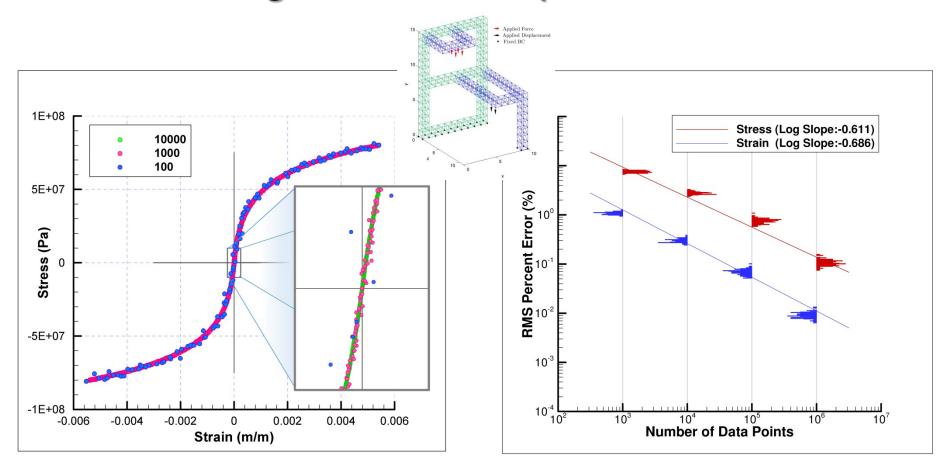
Unsupervised machine learning!



Convergence with respect to the data

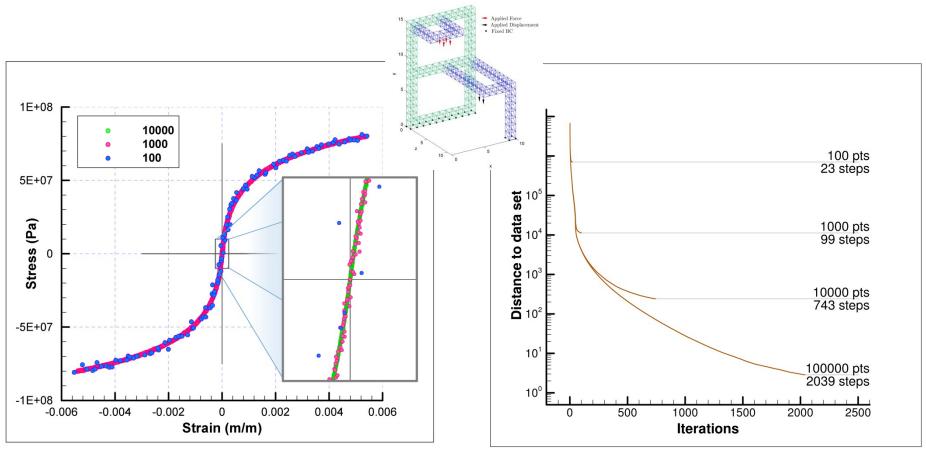


Convergence with respect to the data



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)



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

Convergence of fixed-point solver:

Each iteration requires two backsubstitutions for standard linear systems and one material data search/member Michael Ortiz

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



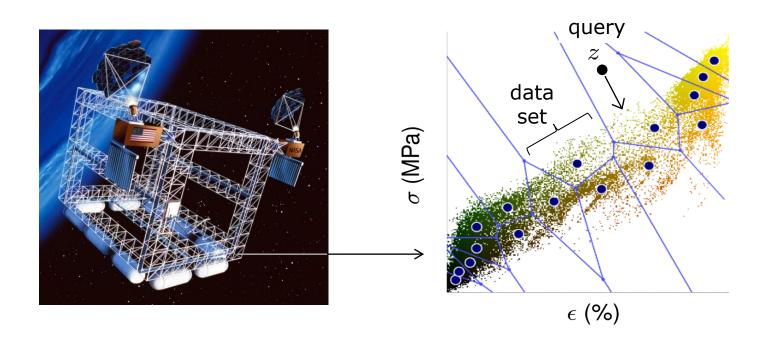




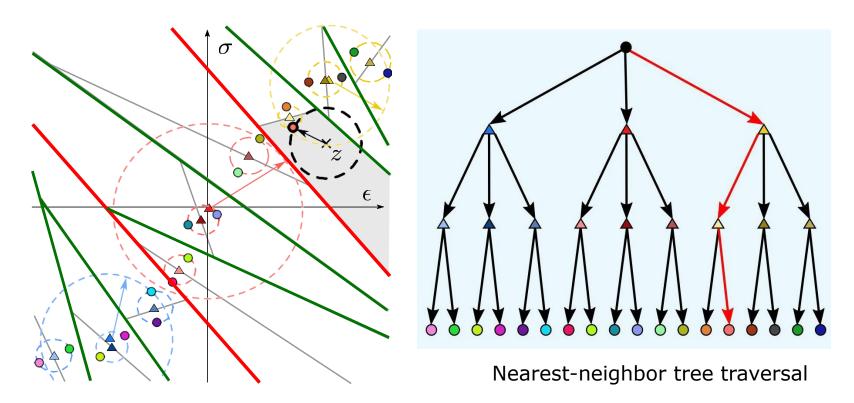




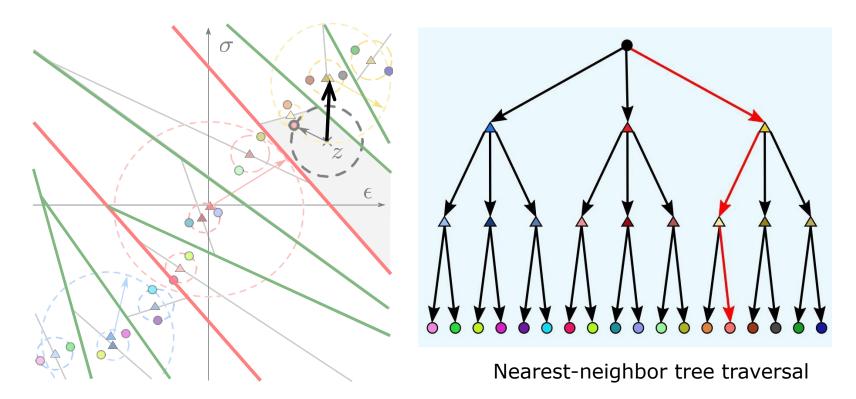
Big data sets – Unsupervised learning



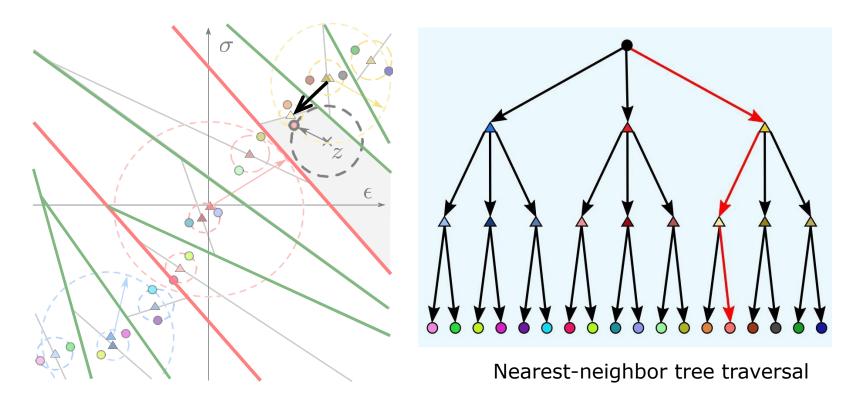
- Material data sets can be very large, cannot do naïve linear lookups!
- *k-means clustering* aims to partition *n* points into *k* clusters in which each point belongs to the cluster with the *nearest mean* (centroid).



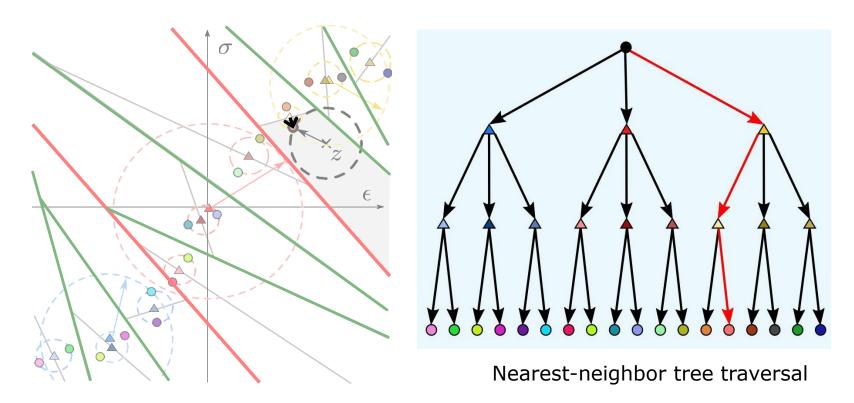
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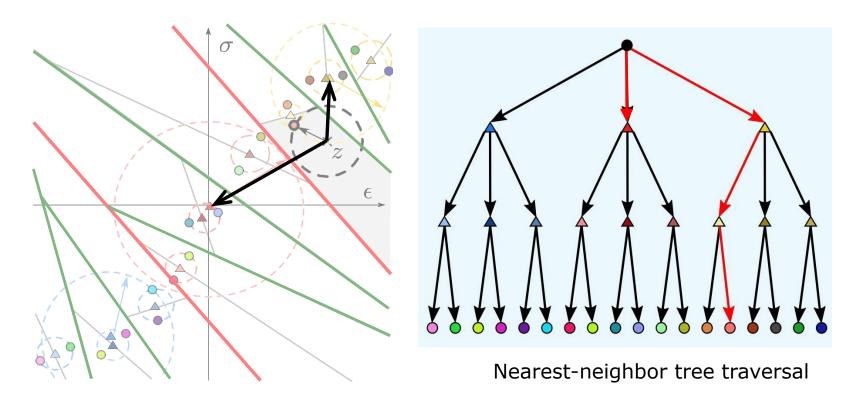
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- Queries can be executed by traversing the k-means tree along nearest neighbors
 Michael Ortiz



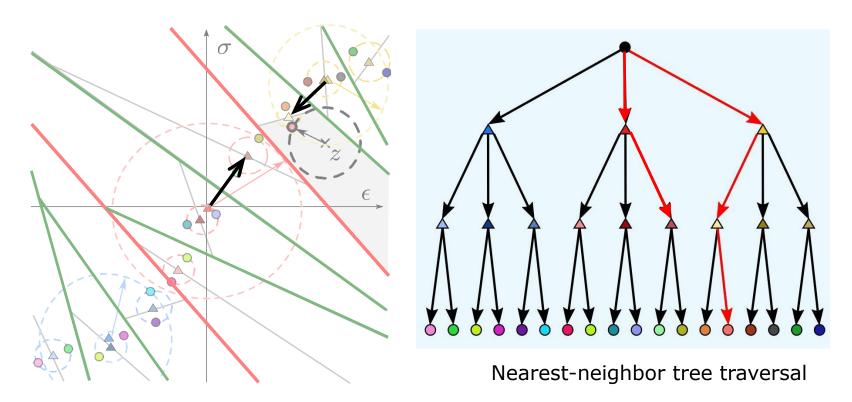
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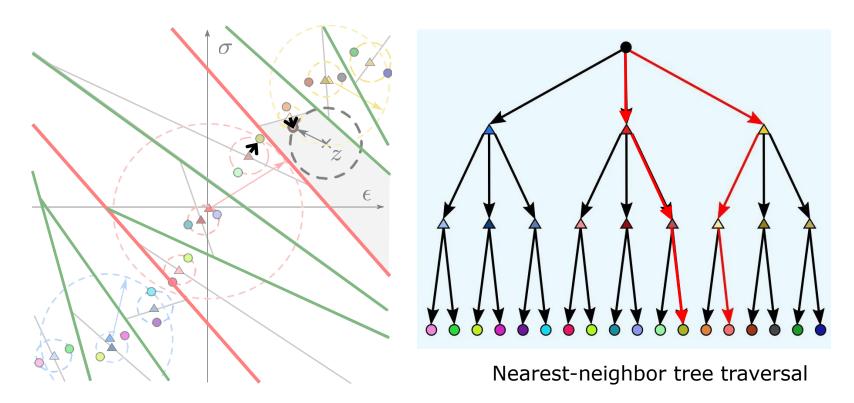


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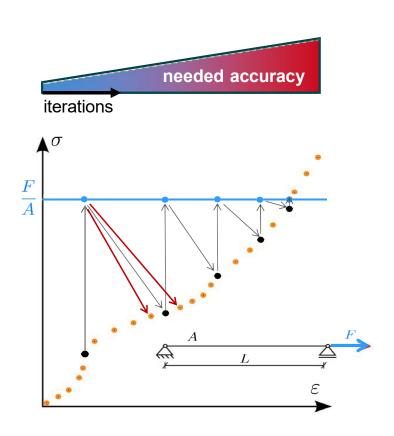
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Big material data sets – k-means

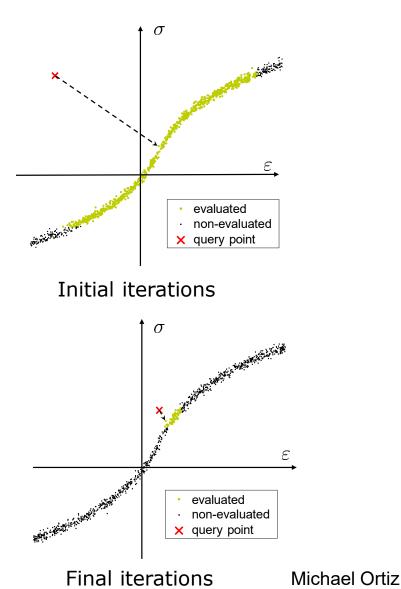


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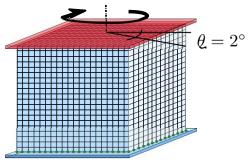
Big material data sets – k-means



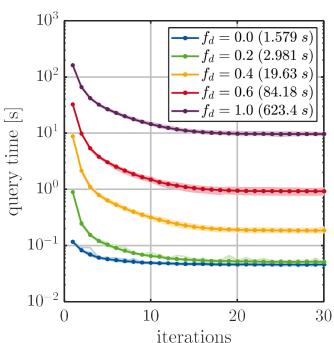
- Accuracy-speed tradeoff
- Initial iterations: Low query accuracy, minimize backtracking
- Final iterations: High query accuracy, maximize backtracking

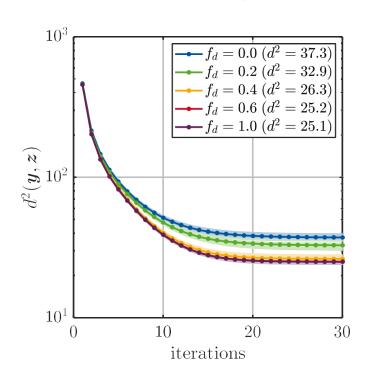


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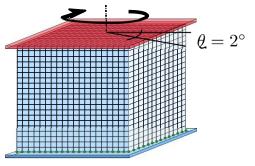


- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- 1 million material data points

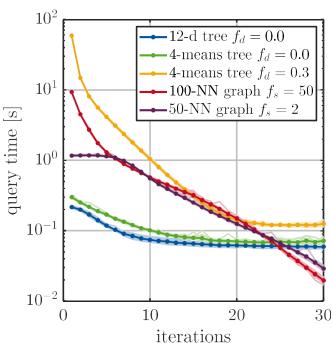


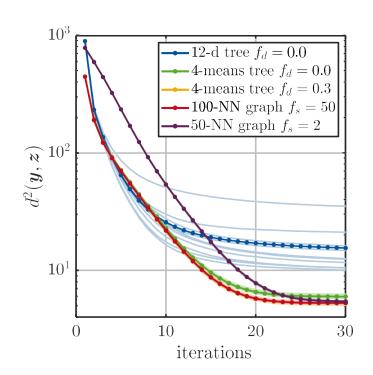


Effect of backtracking on k-means search speed and accuracy $(f_d = 0)$: no backtracking; $f_d = 1$: full backtracking)

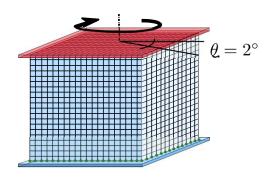


- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- 100 million material data points

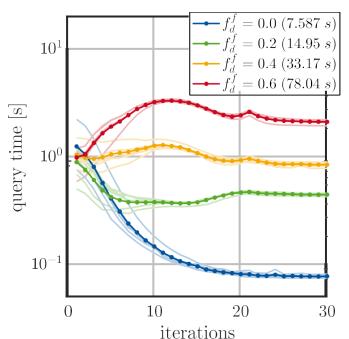


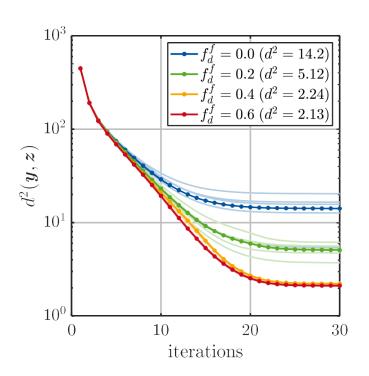


Comparison of search algorithms: kd-tree, k-means and kNN graph algorithms

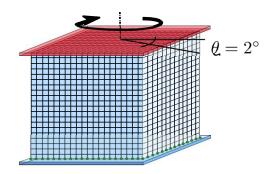


- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
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k-means with different degrees of backtracking. search accuracy set to increase with DD iteration



Total computational times 10^{5} NR-solver (ref. material model) exact k-d tree approx. k-means tree 10^{4} $\lim_{[\mathbf{S}]} 10^3$ 10^{2} 10^{1} 10^{0} $10^4 pts$. $10^5 pts$. $10^6 pts$. $10^3 pts$. number of data points N

- DD nonlinear-elastic cube
- 20x20x20= 8000 elements
- 64,000 material (Gauss) points
- 10³-10⁶ 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 backsubstitution operations only
 - Newton-Raphson requires repeated assembly and factorization of stiffness matrix
 - DD factorization advantage offsets data-searching overhead!



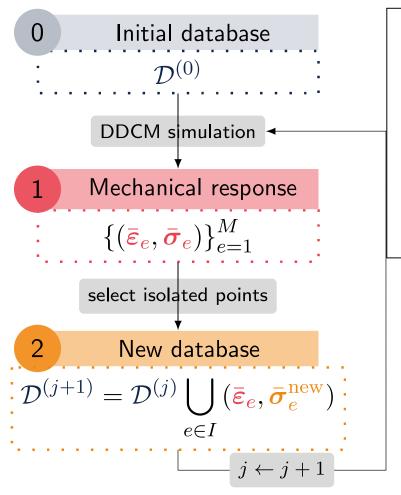


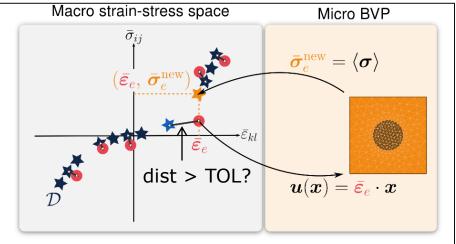






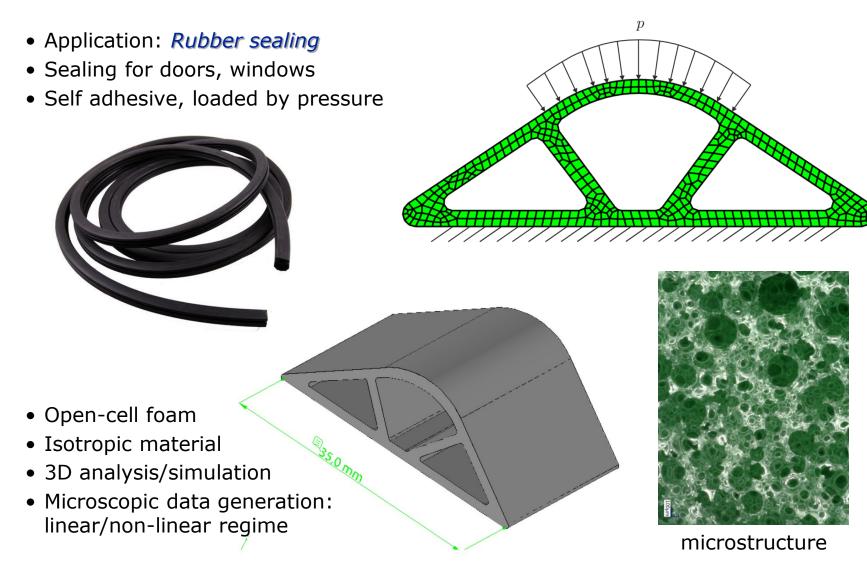
Data-Driven computing with Adaptive Learning





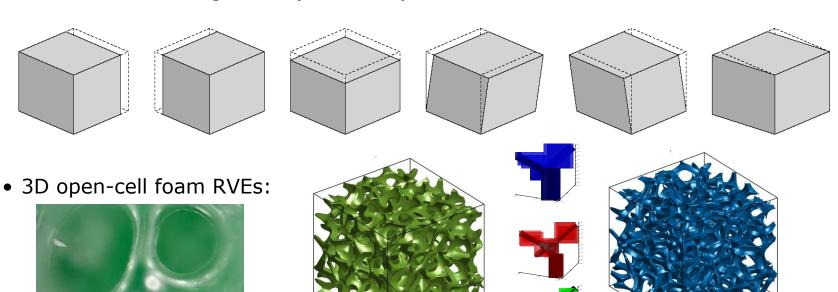
- Generate new data from RVE when local state dist(z_e,D) > TOL!
- Areas of poor coverage in the material data set are detected by DD solver, filled in on-the-fly as needed
- Material data set adapted to solution (goal-oriented adaptive learning)
- Concurrent multiscale analysis with material data re-use (unlike FE²)

Adaptive learning: Open-cell rubber foams



Adaptive learning: Open-cell rubber foams

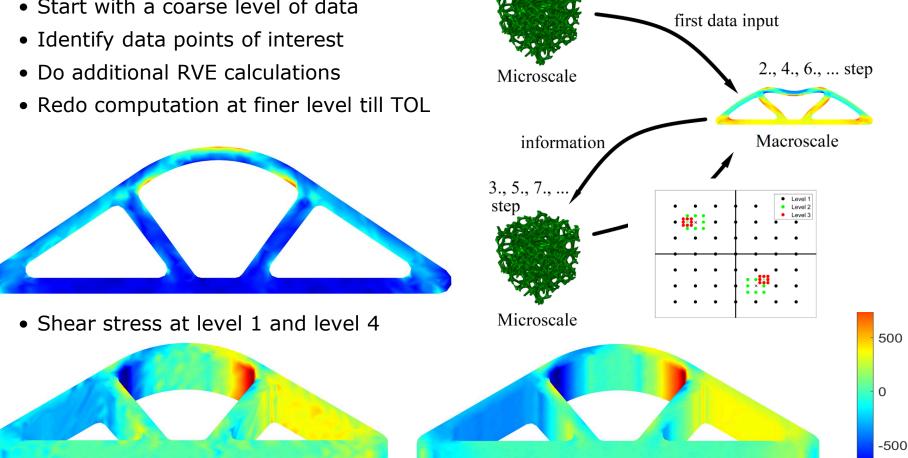
- Data sets: $\mathcal{D} = \{(\epsilon, \sigma)\}$, or $\mathcal{D} = \{(F, P)\}$, or $\mathcal{D} = \{(C, S)\}$.
 - 1.apply deformation
 - 2.compute RVE and determine average stress
 - 3.collect data pairs
- Can generate macroscopic data on demand as required!
- Six different loading cases (unit loads)



Adaptive learning: Open-cell rubber foams

1. step

- Cauchy stress distribution (vertical)
- Start with a coarse level of data











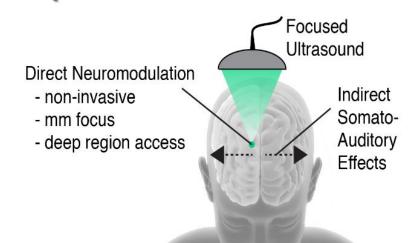


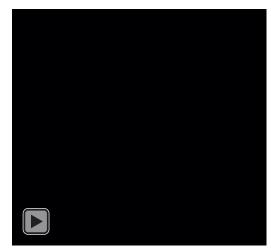
- Ultrasonic neuromodulation (UNM) is a novel non-invasive technique that uses low intensity focused ultrasound (LIFU) to stimulate the brain.
- First proposed in 2002 by A. Bystritsky as possibly having therapeutic benefits.
- W. Tyler and team discovered UNM is able to stimulate high neuron activity.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

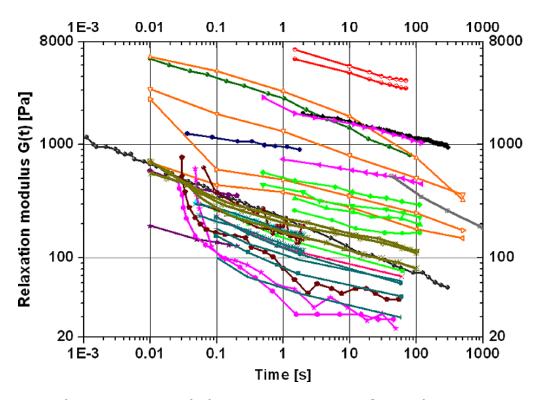
Salahshoor, S., Shapiro, M. and Ortiz, M. Appl. Phys. Lett. **117**, 033702 (2020)





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

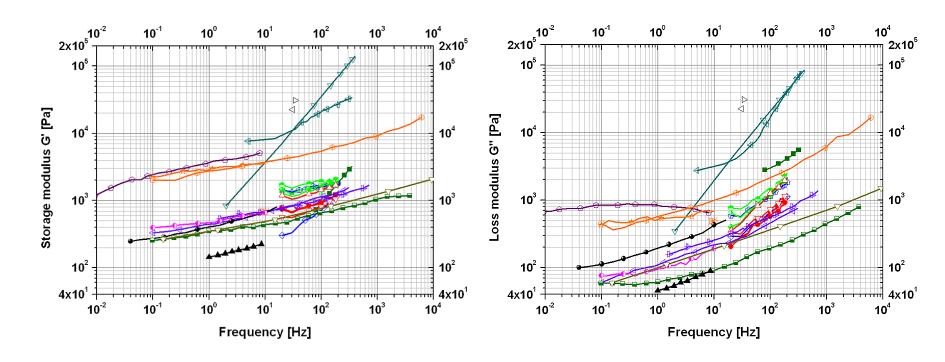
Complexity and variability of brain viscoelasticity defy effective ad hoc modeling!



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

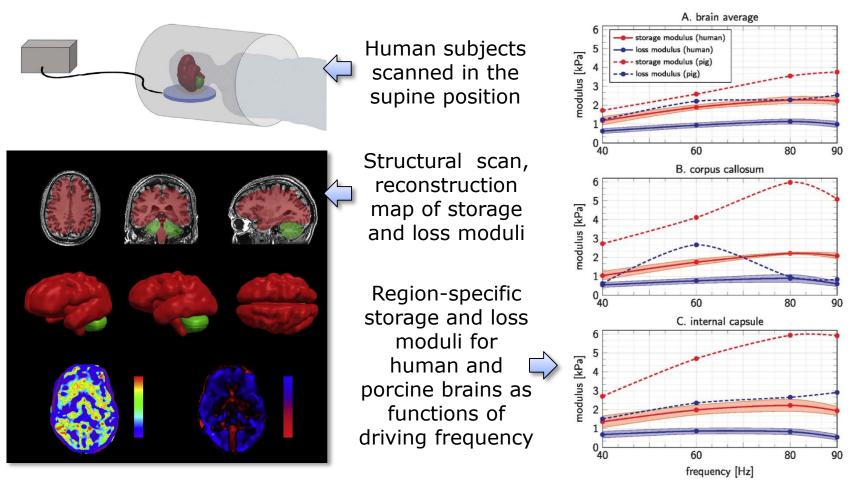
Chatelin, S., Constantinesco, A., Willinger, R., "Fifty years of brain tissue mechanical testing: from in vitro to in vivo investigations." *Biorheology*. 2010;47(5-6):255-76.

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.

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



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

Field equations,

$$\epsilon_e(t) = B_e u(t) + g_e(t), \quad e = 1, \dots m,$$

$$M\ddot{u}(t) + \sum_{e=1}^{m} w_e B_e^T \sigma_e(t) = f(t).$$

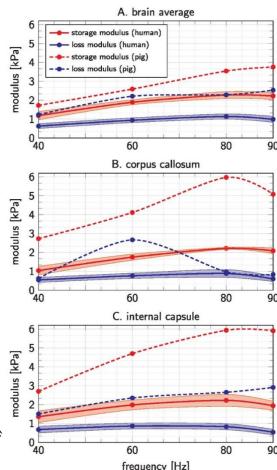
• Fourier-transform representation,

$$\hat{\epsilon}_e(\omega) = B_e \hat{u}(\omega) + \hat{g}_e(\omega), \quad e = 1, \dots m,$$

$$\sum_{e=1}^m w_e B_e^T \hat{\sigma}_e(\omega) - M\omega^2 \hat{u}(\omega) = \hat{f}(\omega).$$

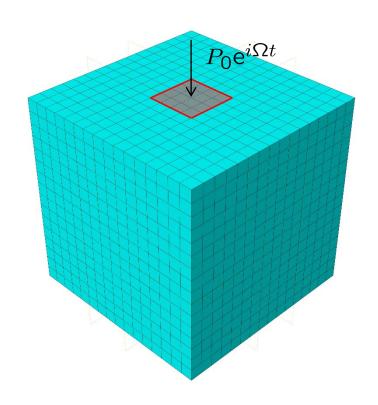
- Complex-modulus: $\hat{\sigma}_e(\omega) = \mathbb{E}(\omega)\hat{\epsilon}_e(\omega)$.
- Displacement problem: For every $\omega \in \mathbb{R}$,

$$\sum_{e=1}^{m} w_e B_e^T \mathbb{E}(\omega) (B_e \hat{u}(\omega) + \hat{g}_e(\omega)) - M\omega^2 \hat{u}(\omega) = \hat{f}$$

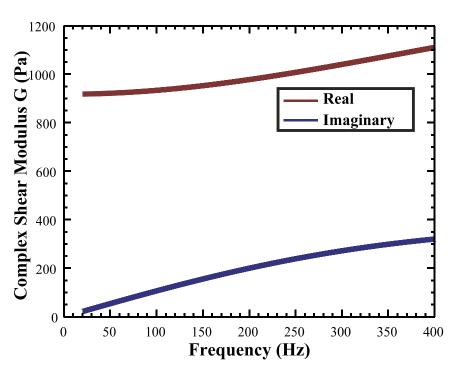


J. Weickenmeier, M. Kurt, E. Ozkaya, M. Wintermark, K.B. Pauly, E. Kuhl, J. Mech. Behav. Biomed. Mater., 77 (2018) 702-710.

Test of convergence: Insonated agarose gel block.



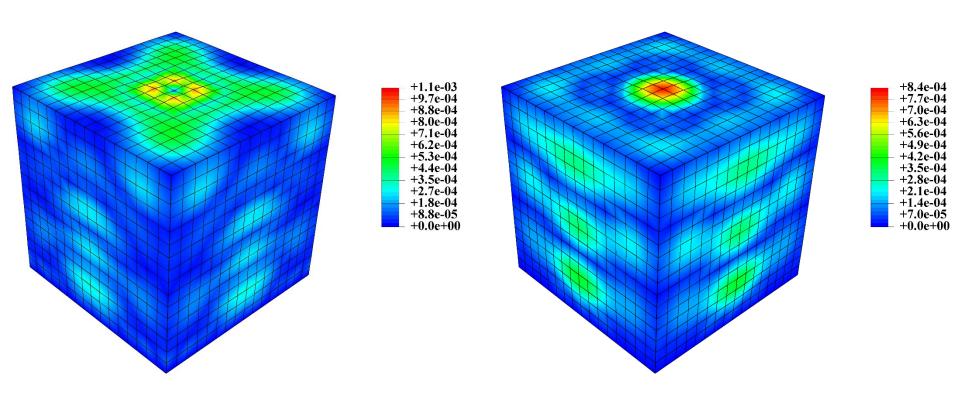
Finite-element discretization of agarose gel block into hex-elements. The square on the top surface marks area of application of harmonic pressure



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

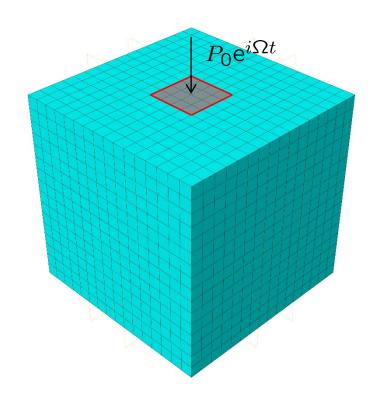
R. J. Okamoto, E. H. Clayton and P. V. Bayly, Physics in Medicine & Biology 56 (19) (2011) 6379.

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

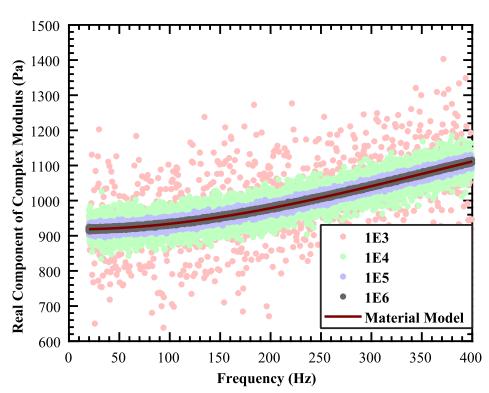


Insonated agarose gel block. Displacements for applied frequency $\Omega = 1000$ Hz. a) Real component. b) Imaginary component.

Test of convergence: Insonated agarose gel block.

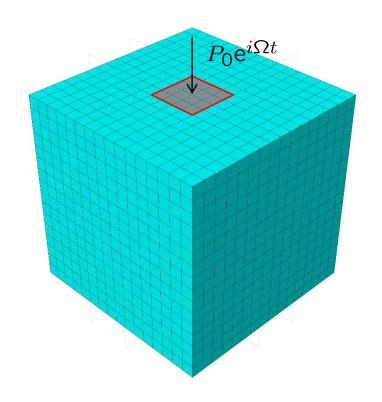


Finite-element discretization of agarose gel block into hex-elements. The square on the top surface marks area of application of harmonic pressure

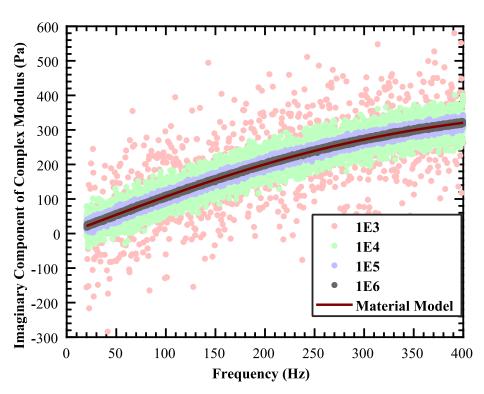


Data of sizes 10³, 10⁴, 10⁵ and 10⁶ used in the DD calculations. Real component of complex modulus.

Test of convergence: Insonated agarose gel block.



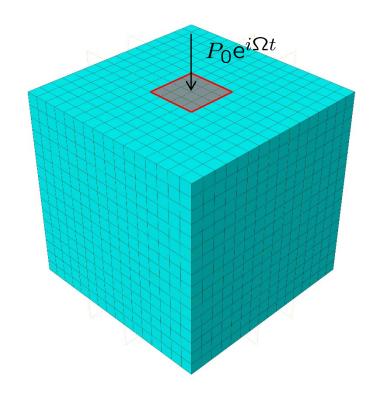
Finite-element discretization of agarose gel block into hex-elements. The square on the top surface marks area of application of harmonic pressure



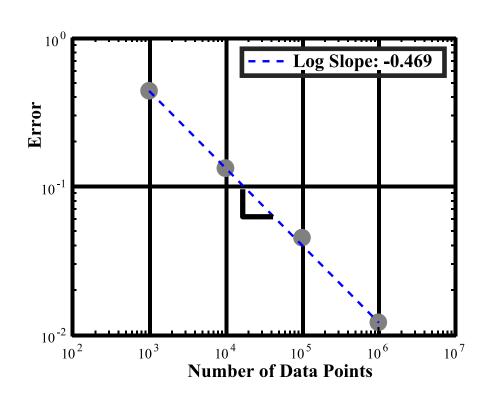
Data of sizes 10³, 10⁴, 10⁵ and 10⁶ used in the DD calculations.

Imaginary component of complex modulus.

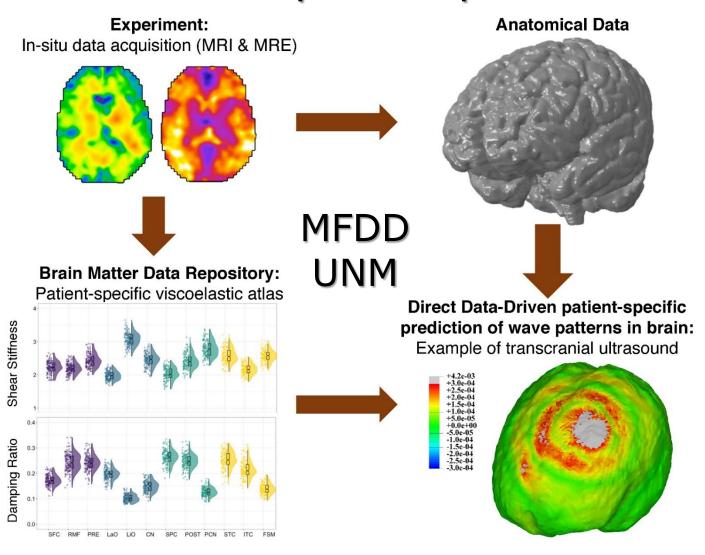
Test of convergence: Insonated agarose gel block.



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

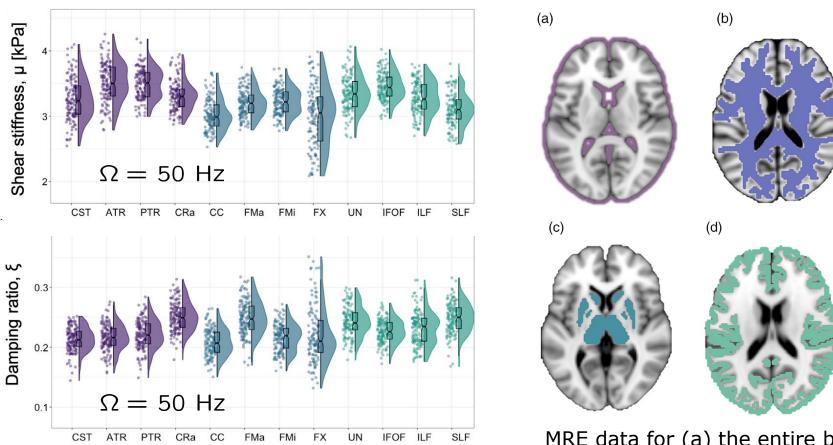


Normalized flat-norm convergence error as a function of the number of data points, showing a clear trend towards convergence.



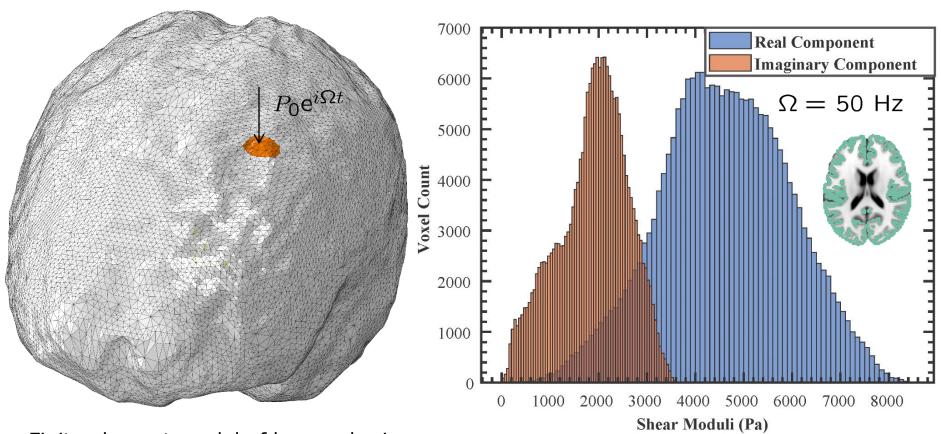
L.V. Hiscox *et al.*, *Hum Brain Mapp.*, 2020;**41**:5282–5300 H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

- Data can be acquired in vivo through Magnetic Resonance Elastography (MRE) .
- 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.



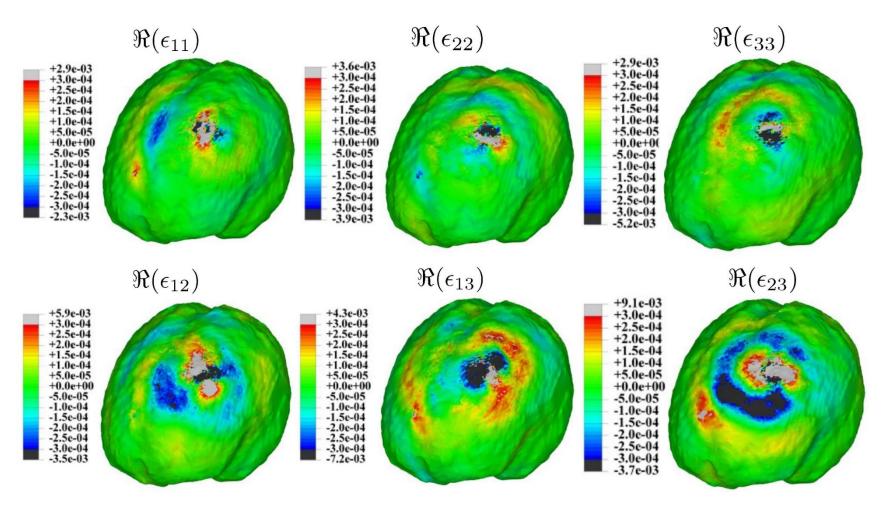
Finite element model of human brain reconstructed from MRI data, 0.2 million tetrahedral elements. Transcranial stimulation is modeled by subjecting the highlighted region to harmonic pressure as a traction boundary condition.

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 Michael Ortiz

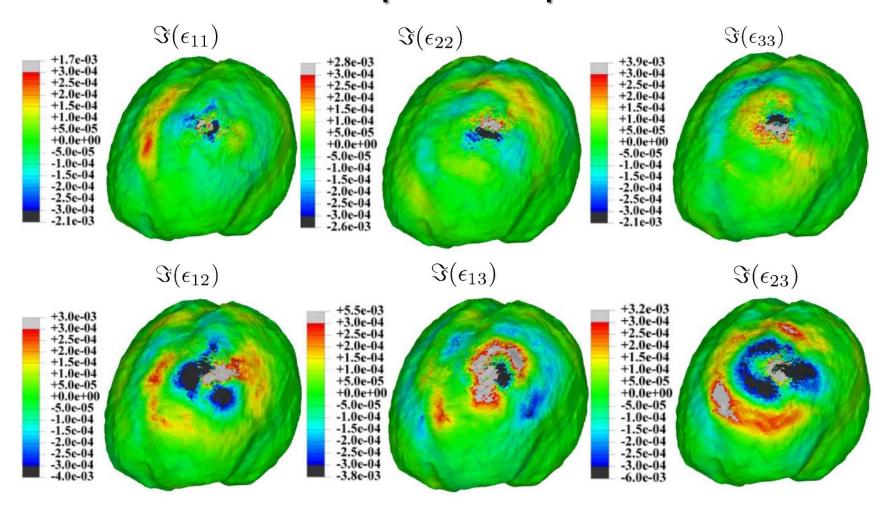
H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

EC25 10/25/22



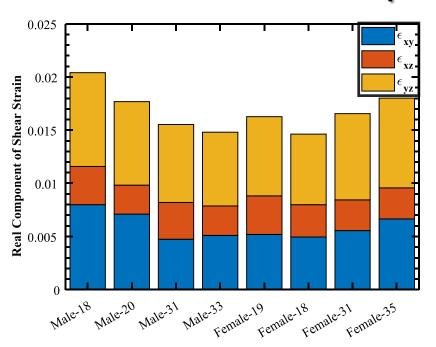
Model-free Data-Driven simulation of transcranial harmonic stimulation on a region on the frontal lobe of the brain at $\Omega=50$ Hz. Real part of the strain field components at steady state.

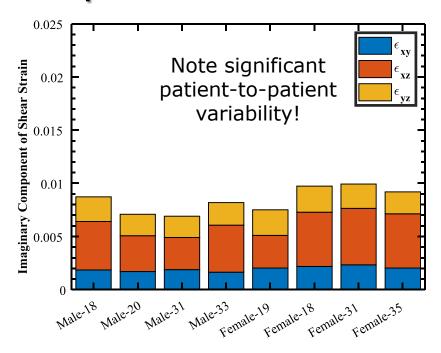
H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.



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.

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





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-thefly integration of in vivo patient-specific data into calculations supporting future UNM clinical applications!

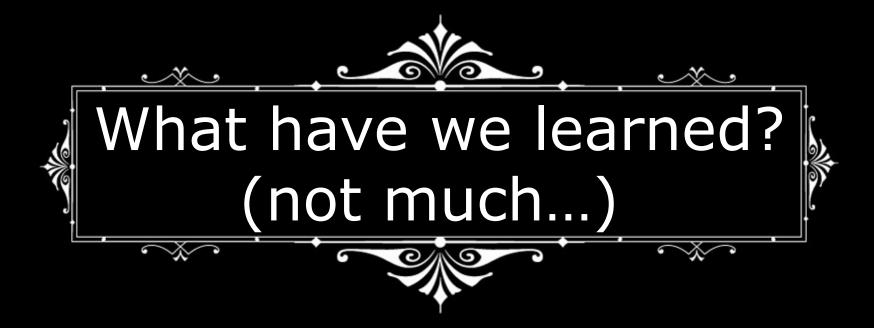
 Michael Ortiz

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

EC25 10/25/22











Empirical vs. epistemic knowledge



Tycho Brahe (1546-1601)

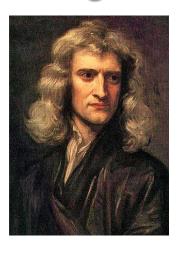




Johannes Kepler (1571-1630)

$$\frac{T^2}{a^3} = \frac{4\pi^2}{G(M+m)}$$

Kepler's laws fit Brahe's data Why?



Sir Issac Newton (1643-1727)

$$\vec{F} = m \, \vec{a}$$

True epistemic knowledge!

- Real knowledge is generated by force of reason!
- Data-Science is just an interim stopgap measure

Concluding remarks

Thank you!