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Data-Driven Mechanics: Constitutive Model-Free Approach

$$\inf_{y\in D}\inf_{z\in E}\|y-z\| = \inf_{z\in E}\inf_{y\in D}\|y-z\|$$

Michael Ortiz – Lecture 4

California Institute of Technology and

Rheinische Friedrich-Wilhelms Universität Bonn

Centre International des Sciences Mécaniques (CSIM)

Udine (Italy), October 10-14, 2022

History-dependent inelastic materials

- *History-dependence* and *inelasticity* of material behavior are exemplified by *viscoelasticity*, rate-independent *plasticity* and *viscoplasticity*.
- Inelastic material behavior is central to many engineering applications.

History-dependent inelastic materials – Crashworthiness

Frontal crash test of
Volvo C30

Frontal crash test of
Chevrolet Venture

Offset frontal crash test of
1998 Toyota Sienna

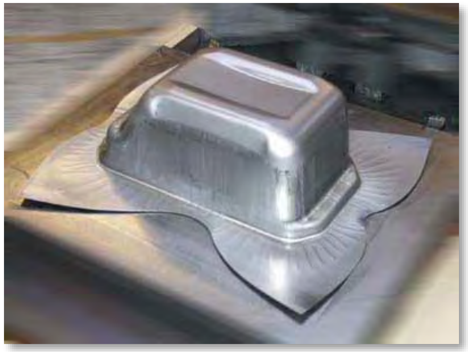
Side-impact test of
1996 Ford Explorer vs.
2000 Ford Focus

Source: http://en.wikipedia.org/wiki/Crash_test

History-dependent inelastic materials – Manufacturing

Metal ingot after forging

Lathe cutting metal from workpiece



Deep-drawing of blank metal sheet (source: ThomasNet)

Cold rolling of steel

Sources: http://en.wikipedia.org/wiki/Forging
http://en.wikipedia.org/wiki/Metal_forming
http://www.kanabco.com/vms/library.html

History-dependent inelastic materials – Collapse

Plastic buckling of storage tank,
1999 Kocaeli earthquake
(PEER 2000/09, Dec. 2000)

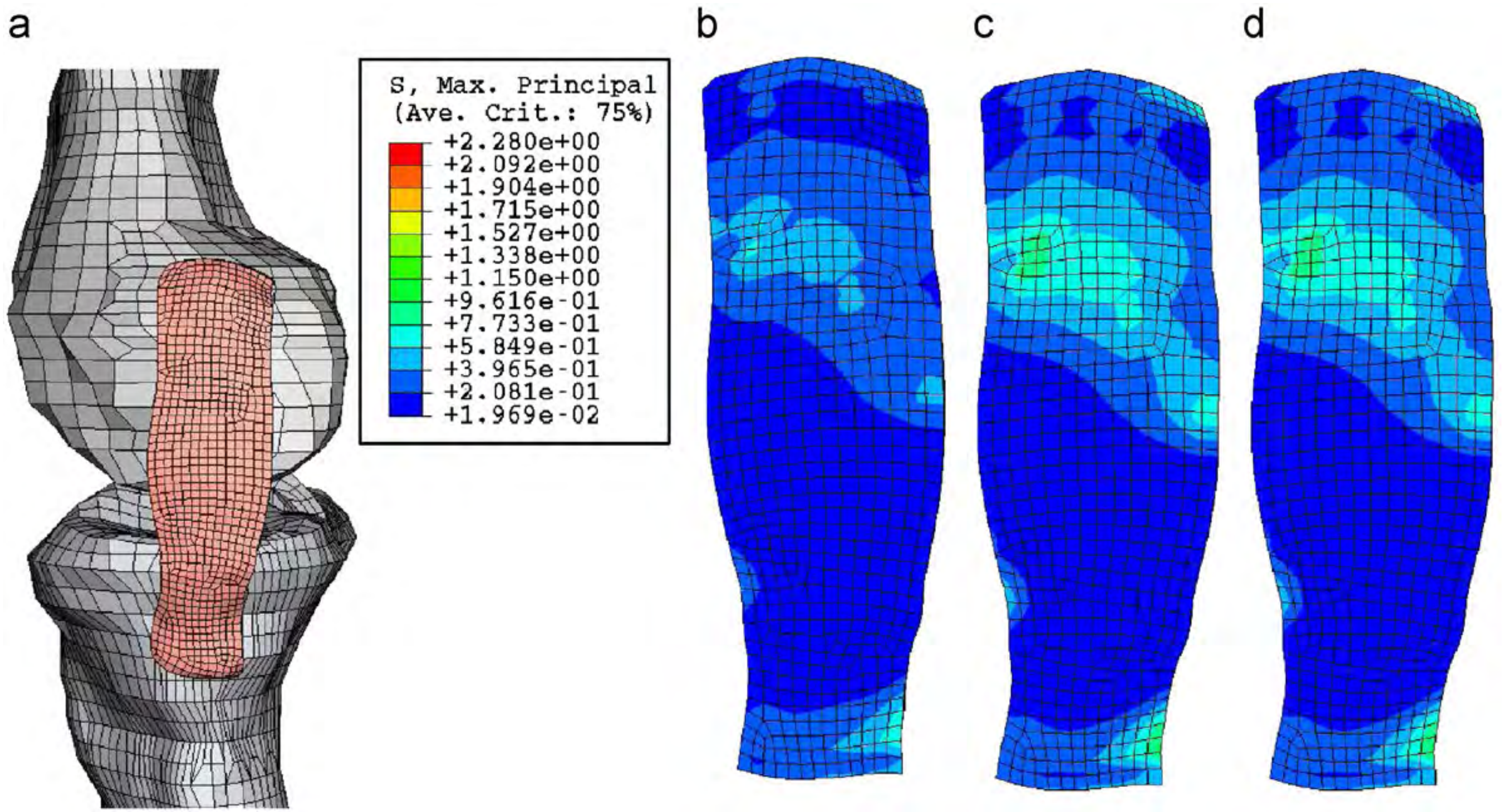
Mid-story collapse,
1995 Kobe earthquake
(EQE Summary Rep., 1995)

History-dependent inelastic materials – Viscoelasticity

Viscoelastic Damping Polymers are used to reduce vibration
in automobiles, disk drives, space craft and commercial aircraft,
sporting goods, appliances and many other industrial products.

 https://www.yumpu.com/en/document/read/48954947/viscoelastic-damping-polymers

History-dependent inelastic materials – Viscoelasticity



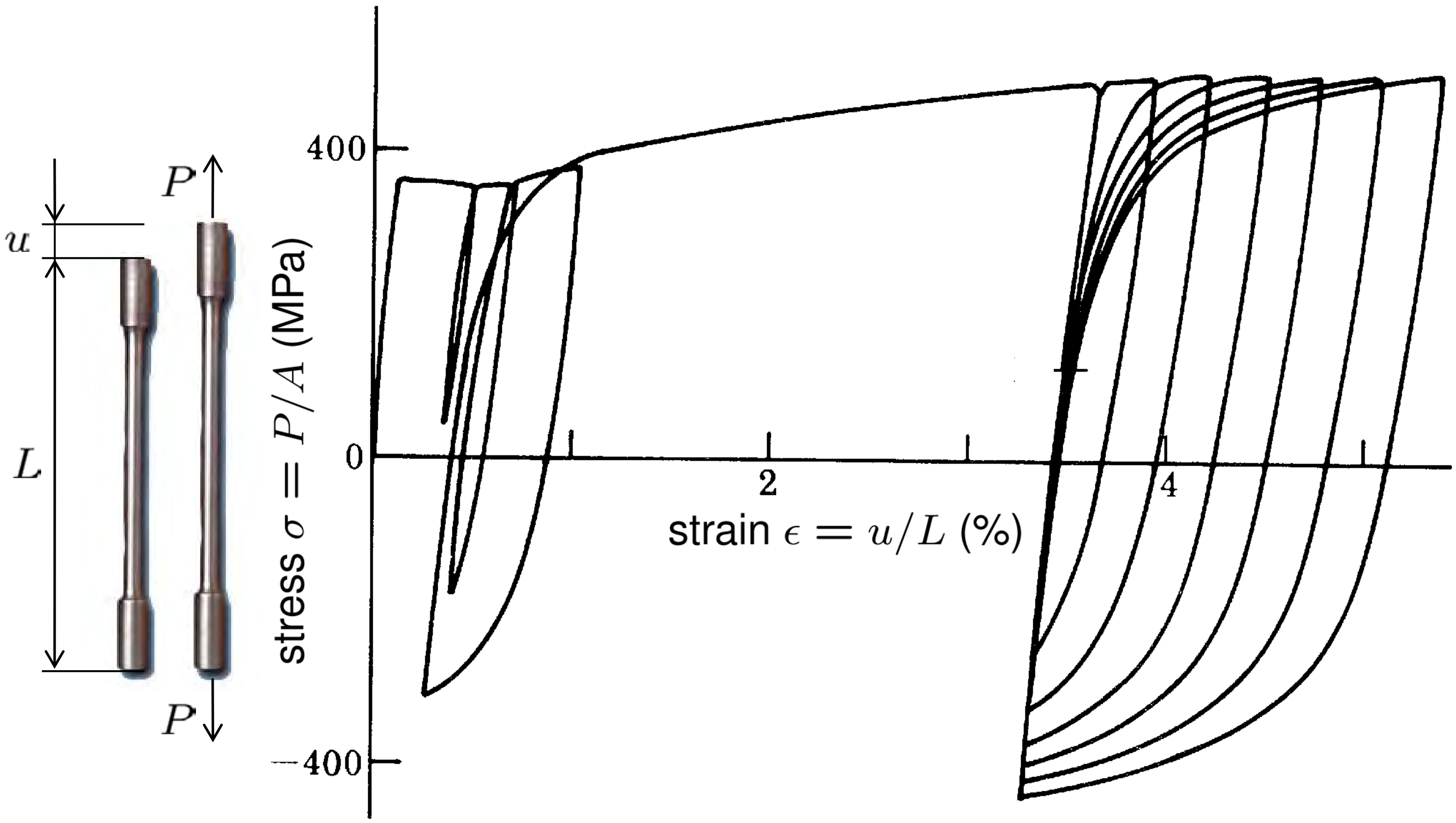
Finite element model (a) of the human medial collateral ligament (MCL)
and stress distribution resulting for the
hyperelastic (b), linear (c) and nonlinear (d) visco-hyperelastic models

E. Peña, J.A. Peña, M. Doblaré, J. Biomechanics, 41 (2008) 2659-2666.

History-dependent inelastic materials

- *History-dependence* and *inelasticity* of material behavior are exemplified by *viscoelasticity*, rate-independent *plasticity* and *viscoplasticity.*
- Inelastic material behavior is central to many engineering applications.
- Inelasticity is characterized by great *complexity* well-documented and characterized *experimentally:*
  - Quasistatic uniaxial tension/compression
    - Elastic domain, yield point
    - Elastic-plastic decomposition of strain
    - Hooke's law for elastic unloading/reloading
    - Reverse yielding and Bauschinger effect
    - Unloading-point fading memory
  - Multiaxial loading, texture anisotropy
  - Rate-sensitivity of the yield stress
  - Temperature-dependence of the yield stress
  - Fraction of work stored as internal energy
  - Fraction of work dissipated as heat
  - Creep and relaxation tests (time domain)
  - Dynamic Material Analysis (frequency domain)

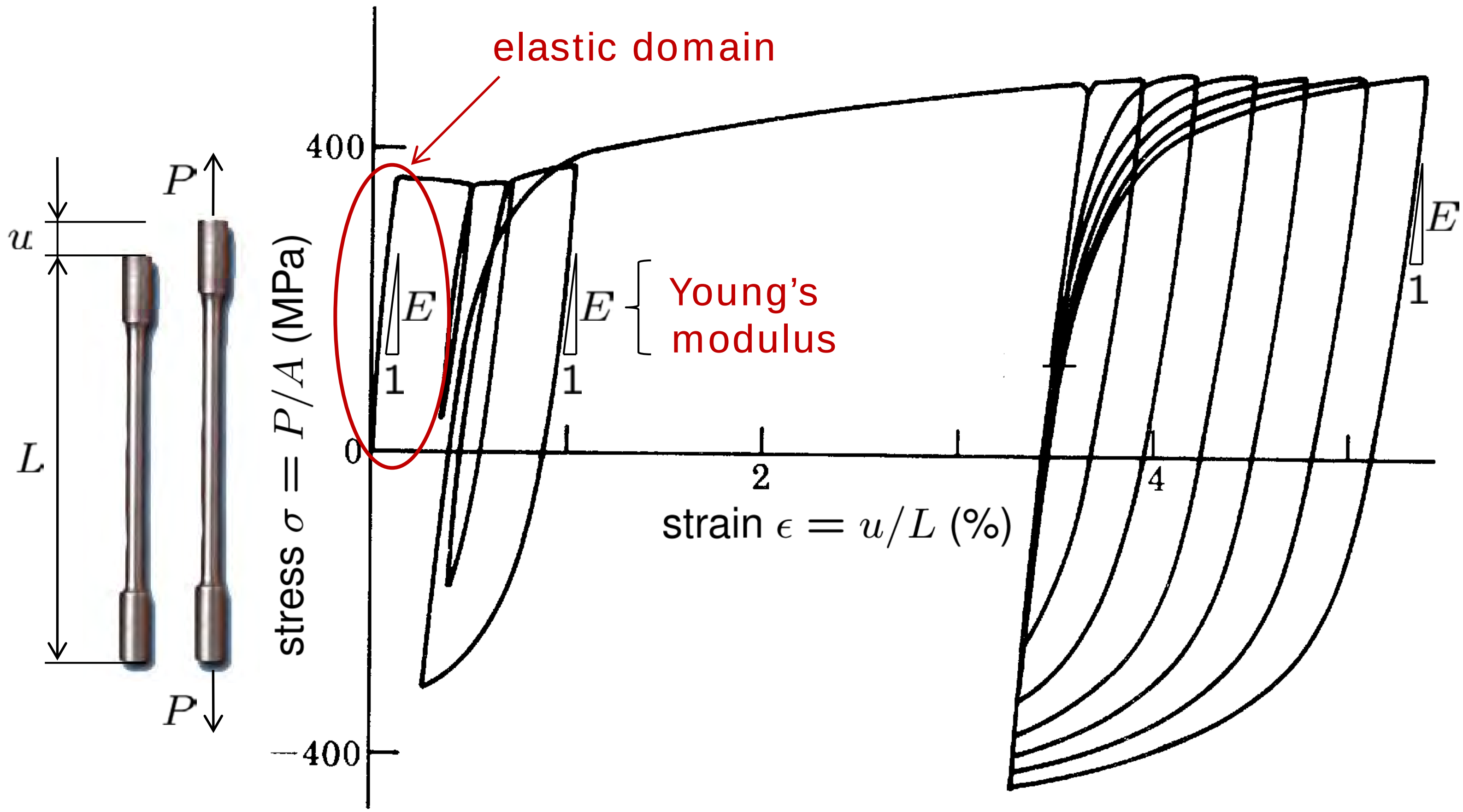
History-dependent inelastic materials – Uniaxial tension/compression



Mild steel under cyclic uniaxial tension/compression loading

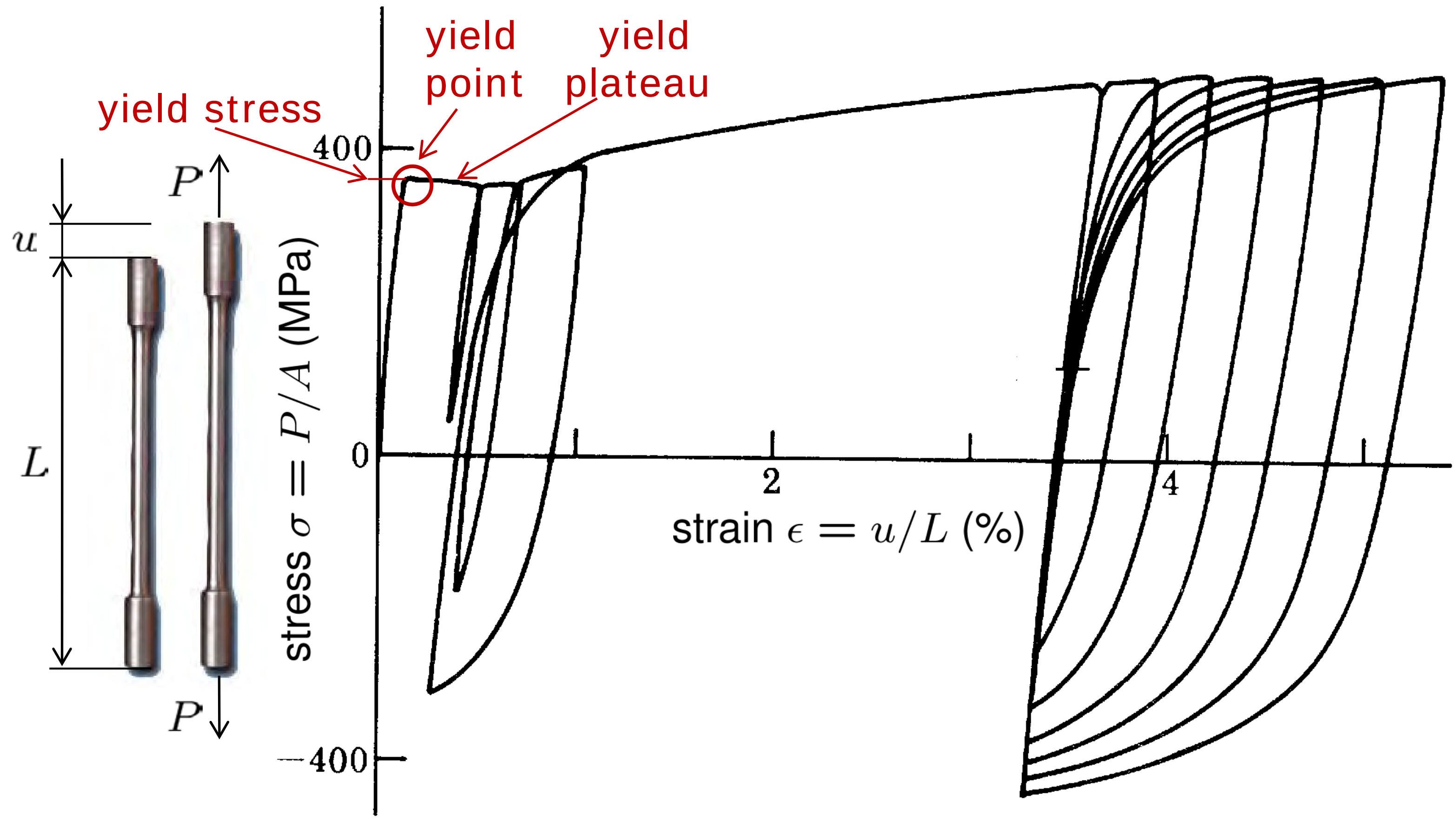
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension / compression



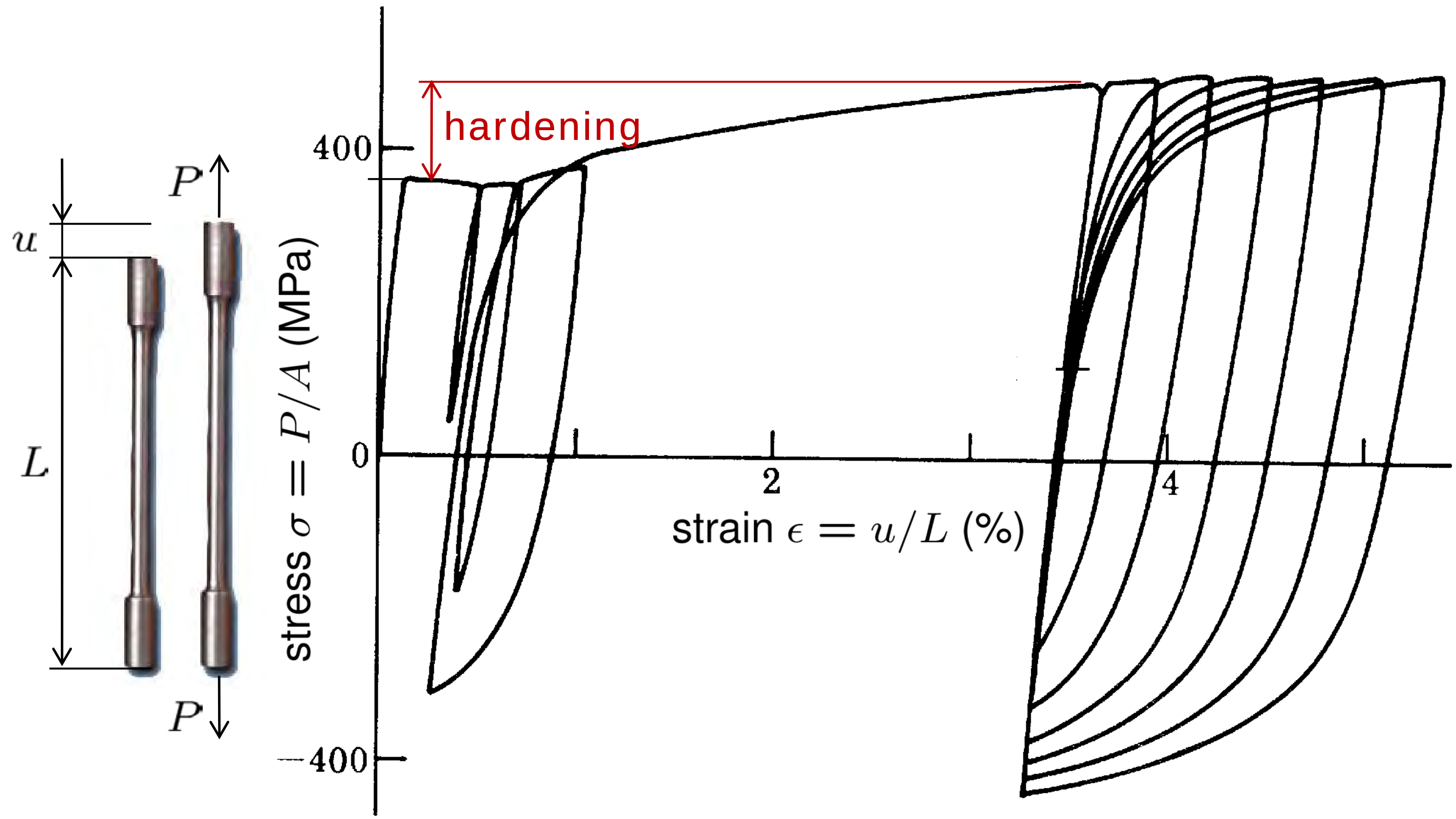
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension / compression



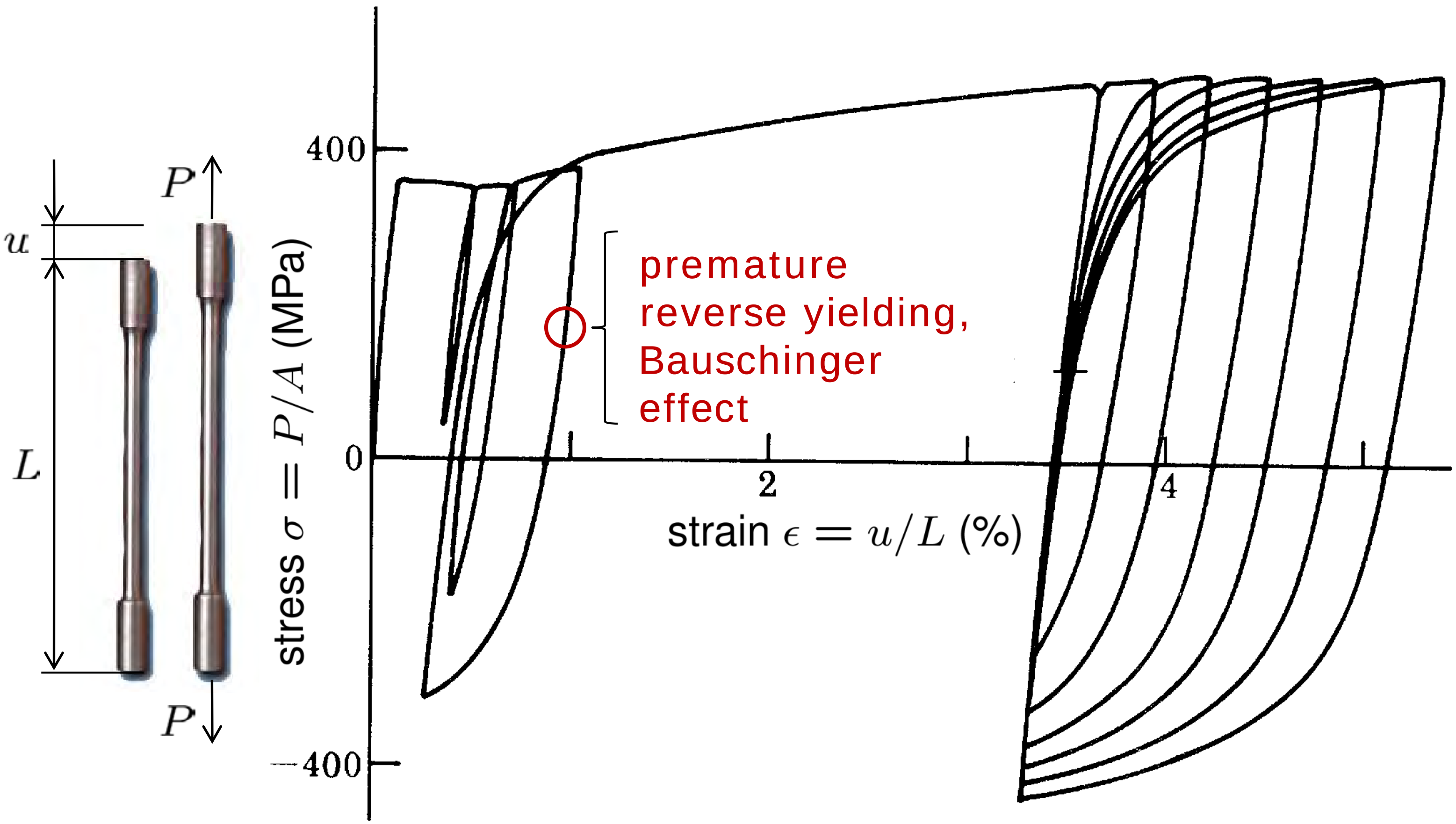
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension / compression



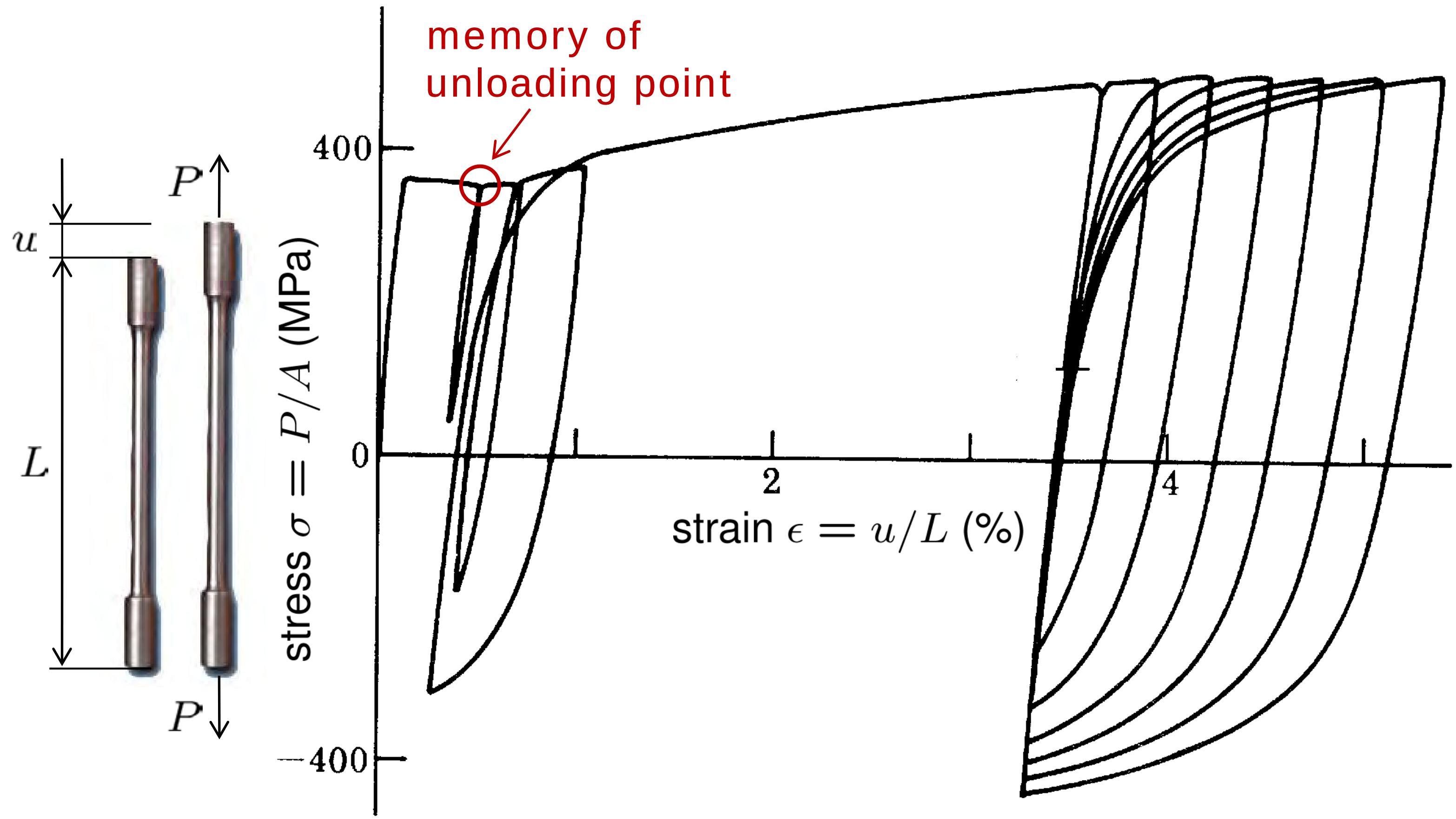
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension / compression



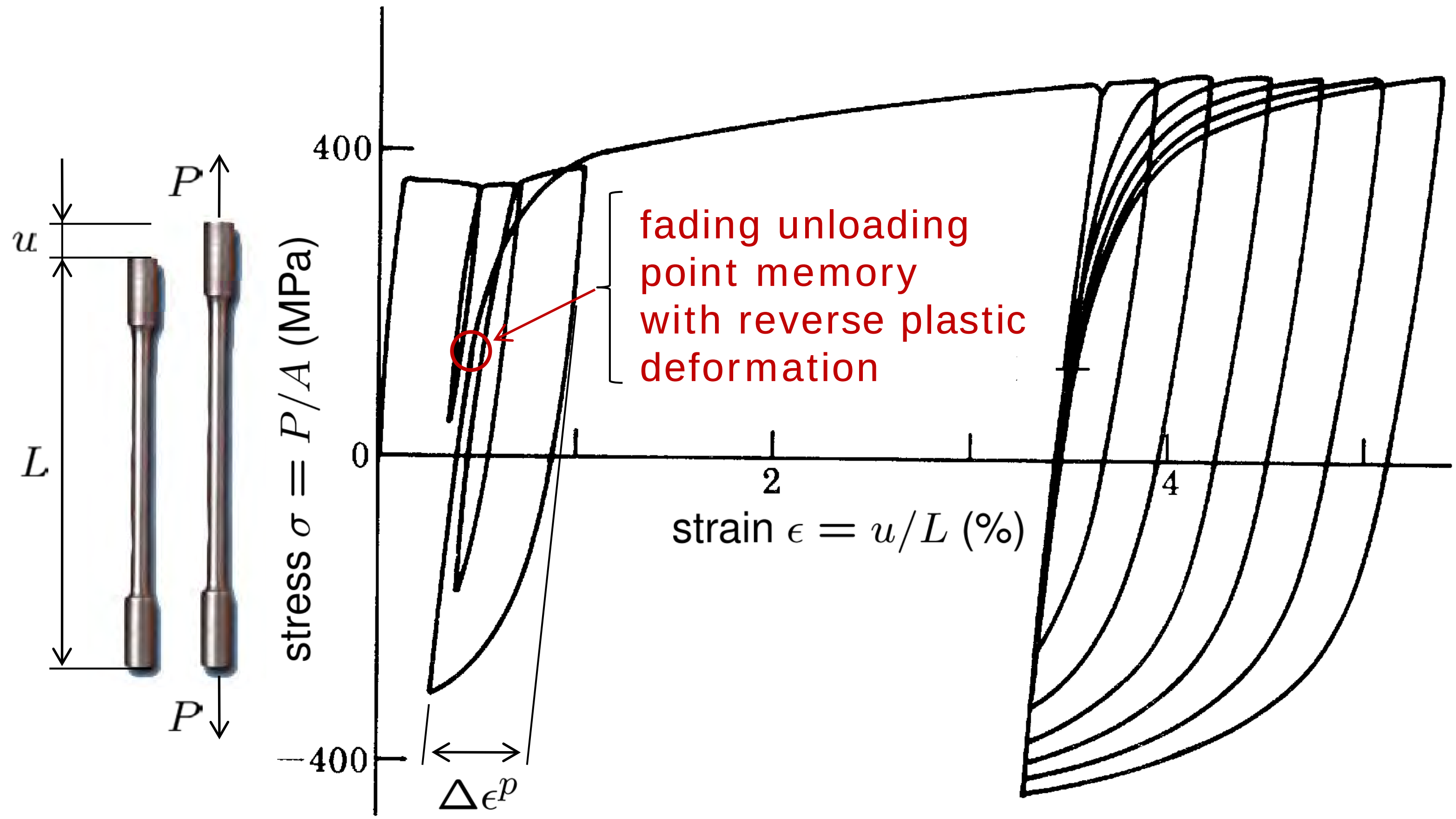
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension/compression



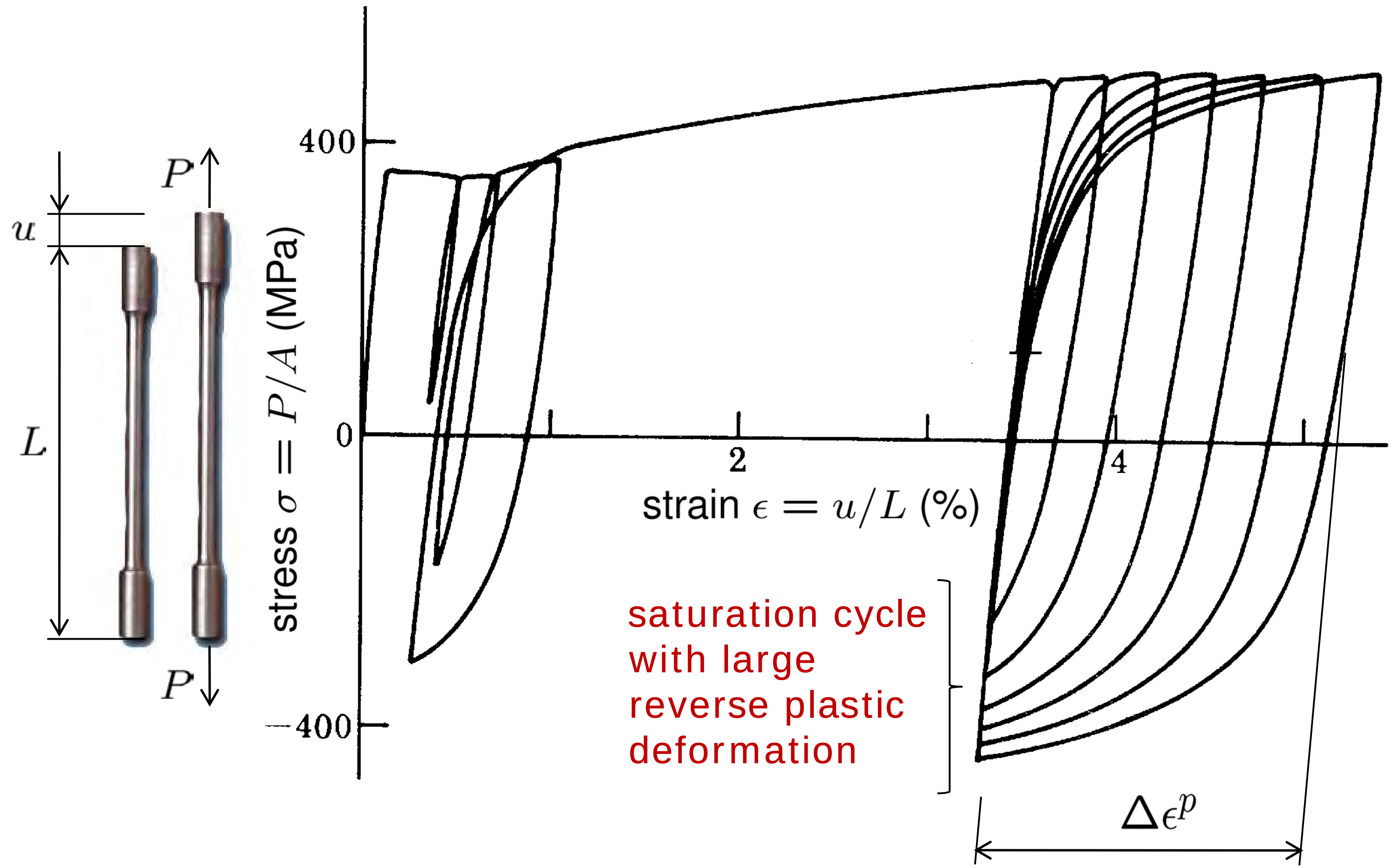
M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Uniaxial tension / compression



M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

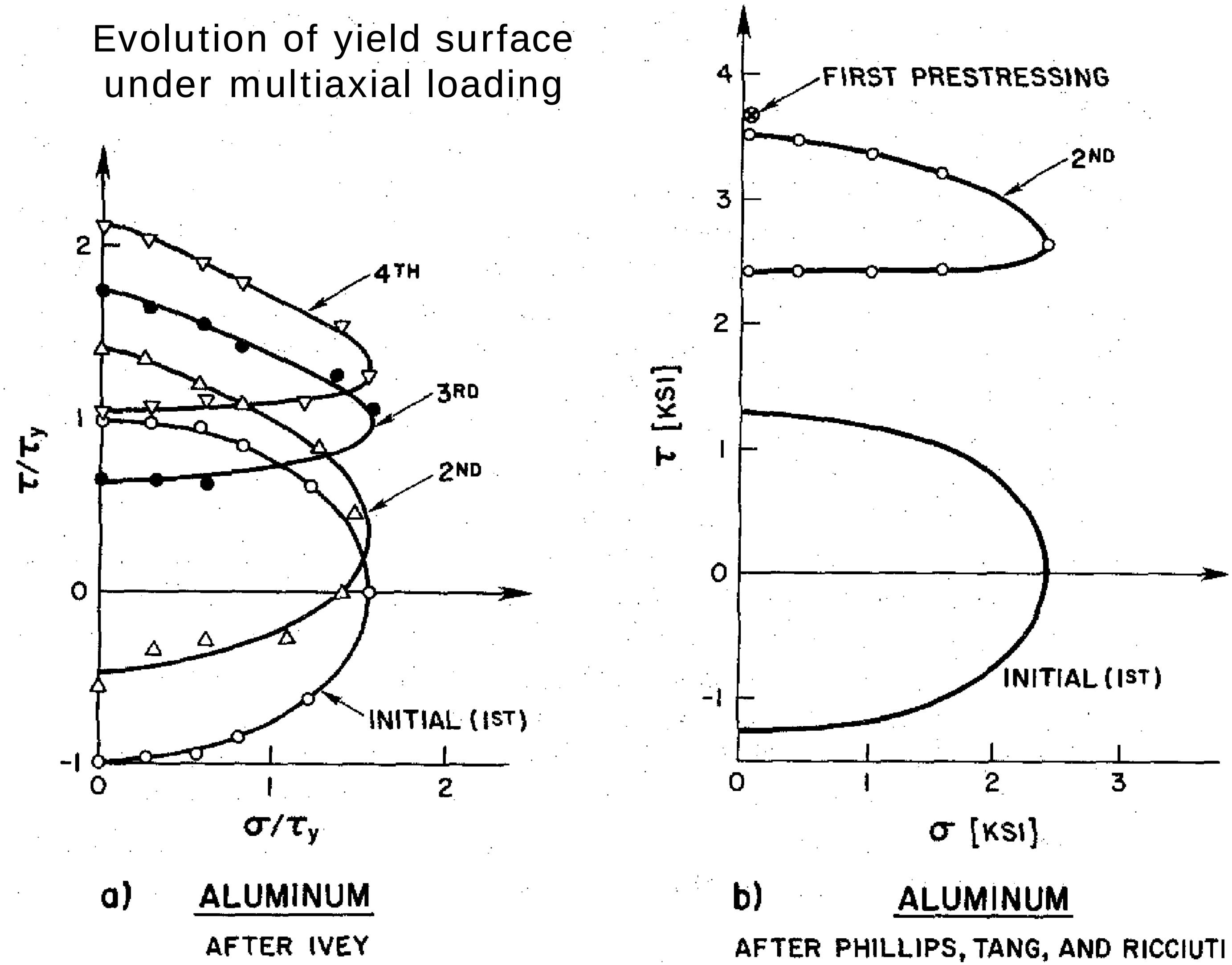
History-dependent inelastic materials – Uniaxial tension / compression



M. Ortiz and E.P. Popov, *Proc. Roy. Soc. Lond.* A **379**, 439-458 (1982)

History-dependent inelastic materials – Multiaxial tension / torsion

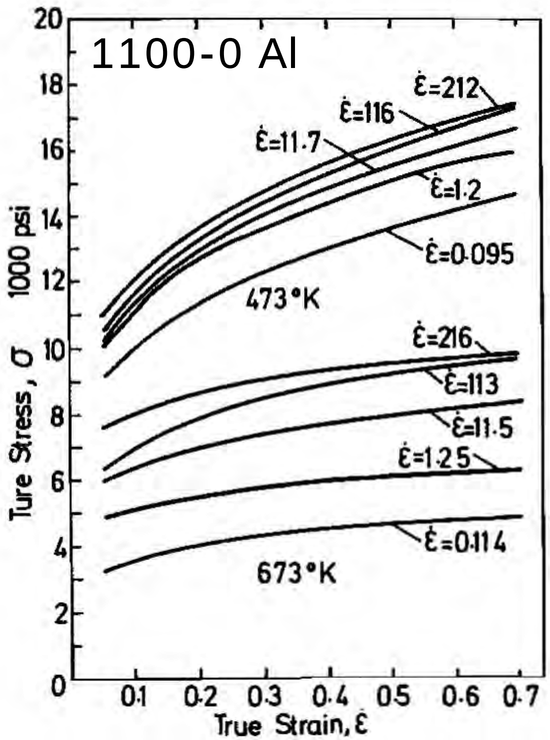
Evolution of yield surface under multiaxial loading

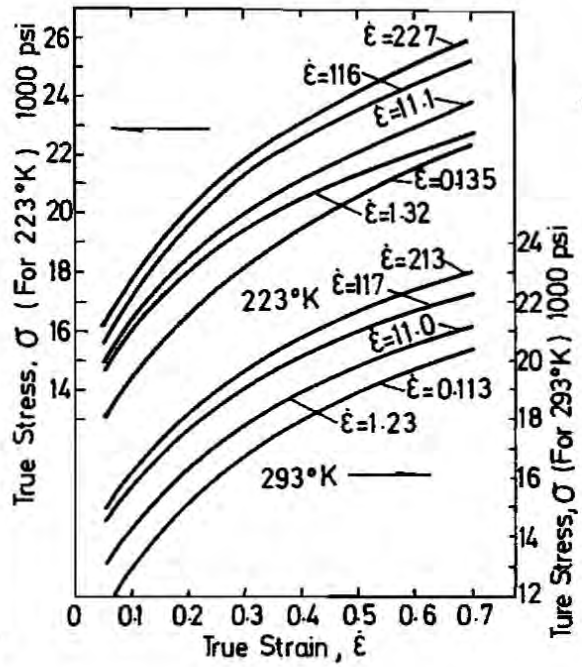


M. Ortiz and E.P. Popov, *J. Eng. Mech. ASCE*. 109(4), 1042-1057 (1983)

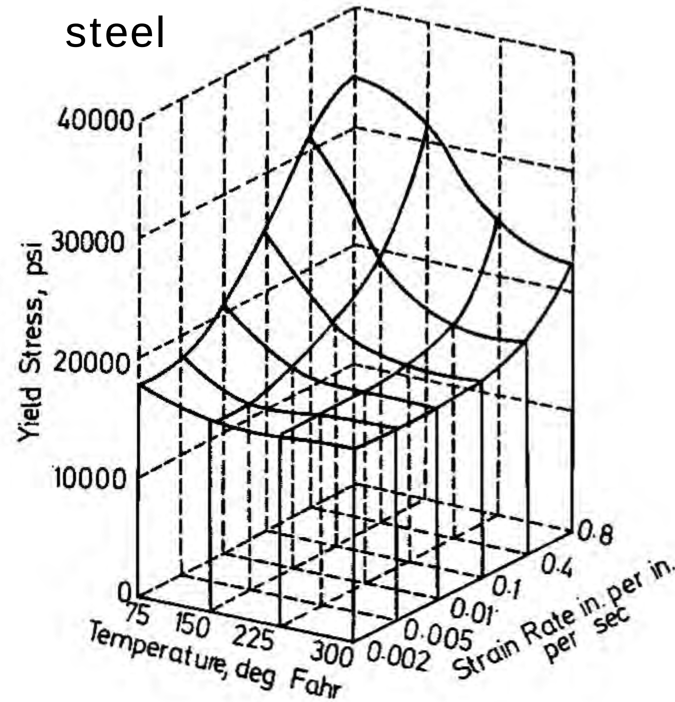
History-dependent inelastic materials – Thermal / rate sensitivity

Servo-hydraulic compression tests





Rolled steel



J.E. Hockett
Trans. AIME Metall. Soc., **239** (1967) 969-976.

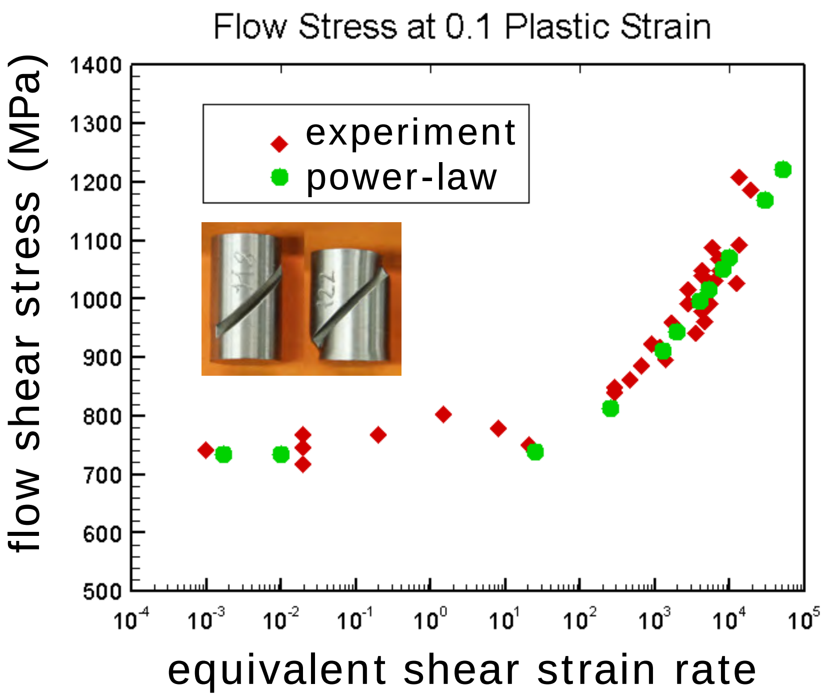
Power-law fit:

$$\sigma = C(\epsilon^p)^n(\dot{\epsilon}^p)^m\theta^{-l}$$

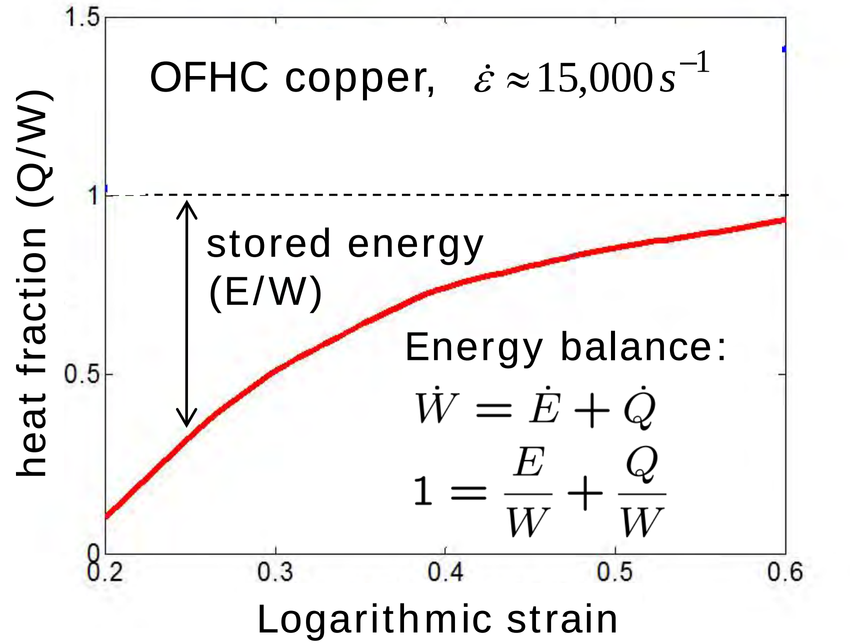
C.E. Work and T.J. Dolan
Proc. Am. Soc. Testing of Materials, **53** (1953) 611-656.

Y. Bai and B. Dodd, *Adiabatic Shear Localization*, Pergamon (1992).

History-dependent inelastic materials – Thermal / rate sensitivity



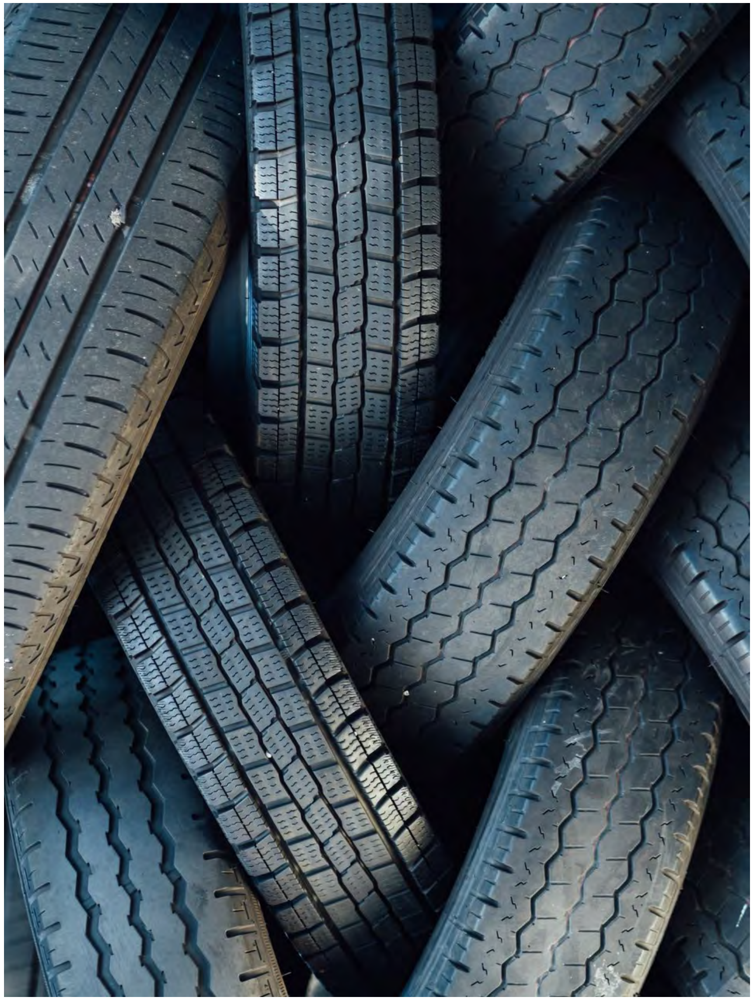
Shear-compression test
Split-Hopkinson (Kolsky)
pressure bar



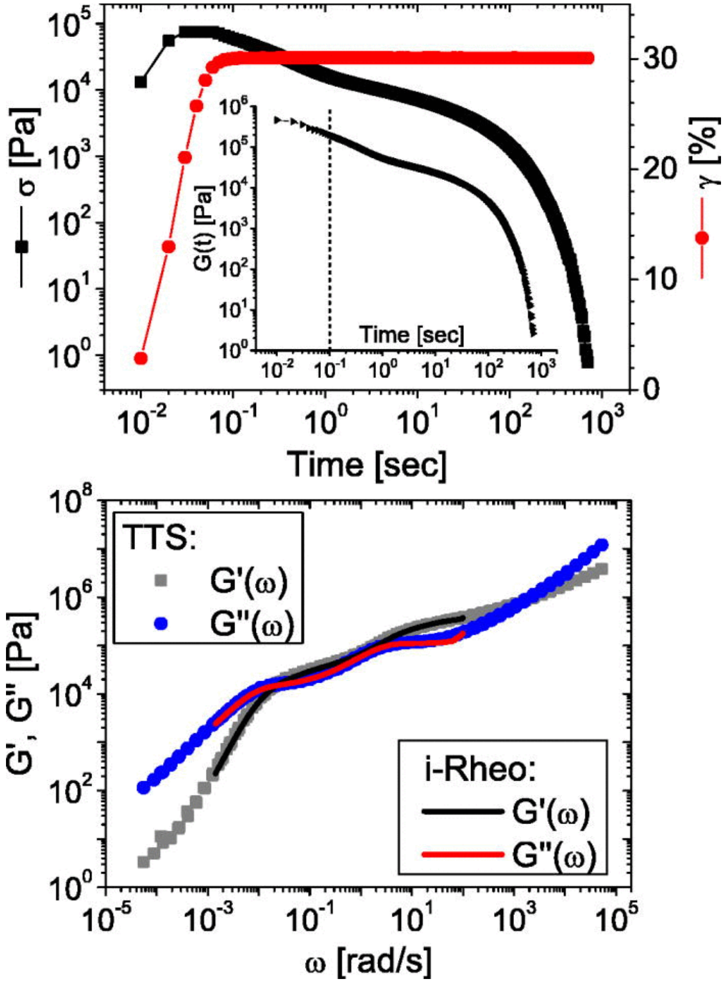
Fraction of total work dissipated as heat
Fraction of total work stored in lattice

M. Vural, D. Rittel and G. Ravichandran, *Metall. Mater. Trans. A*, **34** (2003) 2873.
D. Rittel, G. Ravichandran and S. Lee, *Mechanics of Materials*, **34** (2002) 627-642.

History-dependent inelastic materials – Viscoelasticity



Ultra-high molecular weight polyisoprene rubber
L. Wang et al., Chem. Comms.(2020).



Polyisoprene melt at -20C.
Top: Relaxation curve.
Botton: Complex modulus.
M. Tassieri et al., Journal of Rheology **60**, 649 (2016)

History-dependent inelastic materials

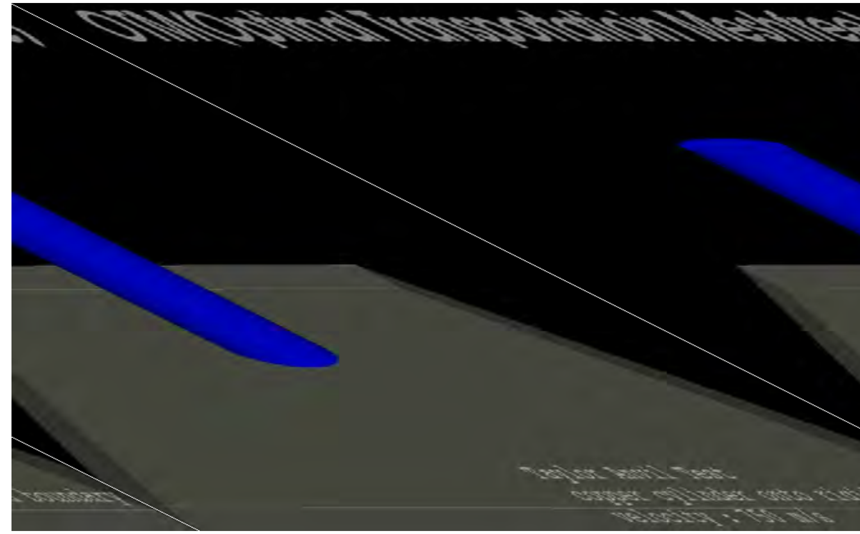
- *The complexity of inelastic behavior defies effective ad hoc modeling!*
- Instead: Extend the *model-free* Data-Driven paradigm to inelastic materials whose response is *history dependent*.

"The characteristic property of inelastic solids which distinguishes them from elastic solids is the fact that the stress measured at time t depends not only on the instantaneous value of the deformation but also on the entire history of deformation[1]."

- The theory of *materials with memory* furnishes the most general representation of inelastic materials.
- Alternative: Replace history by the effects of history, the current *microstructure* (internal state)
- Variables used to describe that microstructure, within a *continuum thermodynamics* framework, are referred to as *internal variables*
- The concept of *internal variable* was introduced into thermodynamics by Onsager (1931), into continuum mechanics by Eckart (1948)...
- *Choice of internal variables* is often *ad hoc,* no notion of *convergence*
- Instead: *Data-Driven* representations that are *history (path) based* and *internal-variable-free. How?*

[1] R. S. Rivlin, "Materials with memory." *Tech. Rep. AD-753 460*, ONR, 1972.

Structural/solid inelasticity



- Phase space: $Z = \mathbb{R}^N \times \mathbb{R}^N$.
- To determine: Histories $z(\cdot)$ over $\mathbb{R}$.
- Space of trial histories:
  $$\mathcal{Z} \equiv \{z(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) : \mathbb{R} \to Z\}.$$
- NB: $z(t) =$ value of $z(\cdot)$ at $t \in \mathbb{R}$.
- Space of physically admissible histories,
  $$\mathcal{E} = \Big\{ z(\cdot) \equiv (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z} \, : \, \text{for } t \in \mathbb{R}, \quad \epsilon_e(t) = B_e u(t), \quad M\ddot{u}(t) + \textstyle\sum_{e=1}^m w_e B_e^T \sigma_e(t) = f(t) \Big\}.$$
- Space of material histories: For specific materials,
  $$\mathcal{D} = \big\{ y(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z} \, : \, \text{attainable by the material} \big\}.$$
- Classical phase-space histories: $z(\cdot) \in \mathcal{D} \cap \mathcal{E}$,
  - Admissible histories that are material!
  - Material histories that are admissible!

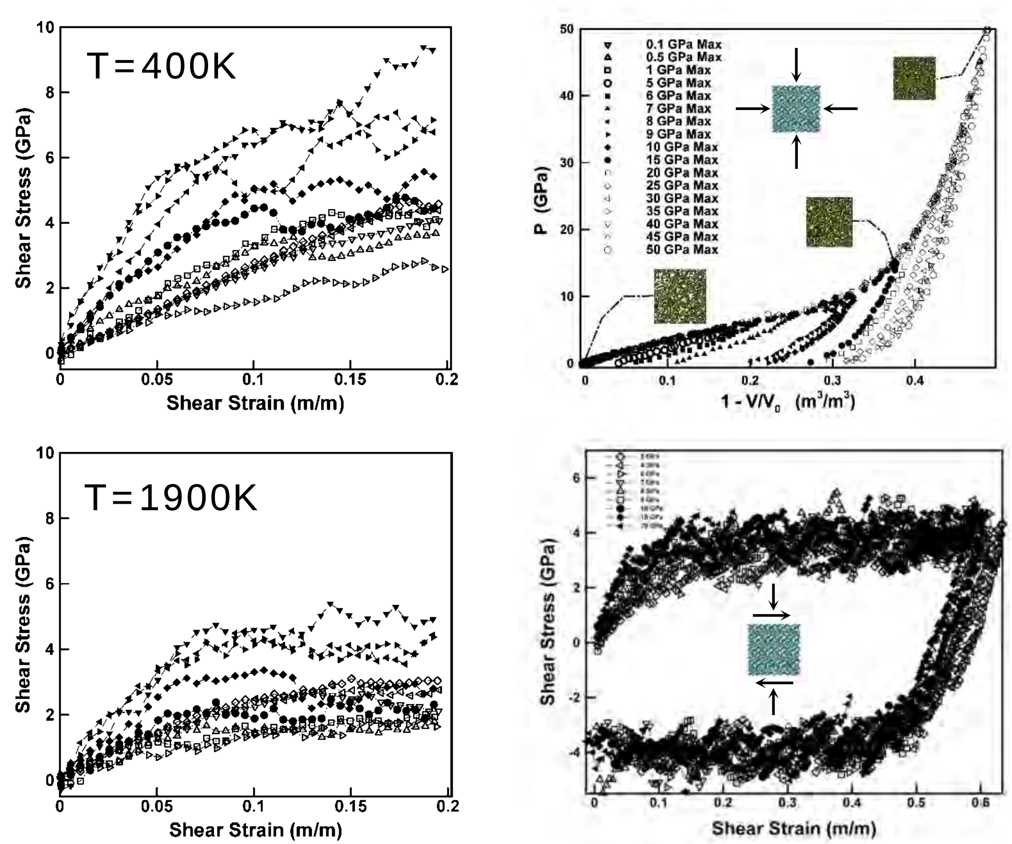
Structural/solid inelasticity – Data acquisition

- Acquire material history set $\mathfrak{D}$ by recourse to experimental testing
- Material history data can also be acquired in large quantities from high-fidelity *micromechanical calculations*

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.

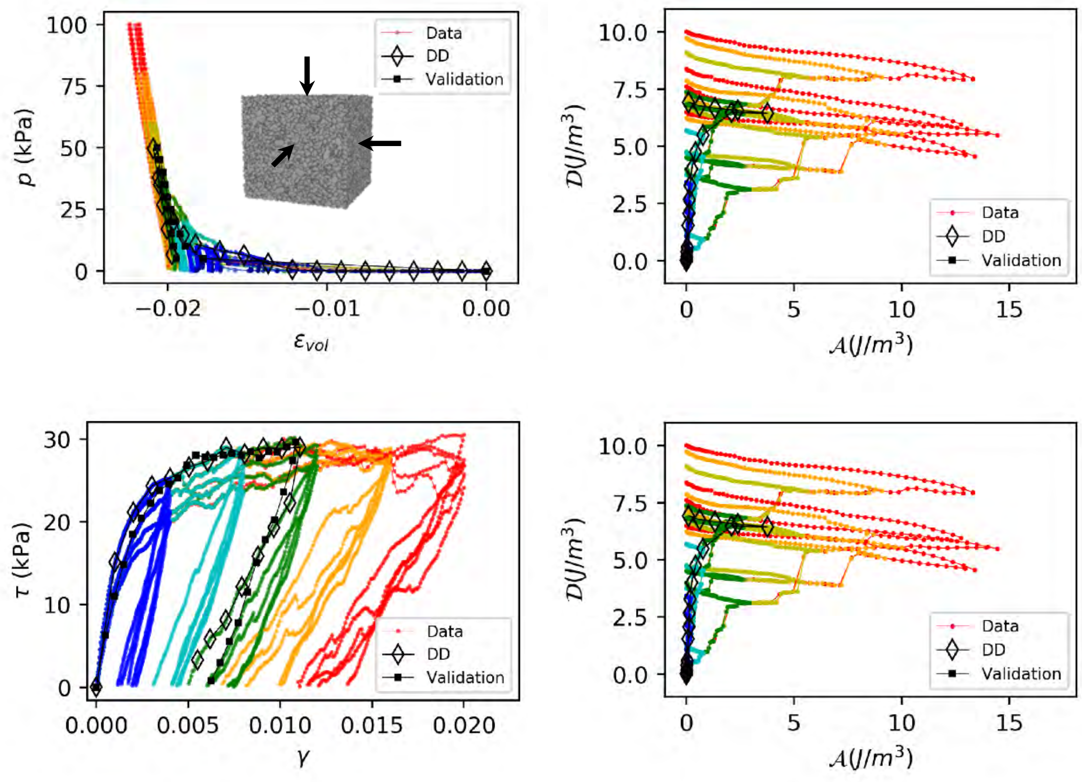


Structural/solid inelasticity

(cf. L. Stainier, Nov 13, 14:00-14:45)
(cf. S. Reese, Nov 13, 15:30-17:30)

- Acquire material history set $\mathfrak{D}$ by means of experimental testing
- Material history data can also be acquired in large quantities from high-fidelity *micromechanical calculations*

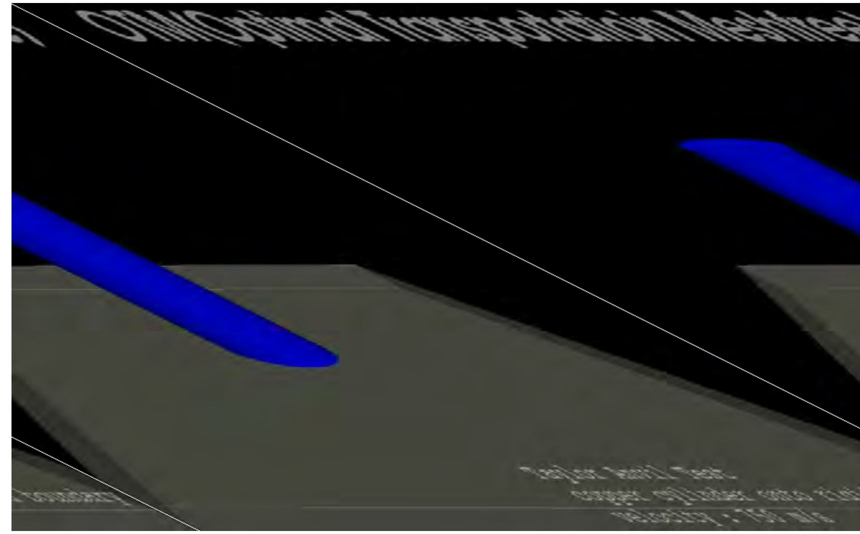
Granular matls. (dry sand): Level-Set Discrete Element Method (LS-DEM) simulation of granular material samples. 3D irregular *rigid particles* interact through *frictional contact*. Particle morphology described by level-set functions. Note calculation of *dissipation and free energy*.



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

Structural/solid inelasticity



- $\mathcal{D}$ may consist of sampled history data.
- No classical histories! ($\mathcal{D} \cap \mathcal{E} = \emptyset$).
- Need Data-Driven reformulation!
- Metrize space $\mathcal{Z}$ of histories.
- Data-Driven histories:

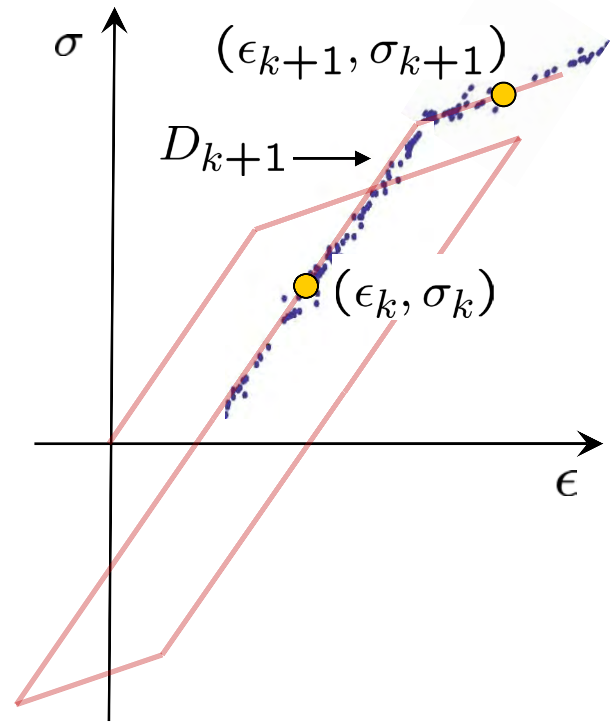
$$\big(y(\cdot), z(\cdot)\big) \in \operatorname{argmin}\Big\{\operatorname{dist}\big(y(\cdot), z(\cdot)\big) \;:\; y(\cdot) \in \mathcal{D},\; z(\cdot) \in \mathcal{E}\Big\},$$

  - Admissible histories that are closest to being material.
  - Material histories that are closest to being admissible.

- Implementation: With $y(\cdot) \in \mathcal{D}$, $z(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z}$,
  - Enforce compatibility strongly by setting $\epsilon_e(t) = B_e u(t)$.
  - Enforce dynamic equilibrium by means of Lagrange multiplier $w(\cdot)$,

$$\delta\Big\{\operatorname{dist}\big(y(\cdot), z(\cdot)\big) + \int_0^T \Big(M\ddot{u}(t) + \sum_{e=1}^m w_e B_e^T \sigma_e(t) - f(t)\Big) \cdot w(t)\, dt\Big\} = 0$$

Structural/solid incremental plasticity



- Time discretization:

$$t_0, \ldots, t_k, t_{k+1} = t_k + \tau, \ldots, t_N.$$

- Space of physically admissible incremental states,

$$E_{k+1} = \Big\{ z_{k+1} \equiv (\epsilon_{k+1}, \sigma_{k+1}) \in Z \, : \, \epsilon_{e,k+1} = B_e u_{k+1}, \quad \sum_{e=1}^{m} w_e B_e^T \sigma_{e,k+1} = f_{k+1} \Big\}.$$

- Space of incremental material states:

$$D_{k+1} = \big\{ y_{k+1} = (\epsilon_{k+1}, \sigma_{k+1}) \in Z \, : \, (\epsilon_k, \sigma_k), \text{ past history} \big\}.$$

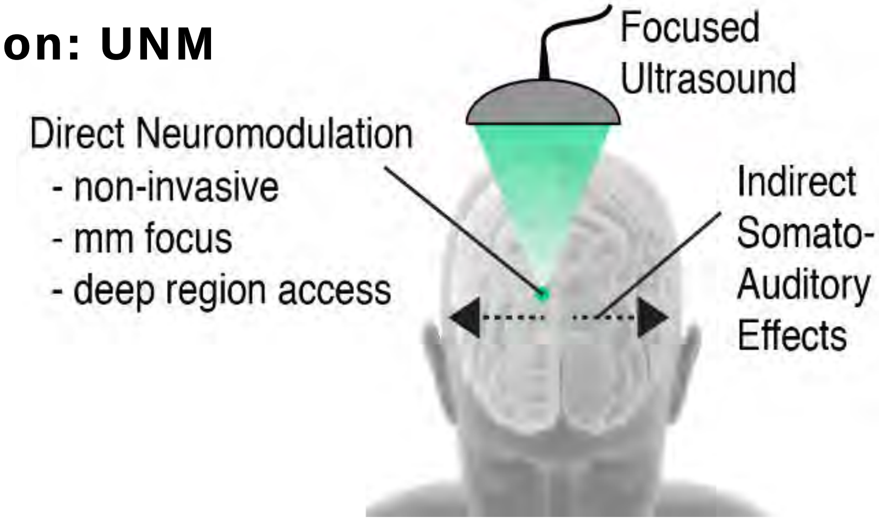
- Incremental Data-Driven problem:

$$\big(y_{k+1}, z_{k+1}\big) \in \operatorname{argmin}\Big\{ \|y_{k+1} - z_{k+1}\|^2 \, : \, y_{k+1} \in D_{k+1}, \; z_{k+1} \in E_{k+1} \Big\}.$$

  - Admissible incremental trajectories that are closest to being material.
  - Material incremental trajectories that are closest to being admissible.
  - Same structure as elastic DD problems: Pseudo-elastic incremental problem.
  - Need to store history data, structure it as a directed graph, define rules for traversing the graph.

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

Data-Driven viscoelasticity – Motivation: UNM

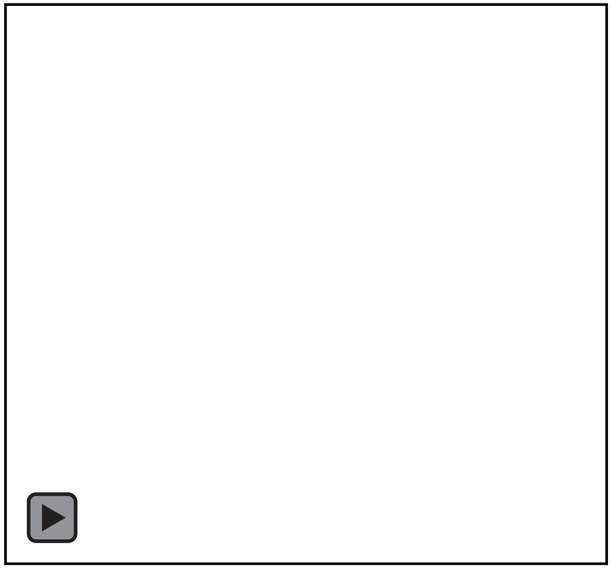


- *Ultrasonic neuromodulation* (UNM) is a novel non-invasive technique that uses *low intensity focused ultrasound* (LIFU) to stimulate the brain.
- First proposed in 2002 by A. Bystritsky as possibly having therapeutic benefits.
- W. Tyler and team discovered UNM is able to stimulate high neuron activity.
- 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.

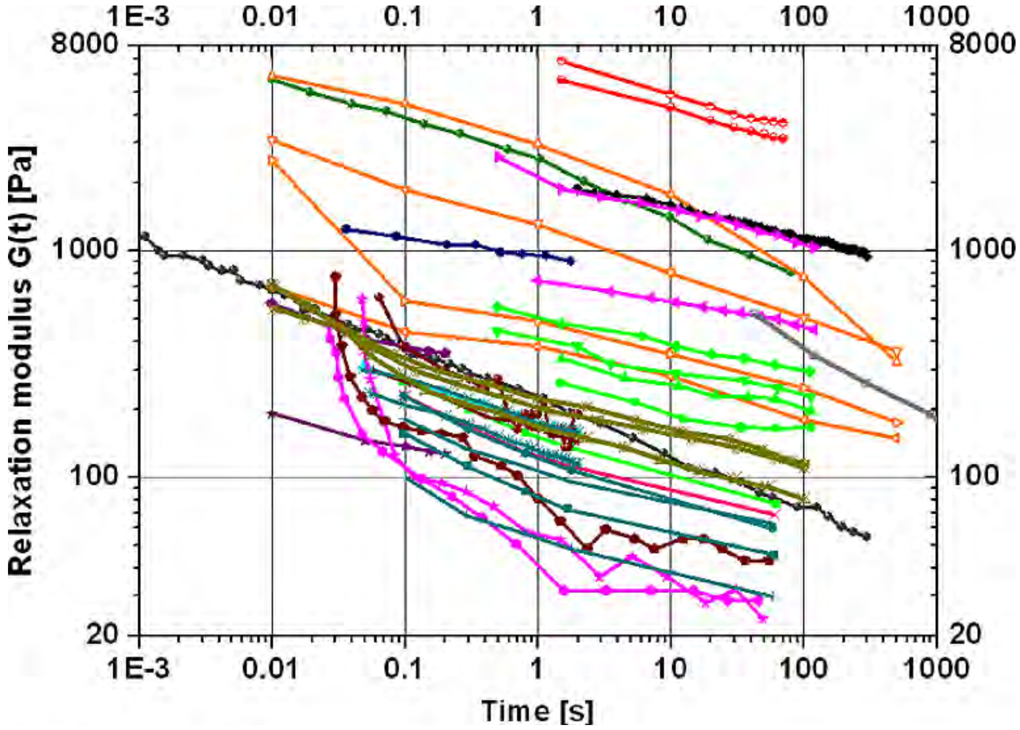
Salahshoor, S., Shapiro, M. and Ortiz, M. Appl. Phys. Lett. **117**, 033702 (2020)



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

Data-Driven viscoelasticity – Motivation: 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.

Data-Driven viscoelasticity – Motivation: UNM

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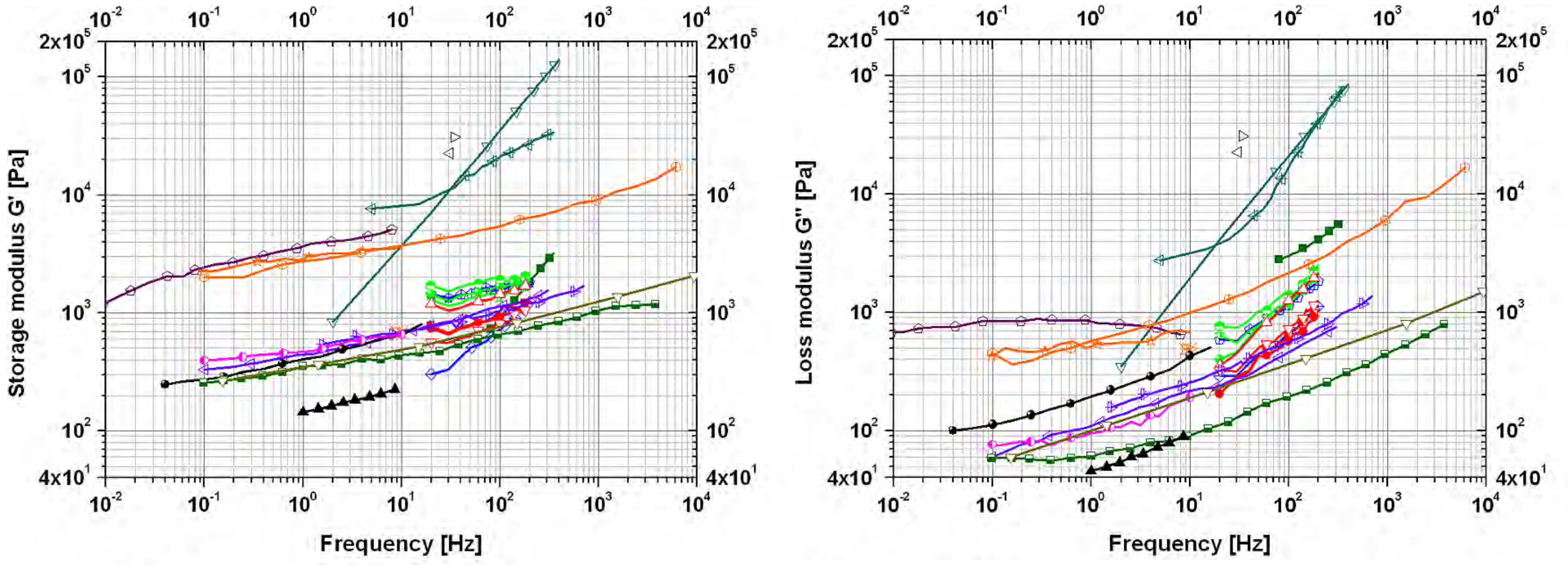
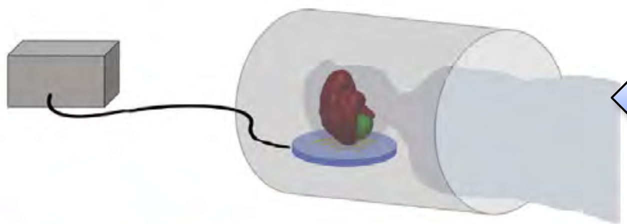


Storage and loss moduli of brain tissue compiled from literature survey of *in vitro* dynamic frequency sweep tests in shear.

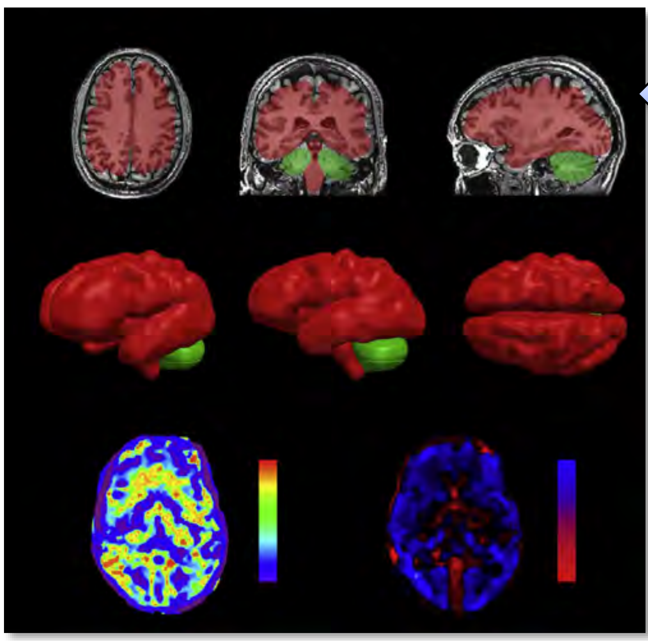
Chatelin, S., Constantinesco, A., Willinger, R.,
"Fifty years of brain tissue mechanical testing: from in vitro to in vivo investigations."
Biorheology. 2010;**47**(5-6):255-76.

Data-Driven viscoelasticity – Motivation: UNM

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

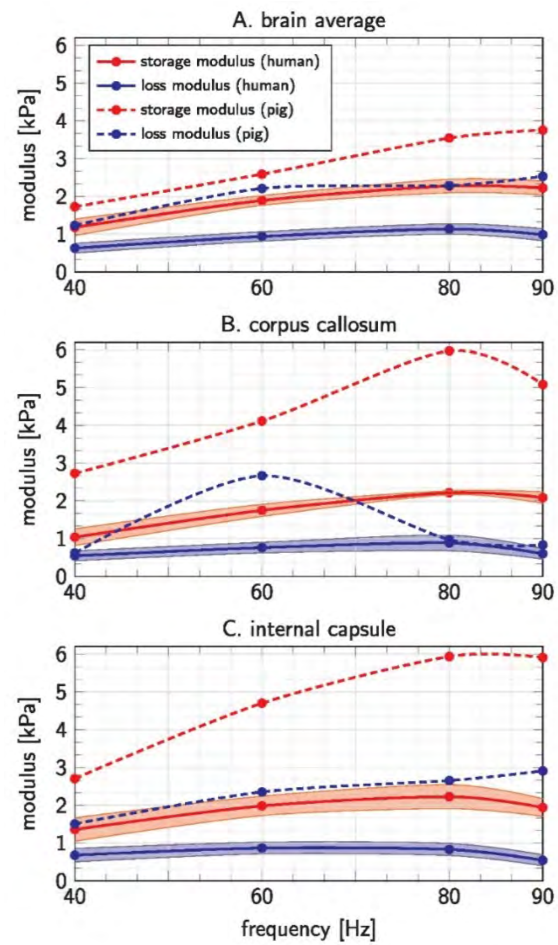


Human subjects scanned in the supine position



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.

Structural/solid linear viscoelasticity

- 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,

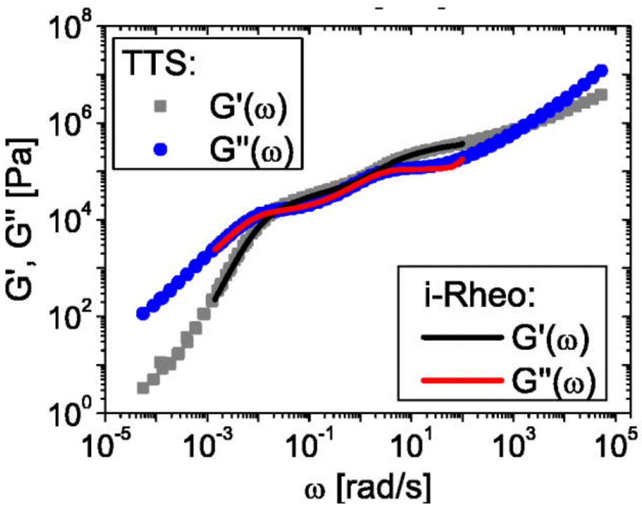
$$\hat{\epsilon}_e(\omega) = B_e \hat{u}(\omega) + \hat{g}_e(\omega), \quad e = 1, \dots m,$$

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

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

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

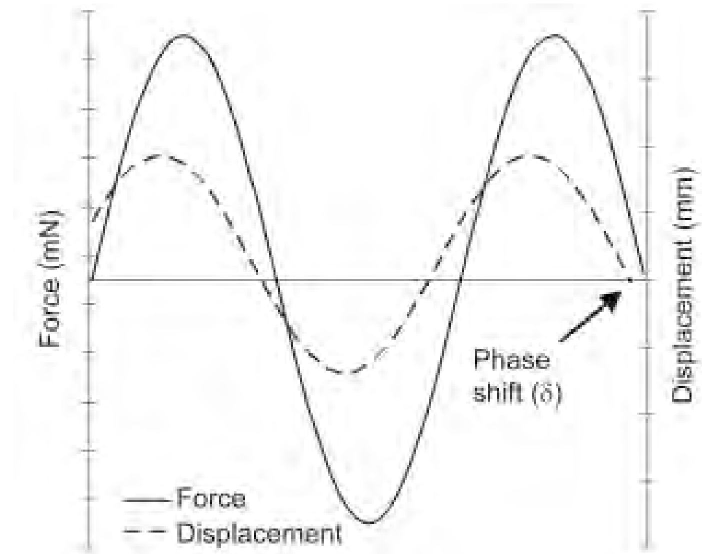
Polyisoprene rubber.



Dynamic Mechanical Analysis (DMA)

L. Wang et al., Chem. Comms.(2020).
M. Tassieri et al., Journal of Rheology **60**, 649 (2016)

Structural/solid linear viscoelasticity – Steady state



- Suppose that the forcing is harmonic,

$$\hat{f} = 2\pi F \delta_\Omega, \quad \hat{g} = 2\pi G \delta_\Omega. \quad \text{NB: Measures!}$$

  - $F \in \mathbb{C}^n$; $G \in \mathbb{C}^N$ $\equiv$ complex amplitudes.
  - $\Omega \equiv$ applied transduction frequency.

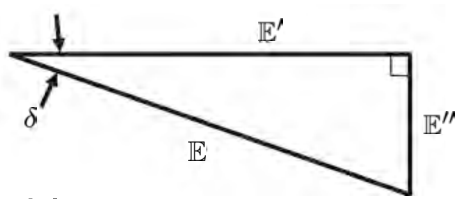
- Monochromatic *ansatz* (in space of measures!),

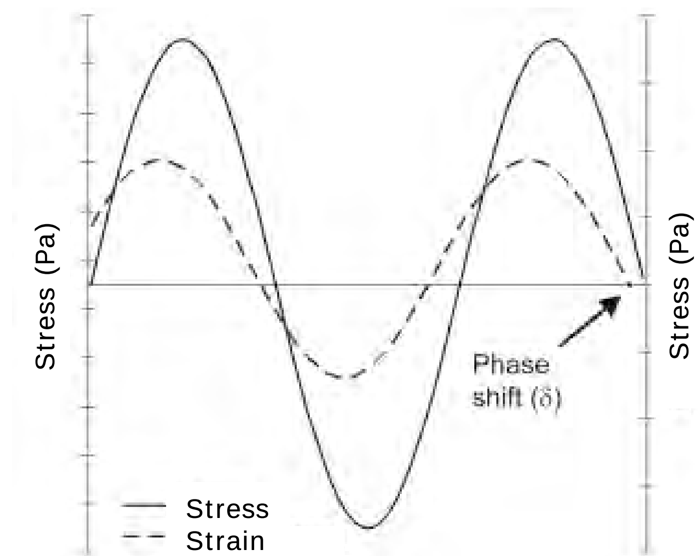
$$\hat{u} = 2\pi U \delta_\Omega, \quad \hat{\epsilon} = 2\pi E \delta_\Omega, \quad \hat{\sigma} = 2\pi S \delta_\Omega.$$

  - $U \in \mathbb{C}^n$; E, $S \in \mathbb{C}^N$ $\equiv$ complex amplitudes

- Steady-state problem,

$$E = BU + G,$$
$$B^T W S - M\Omega^2 U = F,$$
$$S = \mathbb{E}(\Omega)\, E.$$





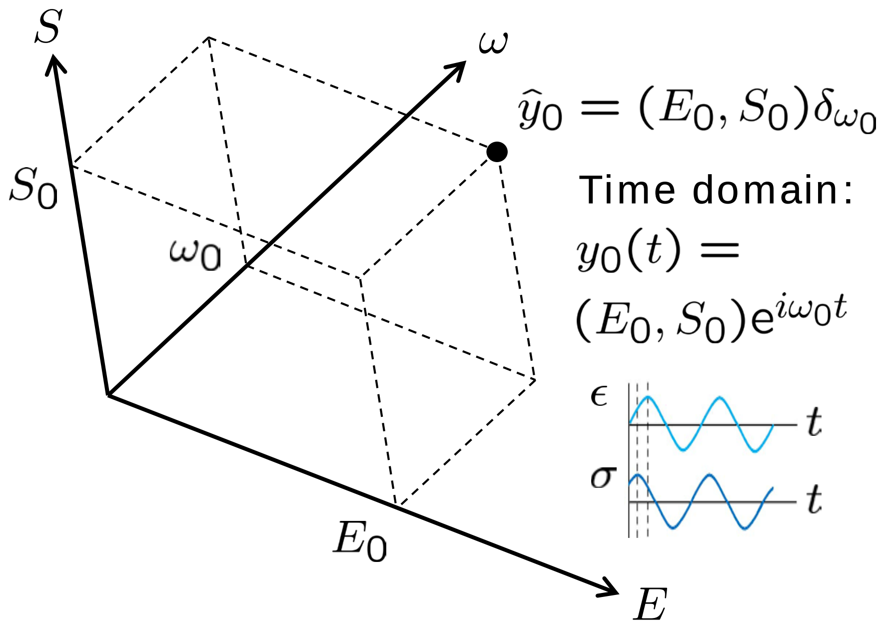
- Steady-state displacement problem,

$$B^T W \mathbb{E}(\Omega)(BU + G) - M\Omega^2 U = F.$$

Structural/solid linear viscoelasticity

- $\mathcal{Z} \equiv$ space of 'infinite wave trains',

  $\mathcal{Z} = \{(\epsilon(\cdot), \sigma(\cdot)) \,:\, (\hat{\epsilon}, \hat{\sigma}) \equiv$ finite Radon measures on $\mathbb{R}$, e.g., Diracs$\}$.



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- Material history set (linear viscoelasticity),

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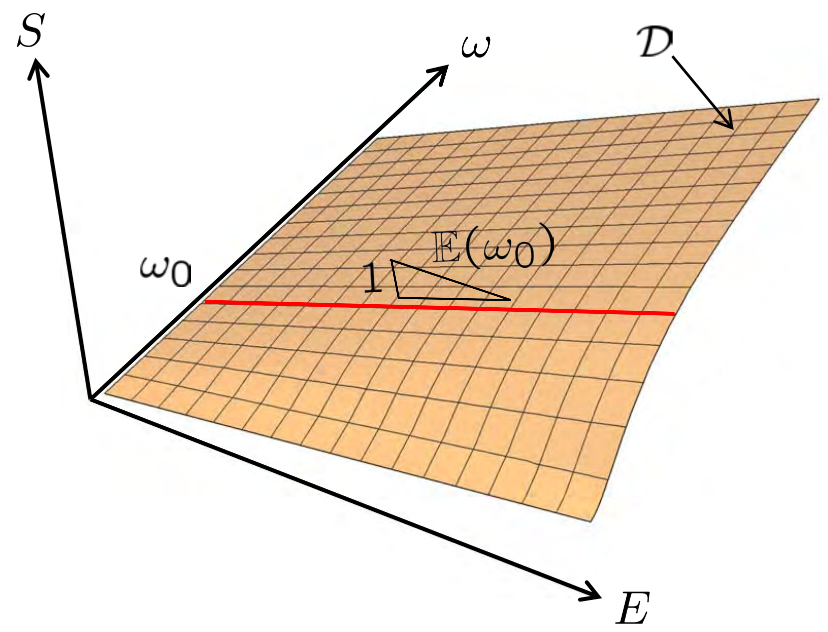
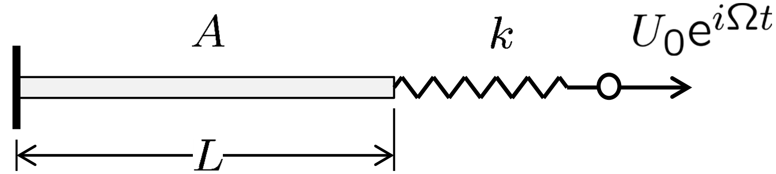
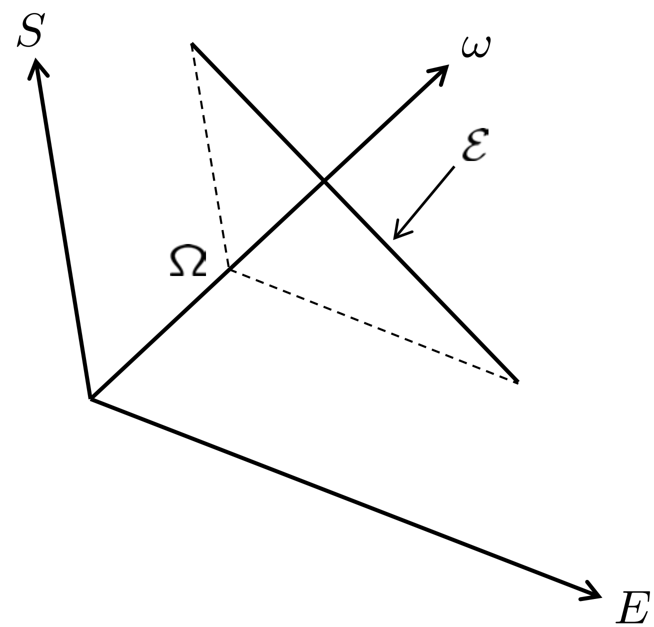


Structural/solid linear viscoelasticity





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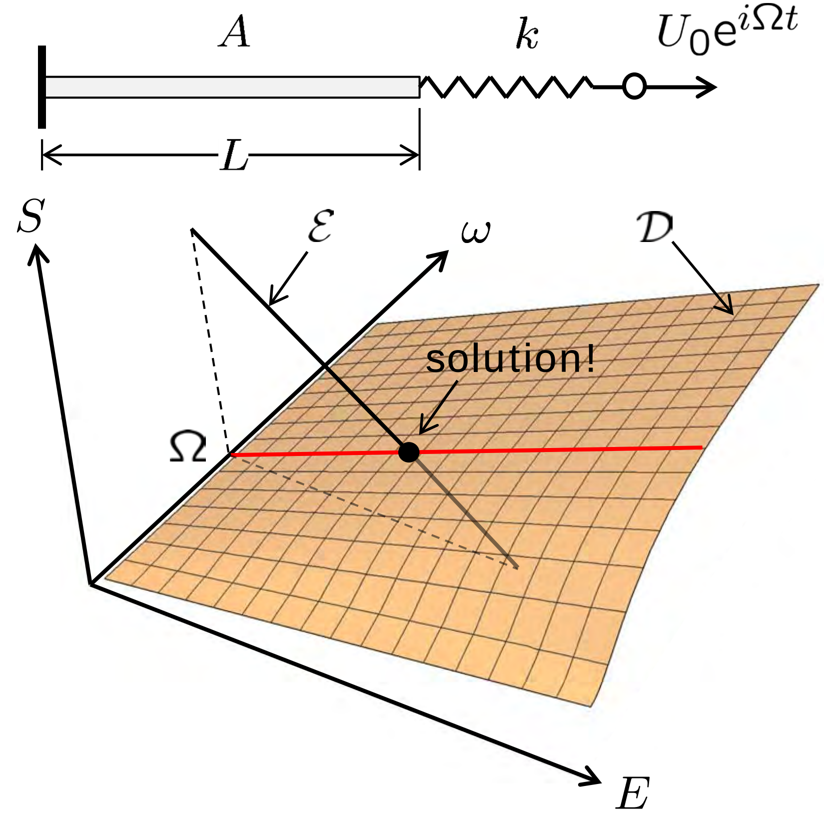
- Admissible history set (harmonic loading):
  For given $F \in \mathbb{C}^n$, $G \in \mathbb{C}^N$, $\Omega \in \mathbb{R}$,

$$\mathcal{E} = \{(\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z} \, : \, (\epsilon(t), \sigma(t)) = (E, S) \, \mathrm{e}^{i\Omega t},$$
$$(\hat{\epsilon}, \hat{\sigma}) = (E, S) \, \delta_\Omega; \quad E = BU + G; \quad B^T W S - M\Omega^2 U = F\}.$$

Structural/solid linear viscoelasticity



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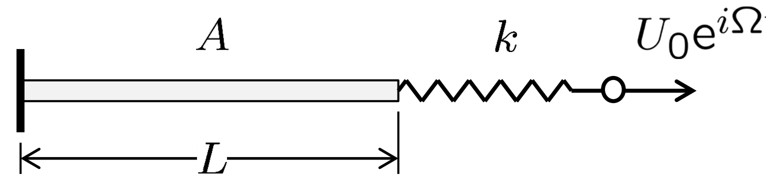
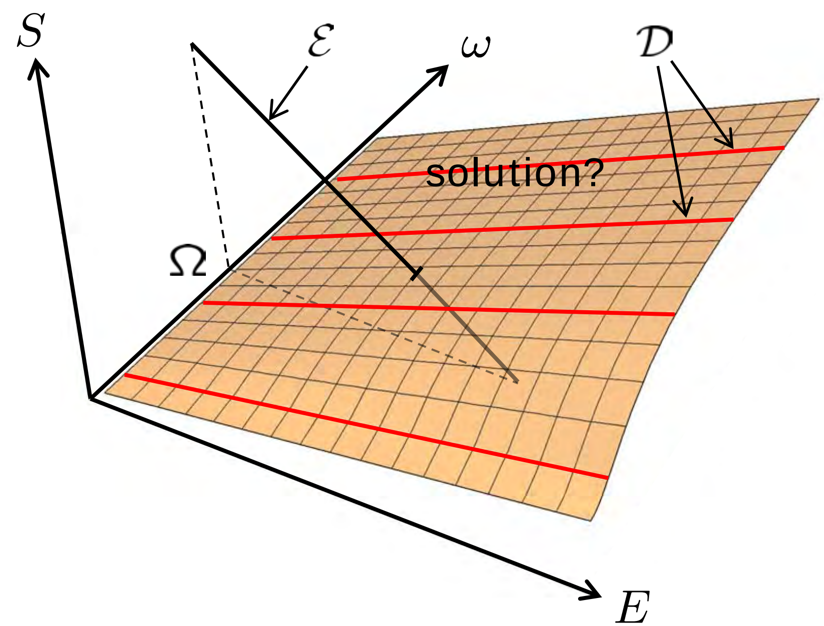
- Classical solution: $(\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{D} \cap \mathcal{E}$.

Structural/solid linear viscoelasticity





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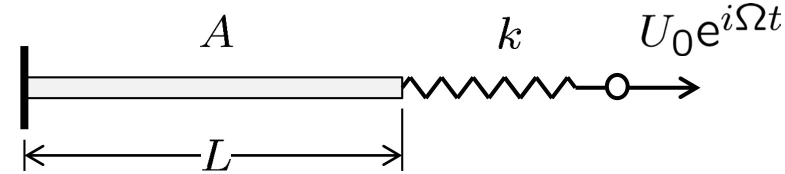
- Classical solution: $(\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{D} \cap \mathcal{E}$.

- Data-Driven solution:

  $$(\epsilon(\cdot), \sigma(\cdot)) \in \operatorname{argmin}\{\mathrm{dist}(y(\cdot), z(\cdot)) \,:\, y(\cdot) \in \mathcal{D},\ z(\cdot) \in \mathcal{E}\}.$$

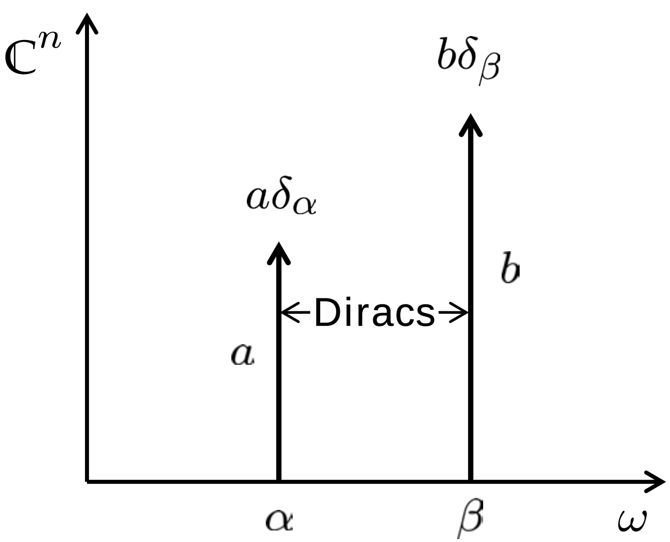
- Appropriate metrization of $\mathcal{Z}$? (need distance between measures, e.g., Diracs).

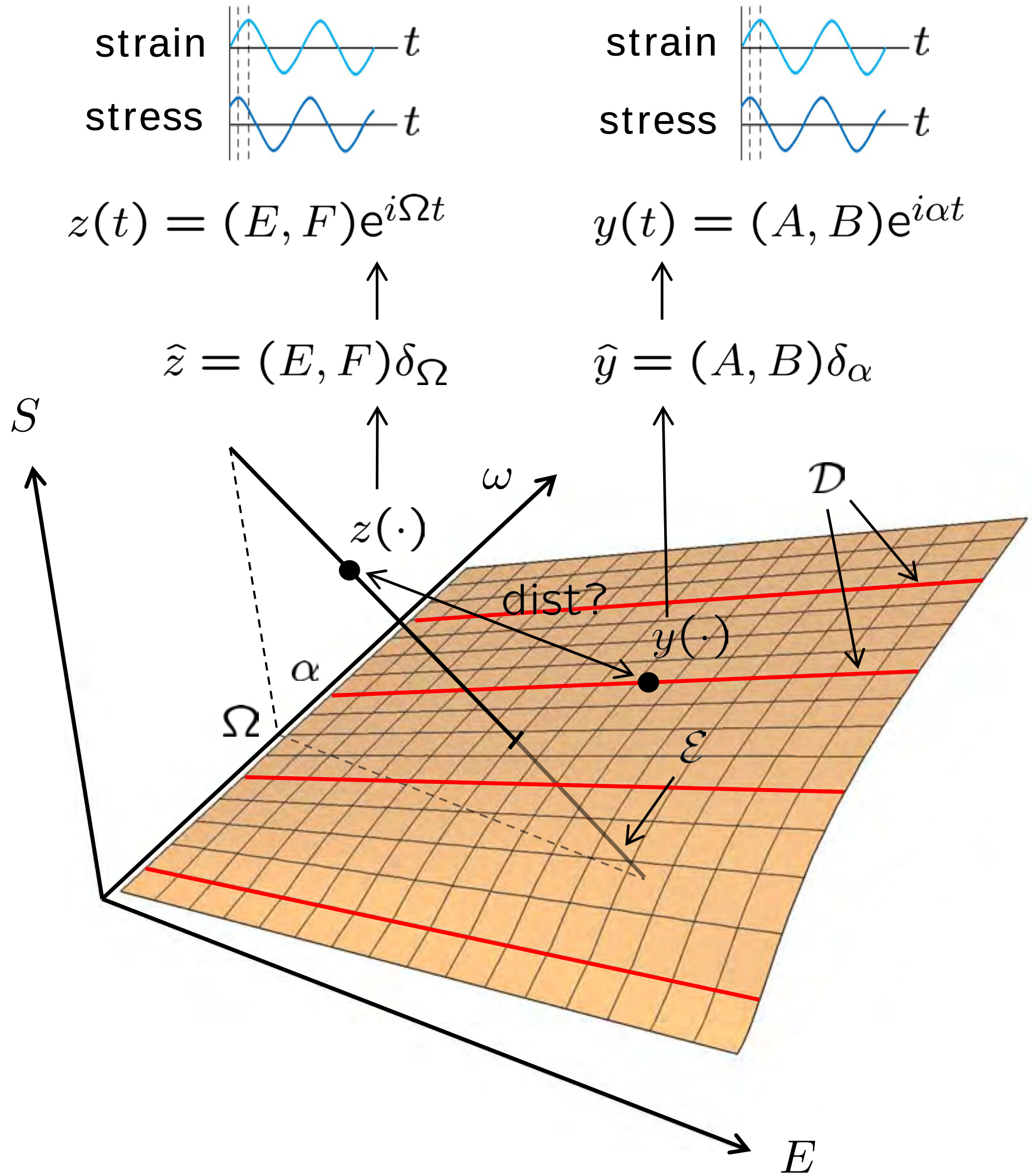
Structural/solid linear viscoelasticity



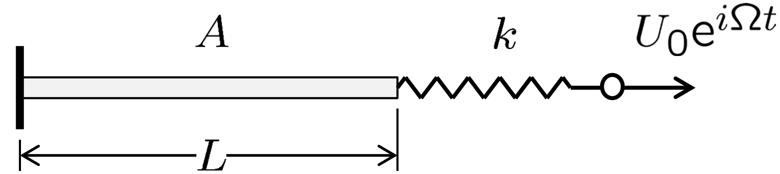
- Need a distance between Diracs.
- Natural distance: Flat norm!
- For $a, b \in \mathbb{C}^n$, $\alpha, \beta \in \mathbb{R}$, $\omega_0 > 0$ (reference frequency),

$$\|a\delta_\alpha - b\delta_\beta\| = \|a - b\| + \min\{\|a\|, \|b\|\} \min\{2, |\alpha - \beta|/\omega_0\}.$$





Structural/solid linear viscoelasticity



- Local DMA data, $e = 1, \dots, m$:

  $\mathcal{P}_e = \{(\omega_{e,i_e}, \mathbb{E}_{e,i_e}),\ i_e = 1, \dots, M_e\}$.

- Local data sets, $e = 1, \dots, m$:

  $\mathcal{D}_e = \cup_{i_e=1}^{M_e} \mathcal{D}_{e,i_e}$, linear subspaces :

  $\mathcal{D}_{e,i_e} = \{S_e = \mathbb{E}_{e,i_e} E_e\}\, \delta_{\omega_{e,i_e}} \subset \mathcal{Z}_e$.

- Global data sets: $\mathcal{D} = \cup_{e=1}^{m} \mathcal{D}_e$.

- Global distance:

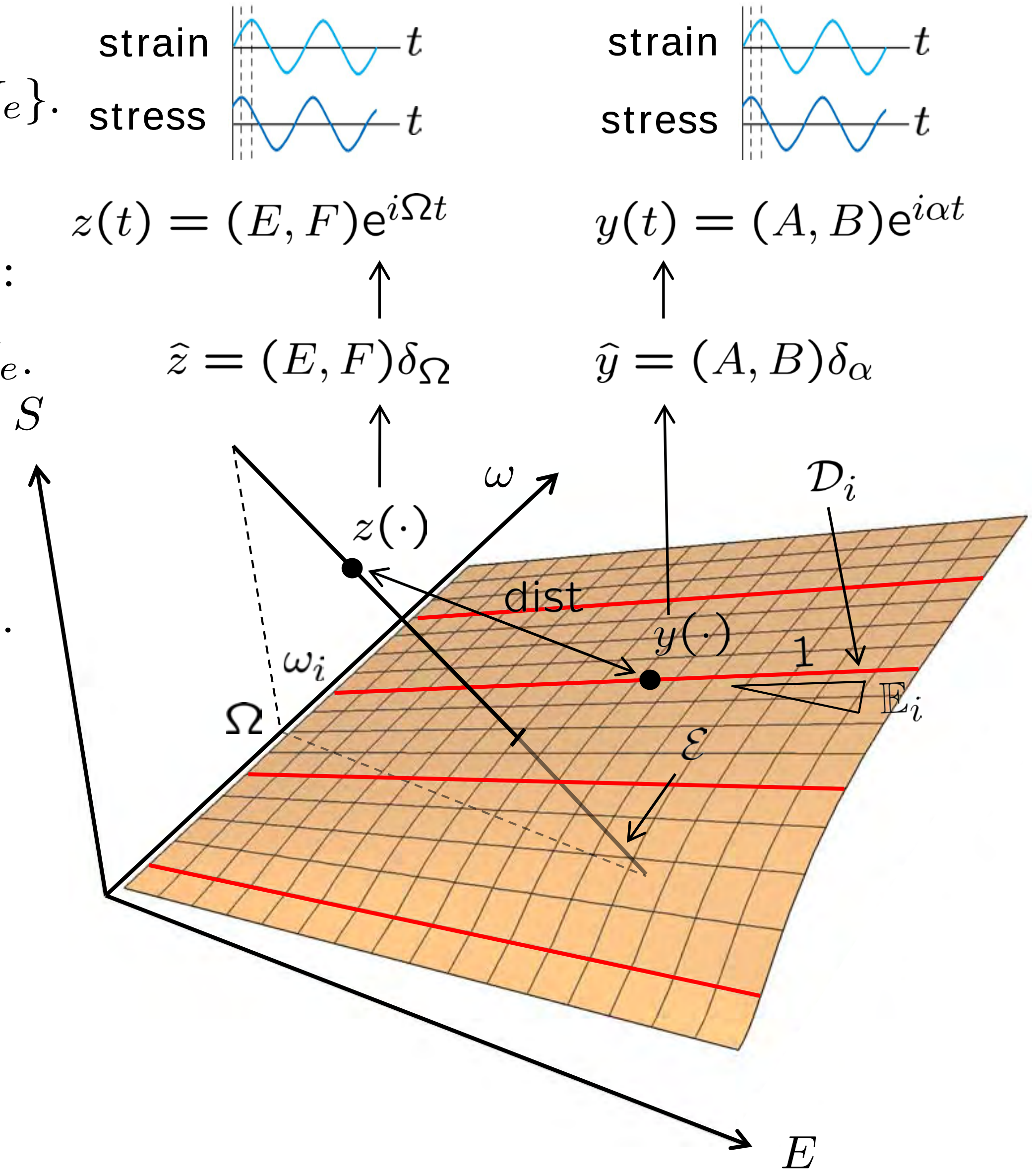
  $\text{dist}(y(\cdot), z(\cdot)) = \Sigma_{e=1}^{m} \|\hat{y}_e - \hat{z}_e\|_{\text{FN}}$.

- Data-Driven problem: Find

  $\text{argmin}\{\Sigma_{e=1}^{m} \text{dist}(\hat{z}_e, \mathcal{D}_{e,i_e})\ :$

  $z(\cdot) \in \mathcal{E},\ i_e = 1, \dots, M_e\}$.

- Subproblem: Compute flat-norm distance in $\mathcal{Z}_e$ from Dirac $\hat{z}_e = (E_e, F_e)\delta_\Omega$ to subspace $\mathcal{D}_{e,i_e}$.



Structural/solid linear viscoelasticity

Theorem

Let $B \in \mathbb{C}^n$, $\alpha, \beta \in \mathbb{R}$. Let S be a proper subspace of $\mathbb{C}^n$ and $\mathcal{S} = \{A\delta_\alpha \,:\, A \in S\}$. Suppose that $\mathbb{C}^n$ is metrized by a norm $\|\cdot\|$ derived from a Hermitian inner product. Then, the flat-norm distance between $B\delta_\beta$ and $\mathcal{S}$ is

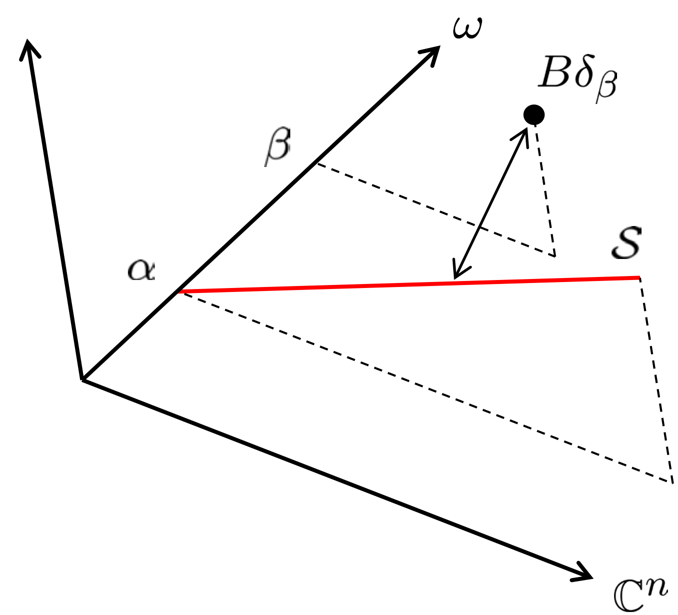
$$\mathrm{dist}(B\delta_\beta, \mathcal{S}) = \min\{\|(\mu - 1)B_{||} - B_\perp\| + c\,\mu\,\|B_{||}\|,\ \|B\|\},$$

with

$$\mu = 1 - \frac{c}{\sqrt{1-c^2}} \frac{\|B_\perp\|}{\|B_{||}\|},$$

and

$$c = \min\{2, |\alpha - \beta|/\omega_0\}.$$



Reading assignment:
Full proof in: H. Salahshoor and M. Ortiz, "Model-Free Data-Driven Viscoelasticity In the Frequency Domain," 13 May 2022, arXiv:2205.06674.

Structural/solid linear viscoelasticity

Algorithm 1 Frequency-domain Data-Driven solver, harmonic loading.

Require: For $e = 1, \dots, m$: Local DMA data set $\mathcal{P}_e$, B_e-matrix, member weights w_e.
Applied amplitudes F and G, applied frequency Ω, cutoff frequency ω_0.

i) **Initialization**. Set $k = 0$. For $e = 1, \dots, m$: Choose $(\omega_e^{(0)}, \mathbb{E}_e^{(0)}) \in \mathcal{P}_e$ randomly.

ii) **Displacement problem**. Solve for $U^{(k)}$ such that

$$B^T W \mathbb{E}^{(k)} (B U^{(k)} + G) - M \Omega^2 U^{(k)} = F,$$

iii) **Local states**. For $e = 1, \dots, m$: $E_e^{(k)} = B_e U^{(k)} + G_e; \quad S_e^{(k)} = \mathbb{E}_e^{(k)} E_e^{(k)}$.

iv) **Data assignment**. For $e = 1, \dots, m$, $Z_e^{(k)} = (E_e^{(k)}, S_e^{(k)})$:

iv.a) Find $(\omega_{e,i}, \mathbb{E}_{e,i}) \in \mathcal{P}_e$ s. t. $\text{dist}(Z_e^{(k)} \delta_\Omega, \{S_e = \mathbb{E}_{e,i} E_e\} \delta_{\omega_{e,i}})$ minimal.

iv.b) Set $(\omega_e^{(k+1)}, \mathbb{E}_e^{(k+1)}) = (\omega_{e,i}, \mathbb{E}_{e,i})$

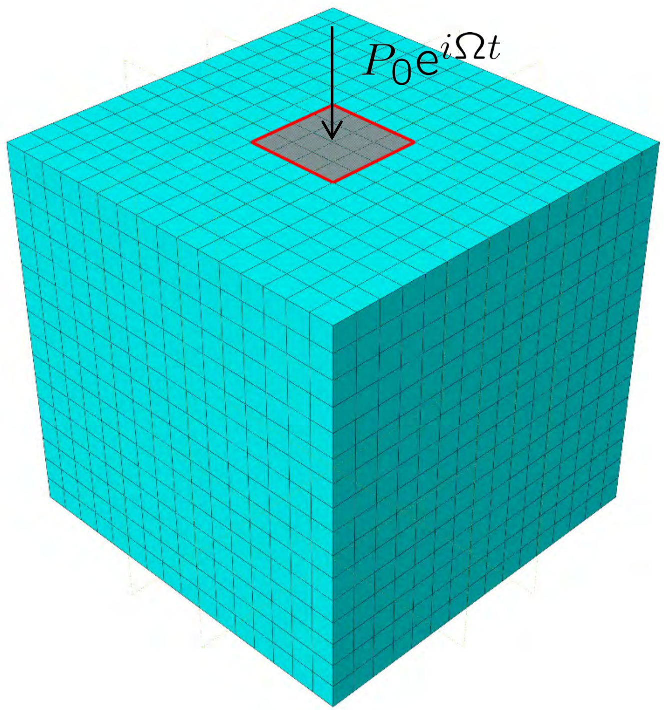
v) **Convergence test**.

if $\mathbb{E}^{(k+1)} = \mathbb{E}^{(k)}$ **then** $U = U^{(k)}$; $E = E^{(k)}$; $S = S^{(k)}$, **exit**.

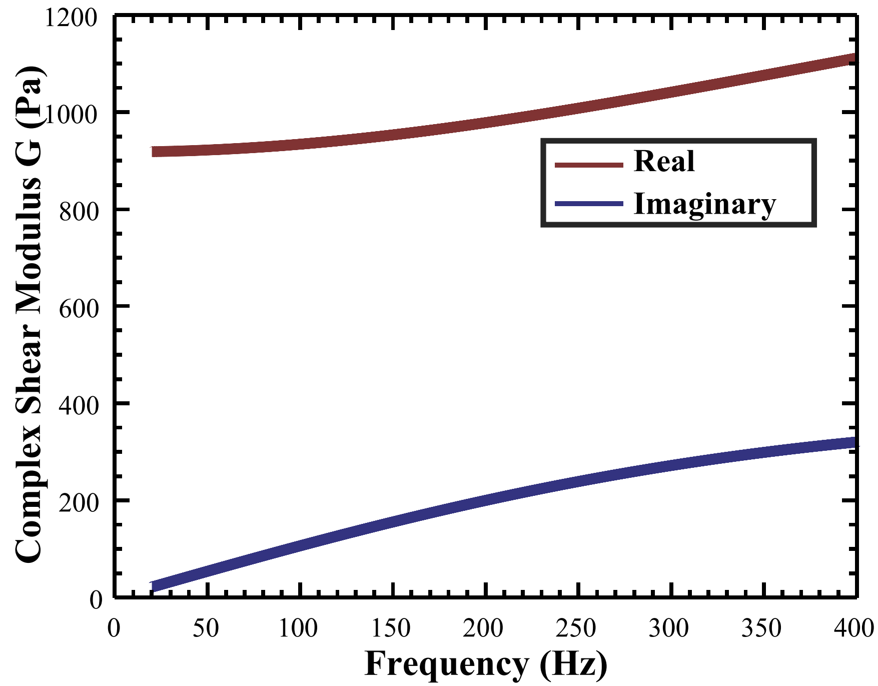
else $k \leftarrow k + 1$, **goto** (ii).

Structural/solid linear viscoelasticity – Convergence test

- 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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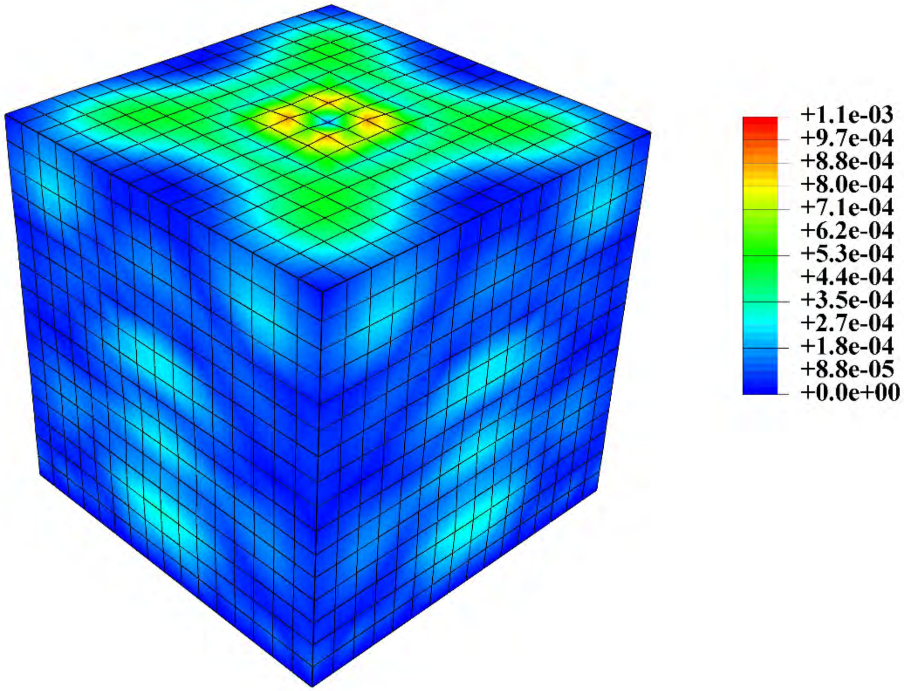

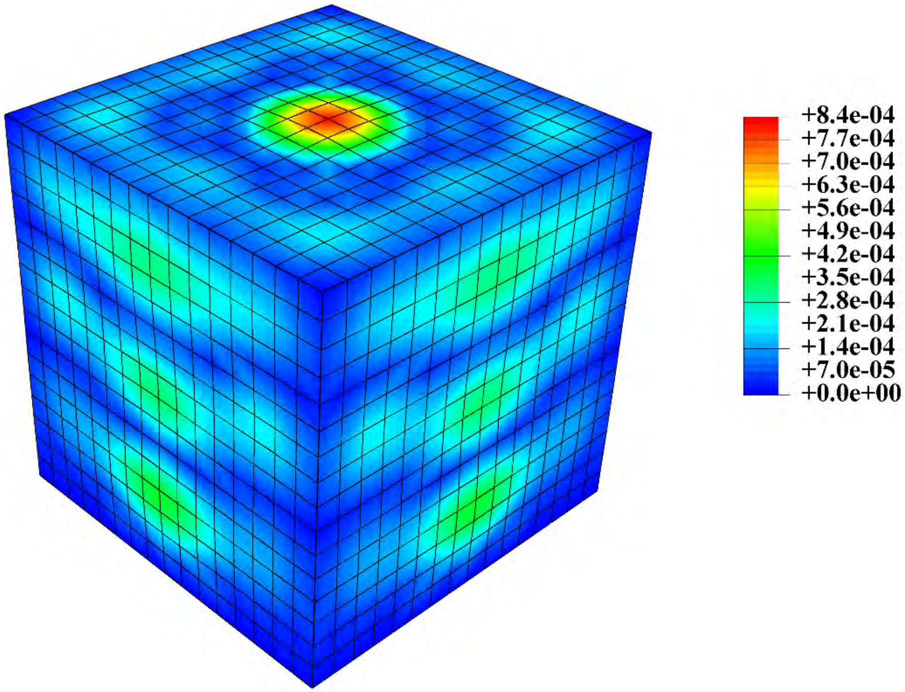

Insonated agarose gel block.
Displacements for applied frequency Ω = 1000 Hz.
a) Real component. b) Imaginary component.

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

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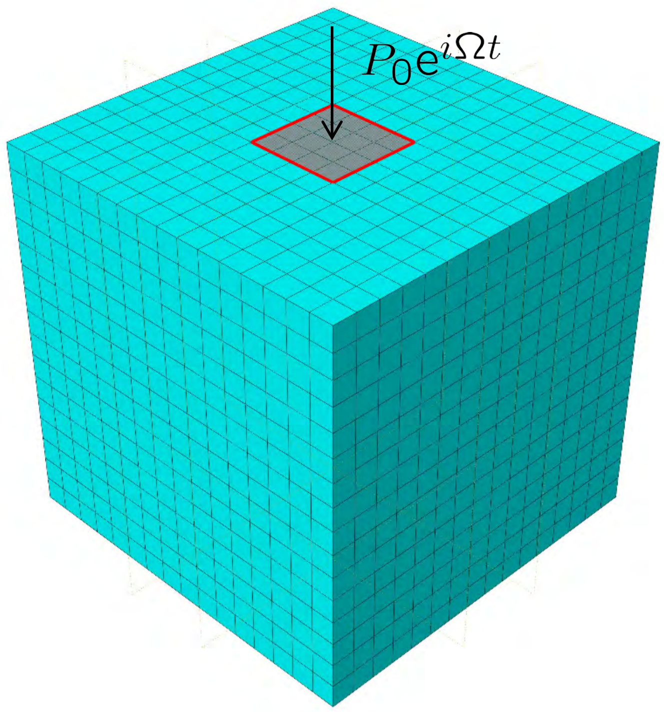

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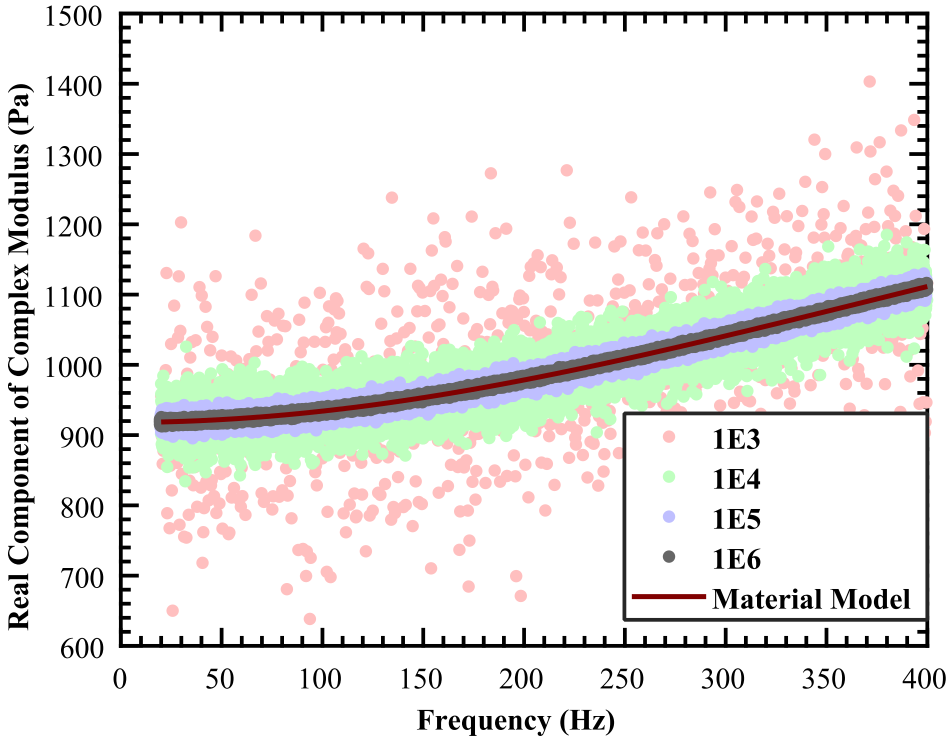

Data of sizes 10^3, 10^4, 10^5 and 10^6 used in the DD calculations. Real component of complex modulus.

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

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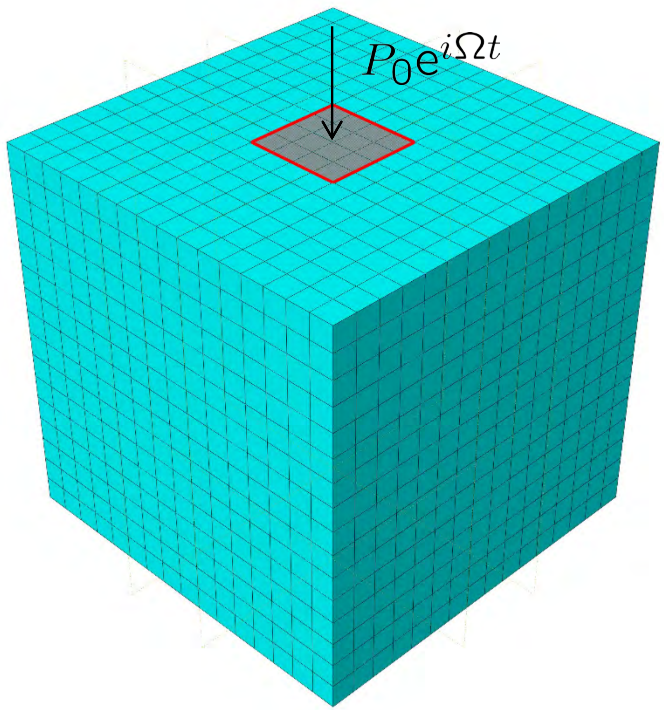

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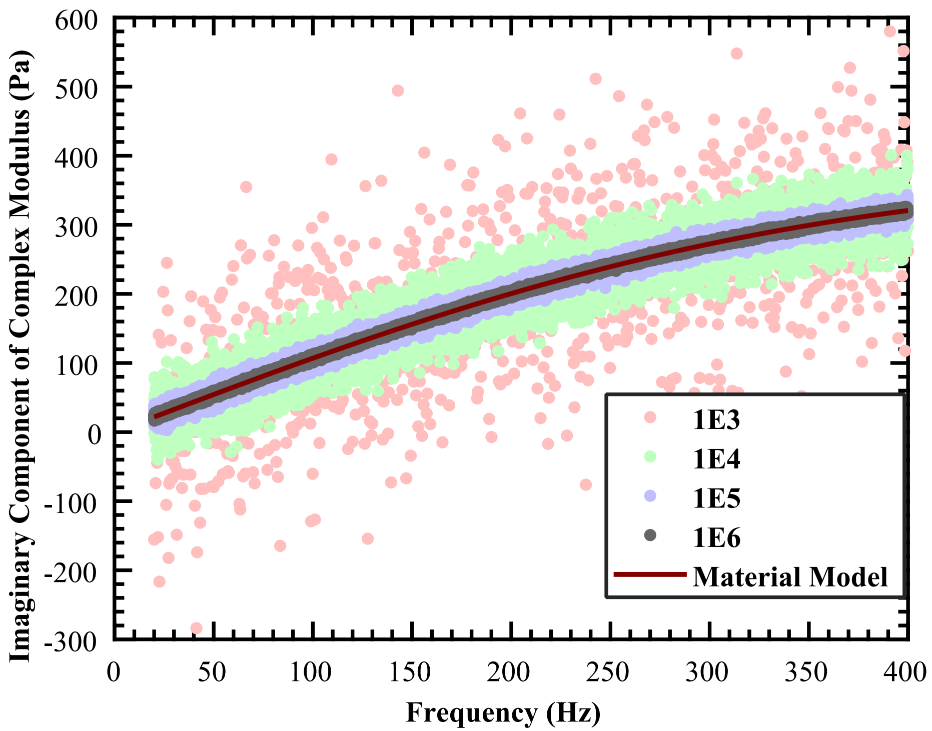

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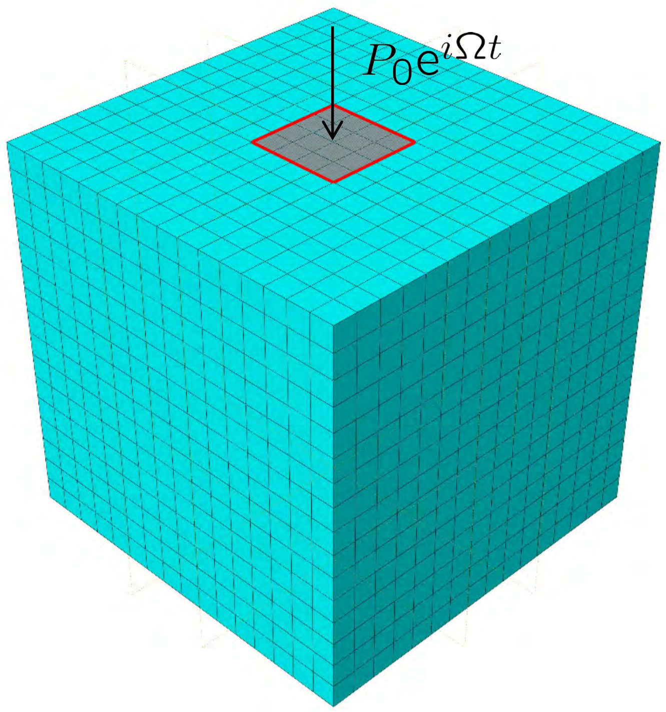

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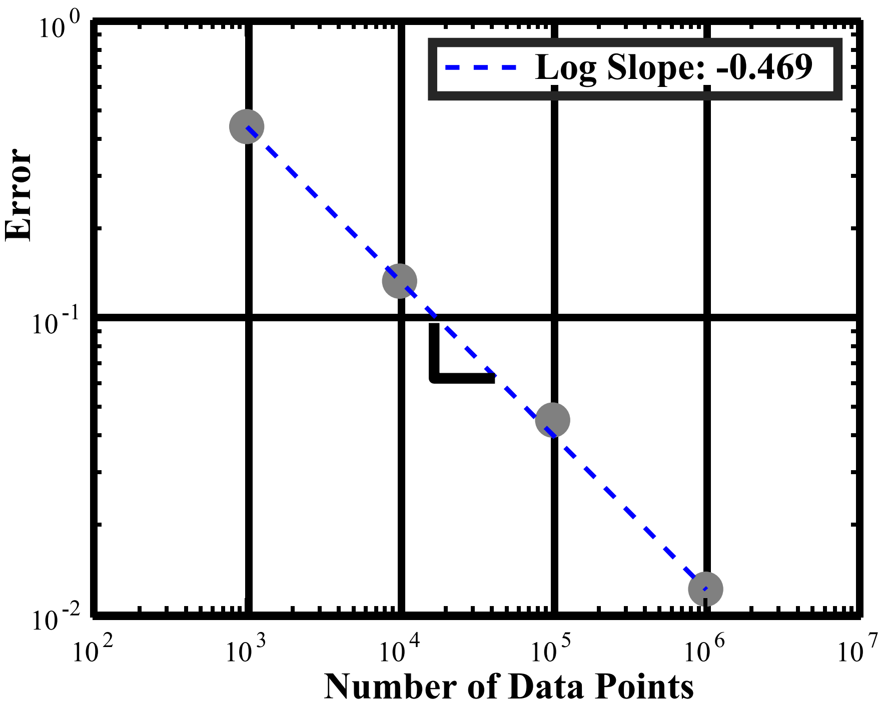
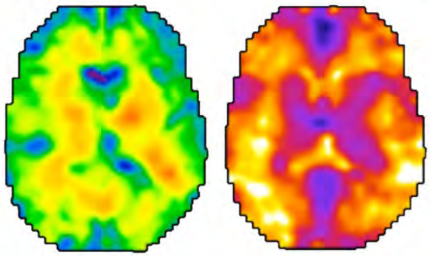


Normalized flat-norm convergence error as a function of the number of data points, showing a clear trend towards convergence.

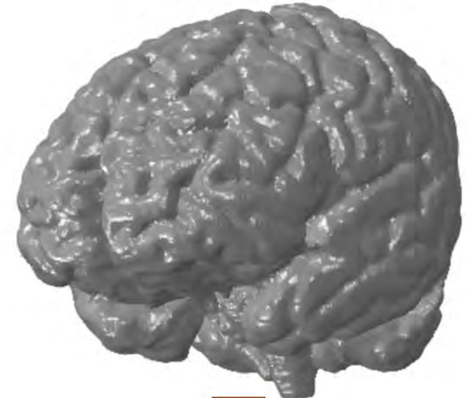
H. Salahshoor and M. Ortiz, arXiv 2205.06674v1, May 13, 2022.

Data-Driven viscoelasticity – Patient-specific UNM

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

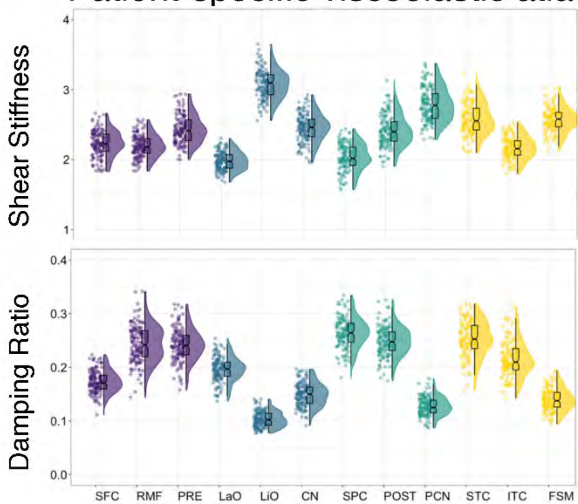


Anatomical Data

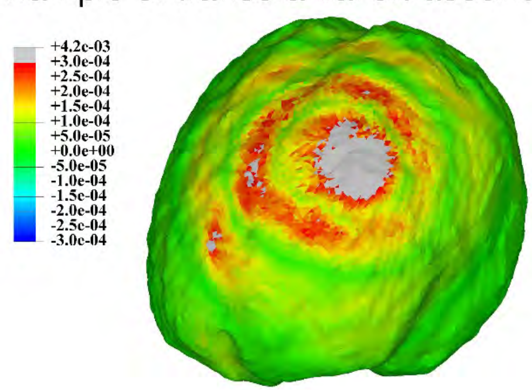


DD
UNM

Brain Matter Data Repository:
Patient-specific viscoelastic atlas



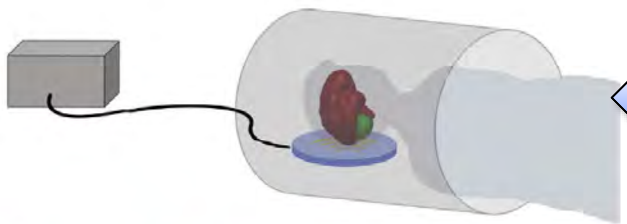
Direct Data-Driven patient-specific prediction of wave patterns in brain:
Example of transcranial ultrasound



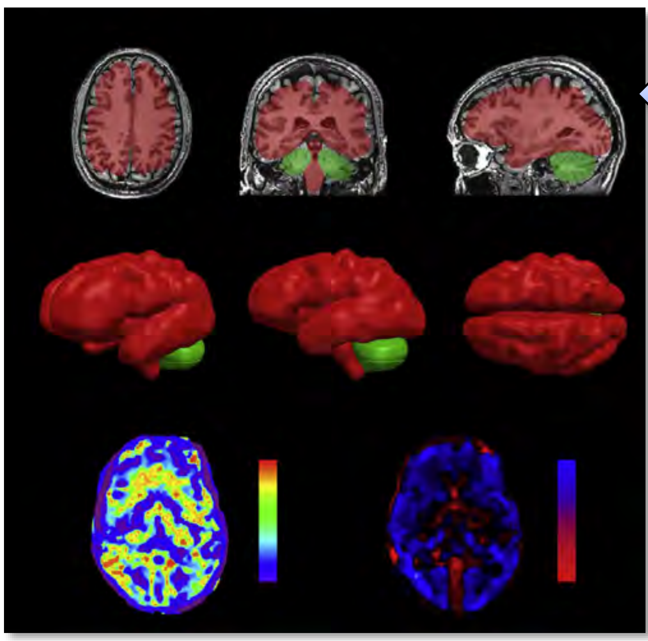
H. Salahshoor and M. Ortiz, bioRxiv 2022.09.01.506248, Sept 1, 2022.

Data-Driven viscoelasticity – 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.

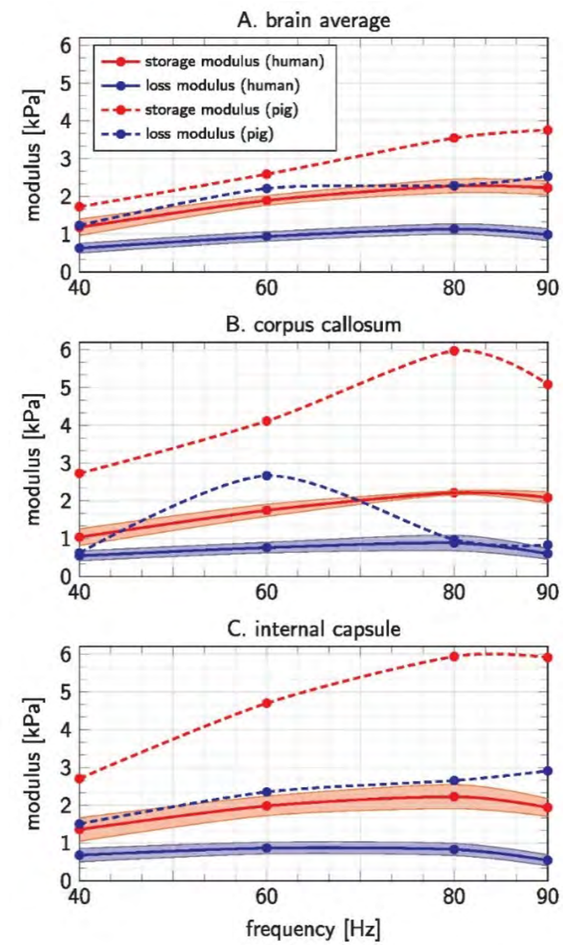


Human subjects scanned in the supine position



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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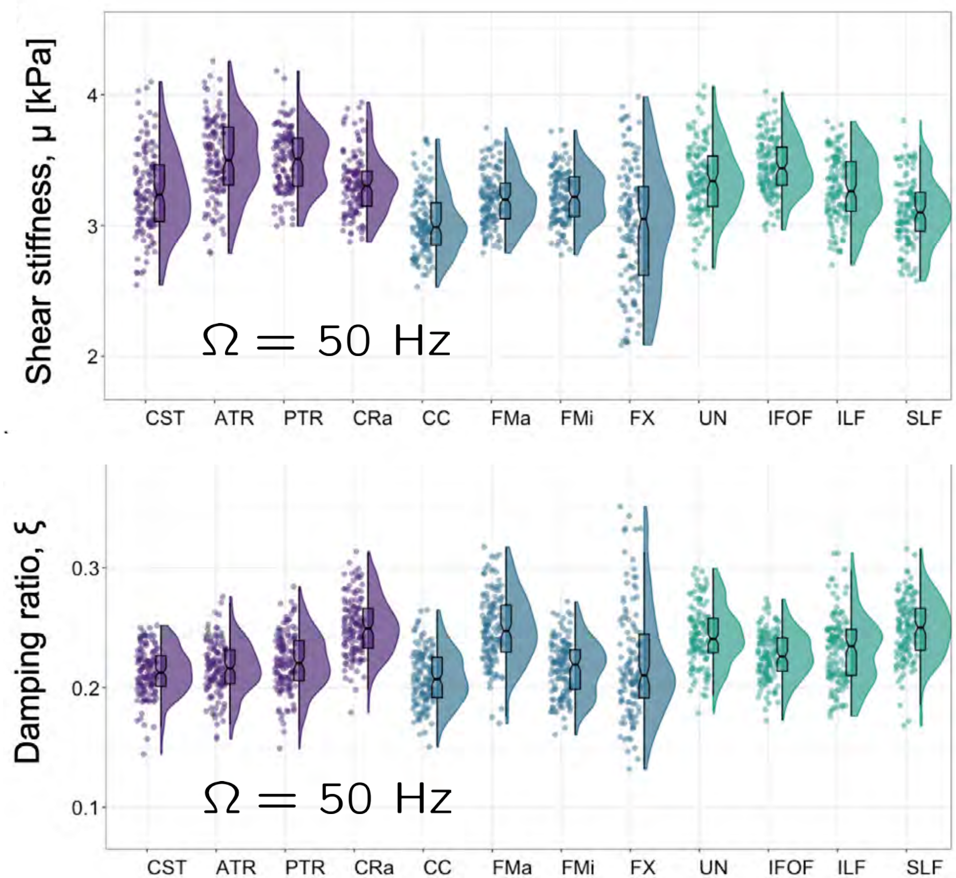
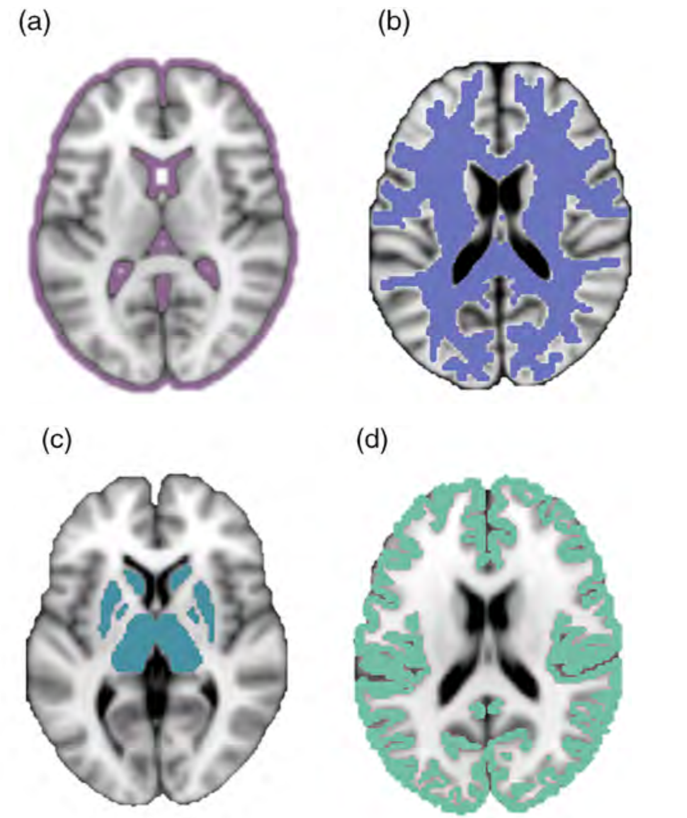


MRE viscoelastic data atlas at 12 regions of interest (Desikan–Killiany–Tourville cortical labelling protocol).

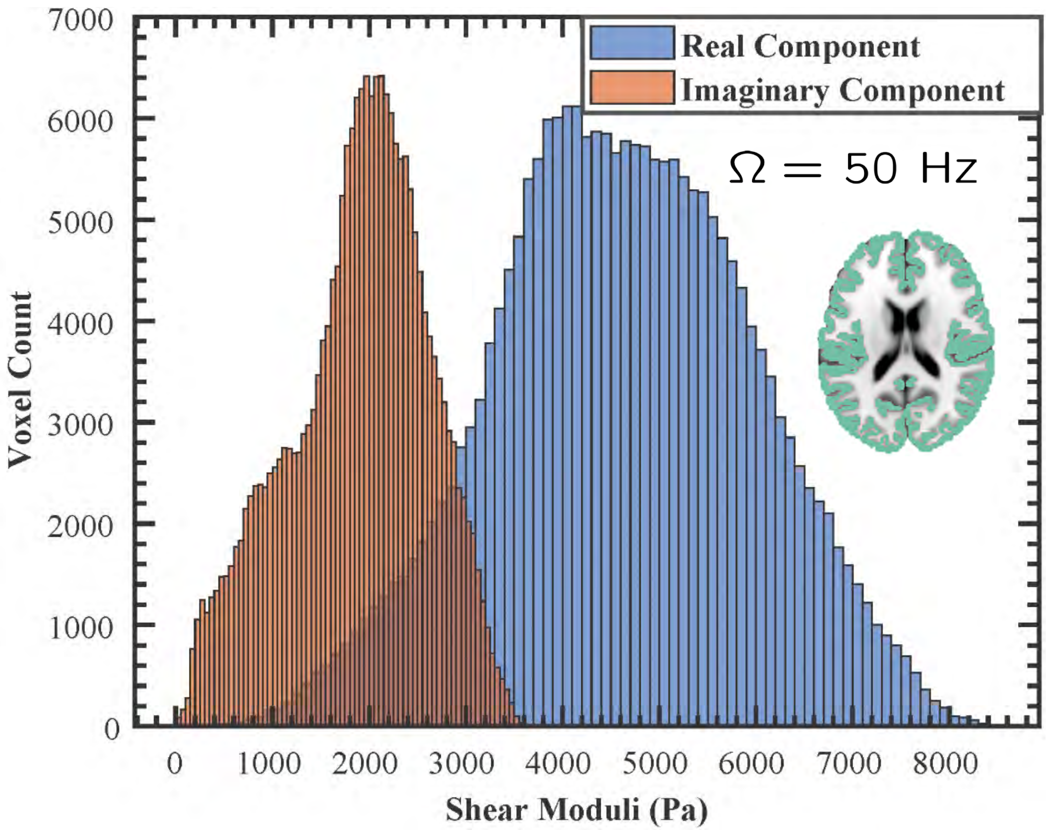


MRE data for (a) the entire brain (b) white matter (c) subcortical gray matter (d) cerebral cortex.

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

Data-Driven viscoelasticity – 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.

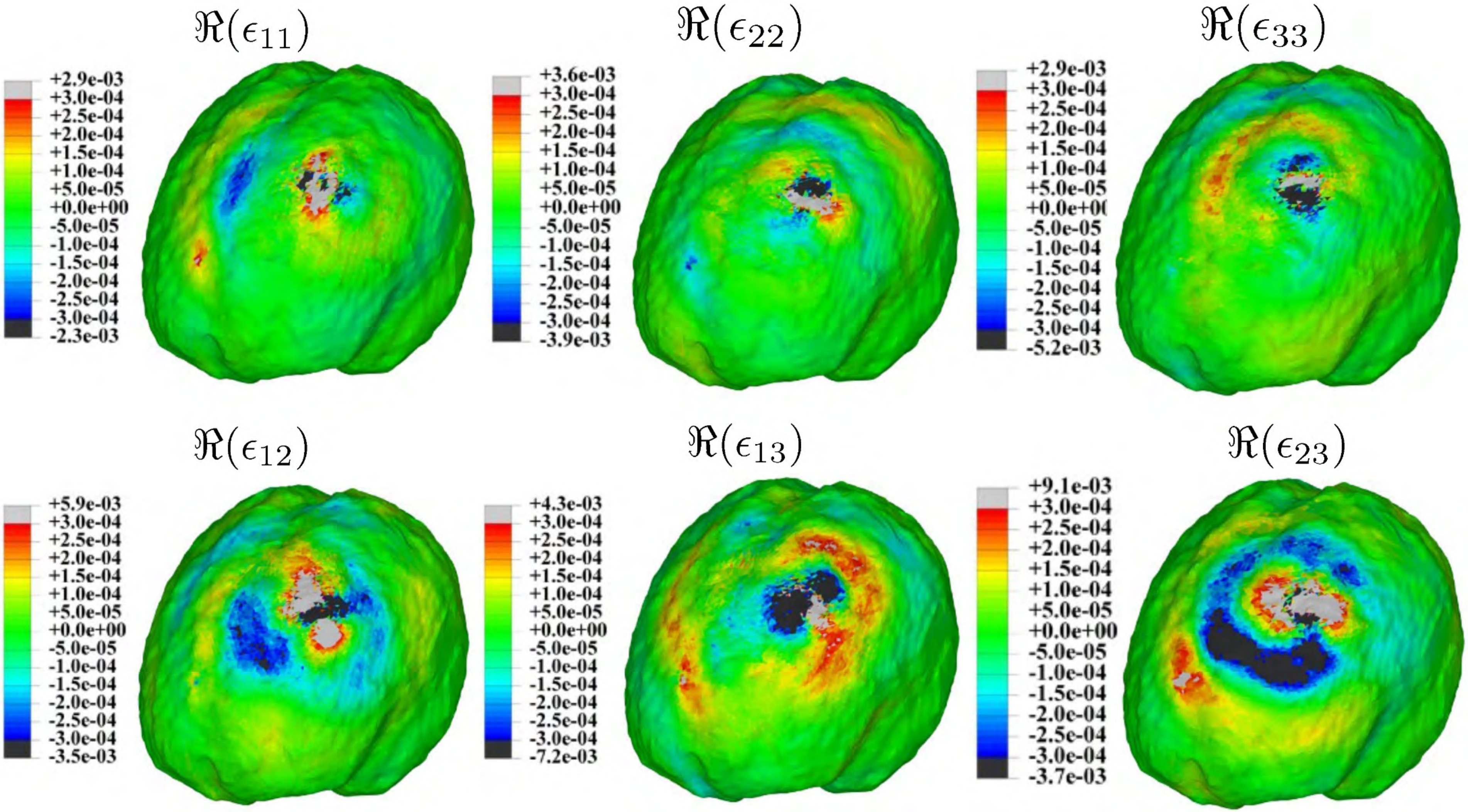


Histogram of complex moduli from in vivo MRE data. The finite-element model is co-registered to the MRE data.

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

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

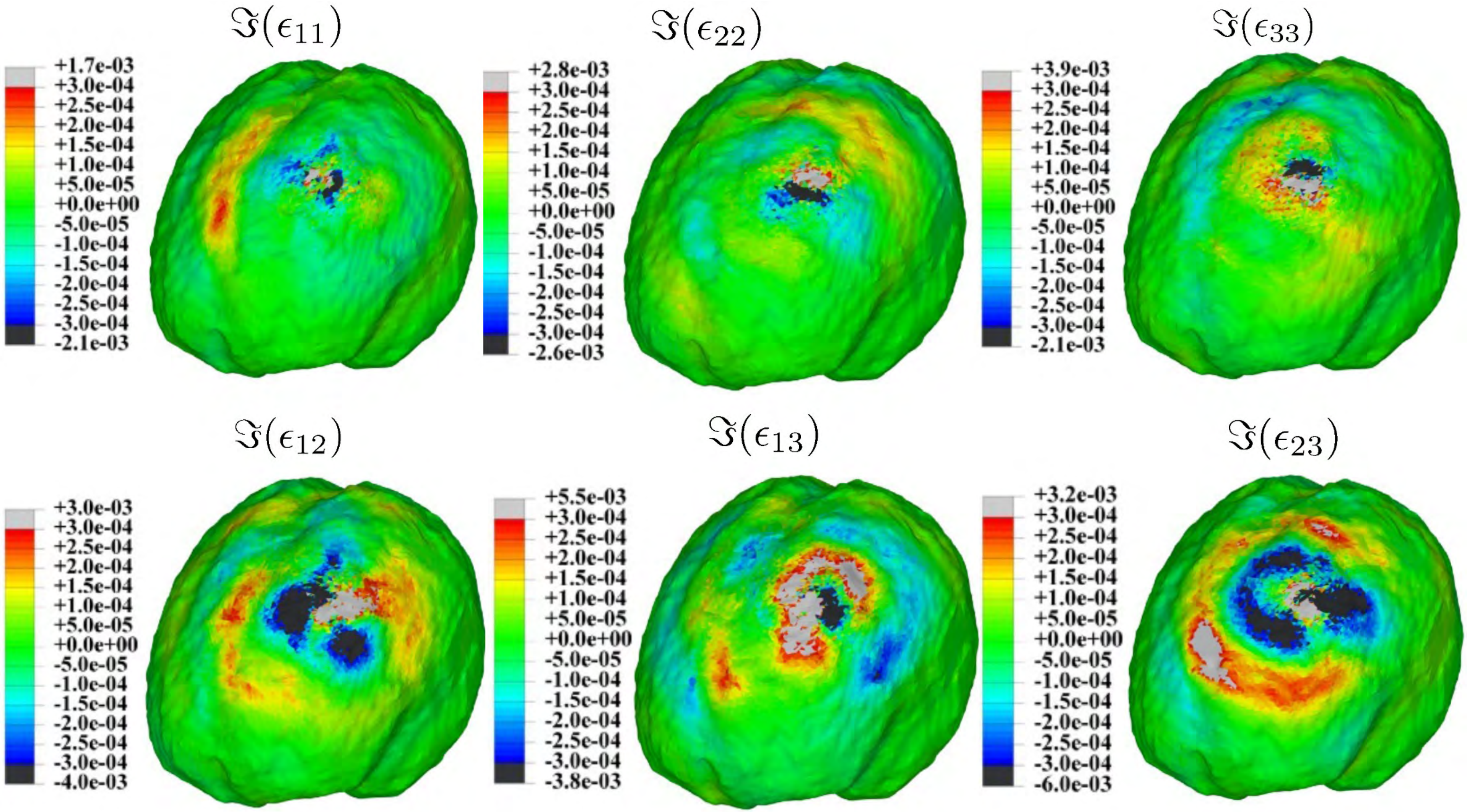
Data-Driven viscoelasticity – Patient-specific UNM



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.

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

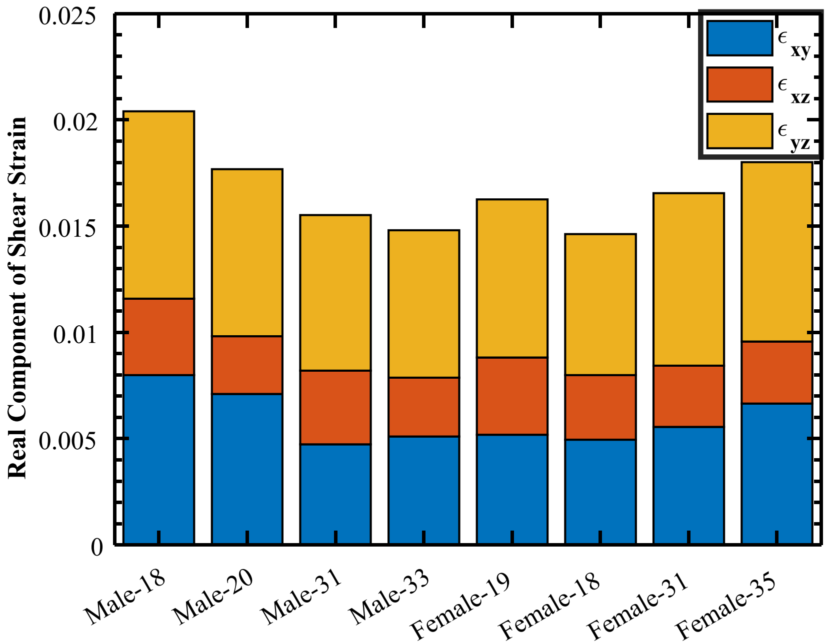
Data-Driven viscoelasticity – Patient-specific UNM

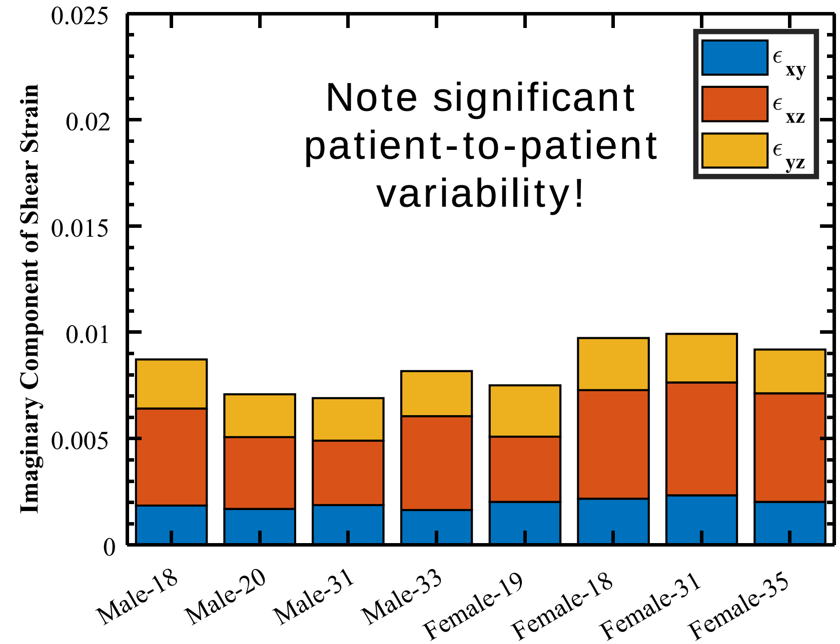


Model-free Data-Driven simulation of transcranial harmonic stimulation on a region on the frontal lobe of the brain at Ω = 50 Hz. Imaginary part of the strain field components at steady state.

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

Data-Driven viscoelasticity – 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***, 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 clinical applications!

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

to be continued...