26th Symposium on Fluid Mechanics and Rheology of Nonlinear Materials and Complex Fluids
International Mechanical Engineering Congress & Exposition (IMECE), November 11-14, 2019, Salt Lake City, Utah

IMECE2019-13370
Continuous Relaxation Spectra and Its Reduced-Dimensionality Descriptions for Engineering Design With Linear Viscoelasticity

Yong Hoon Lee,[1*] R. E. Corman,[1] Randy H. Ewoldt,[1] James T. Allison[2]

* ylee196@Illinois.edu
[1] Dept. of Mechanical Science and Engineering
[2] Dept. of Industrial and Enterprise Systems Engineering

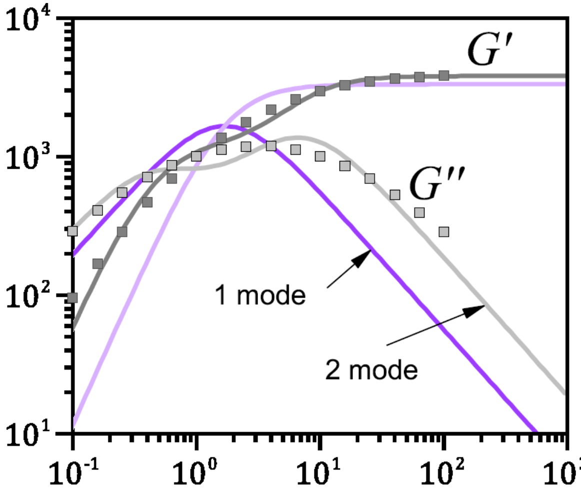
University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA

Table of Contents

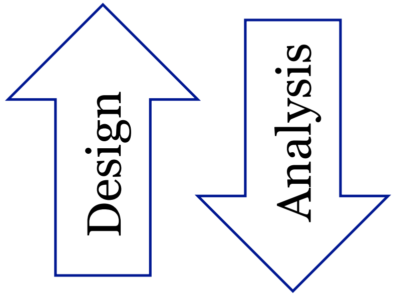
ILLINOIS

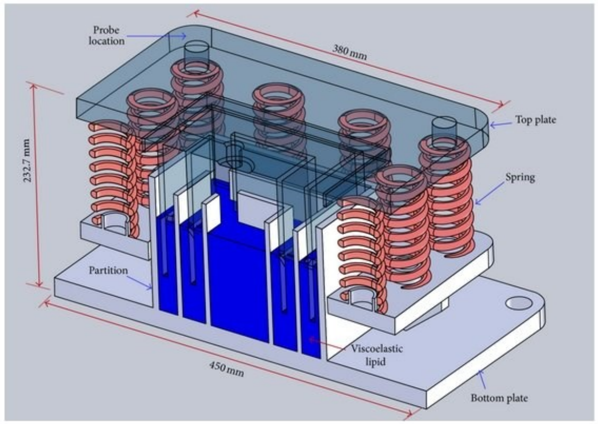
Background and Motivation
: DESIGN PERSPECTIVES

- Engineering design demands **more** performance, efficiency, and reliability, **for less** time, cost, material, and effort.
- Non-traditional (including rheologically-complex) materials may provide novel performance beyond what was available with simple (Newtonian fluids, elastic solids) materials.
- Designing materials (with synthesis of new materials) opens an avenue to unprecedented design innovations.
- Function-valued material properties (material functions): e.g., $\eta(\dot{\gamma})$, $\psi_1(\dot{\gamma})$, $\psi_2(\dot{\gamma})$, $G(t)$, $G'(\omega)$, $G''(\omega)$, etc.
- We limit our study to Linear Viscoelasticity (LVE) here.



Frequency-dependent moduli of PVA Borax (Corman, PhD 2019; Corman et al, JMD 2016)





VDI: Viscoelastic Damping Isolator (Huang et al, 2015)

ILLINOIS

Background and Motivation
: RESEARCH QUESTIONS

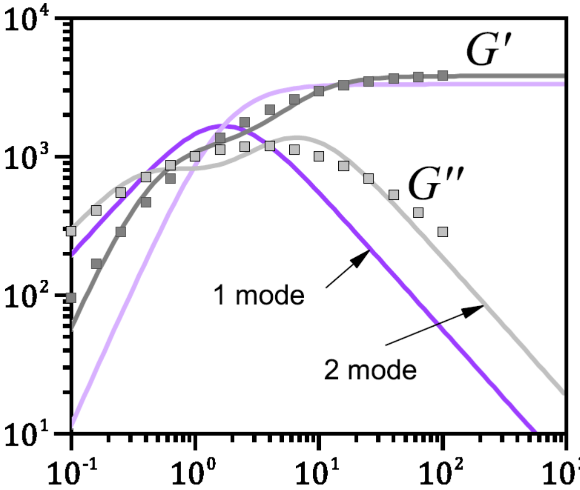
- Rheological Materials Design Challenges:

1. Models that could violate physics laws:
   e.g., directly designing relaxation kernel function
   $\eta(\dot{\gamma})$, $\psi_1(\dot{\gamma})$, $\psi_2(\dot{\gamma})$, $G(t)$, $G'(\omega)$, $G''(\omega)$

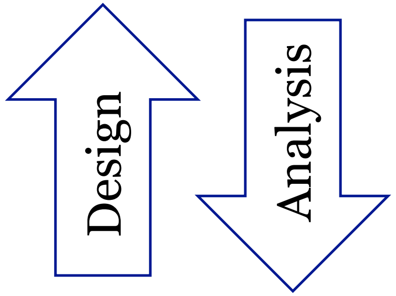
2. Models that do not have unique parameters for identical designs:
   e.g., multimode Maxwell model

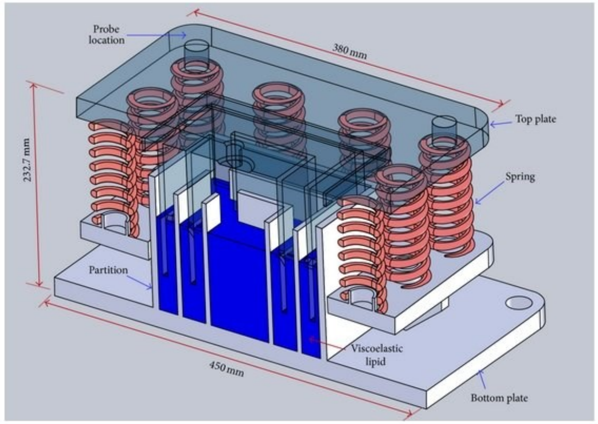
3. Models that limits the type of material systems significantly:
   e.g., Giesekus model (polymeric flow), Baxter's model (colloids)

4. What additional design efforts are needed?
   e.g.,
   - How to parameterize function-valued properties?
   - How many number of design parameters are deeded?



Frequency-dependent moduli of PVA Borax
(Corman, PhD 2019; Corman et al, JMD 2016)



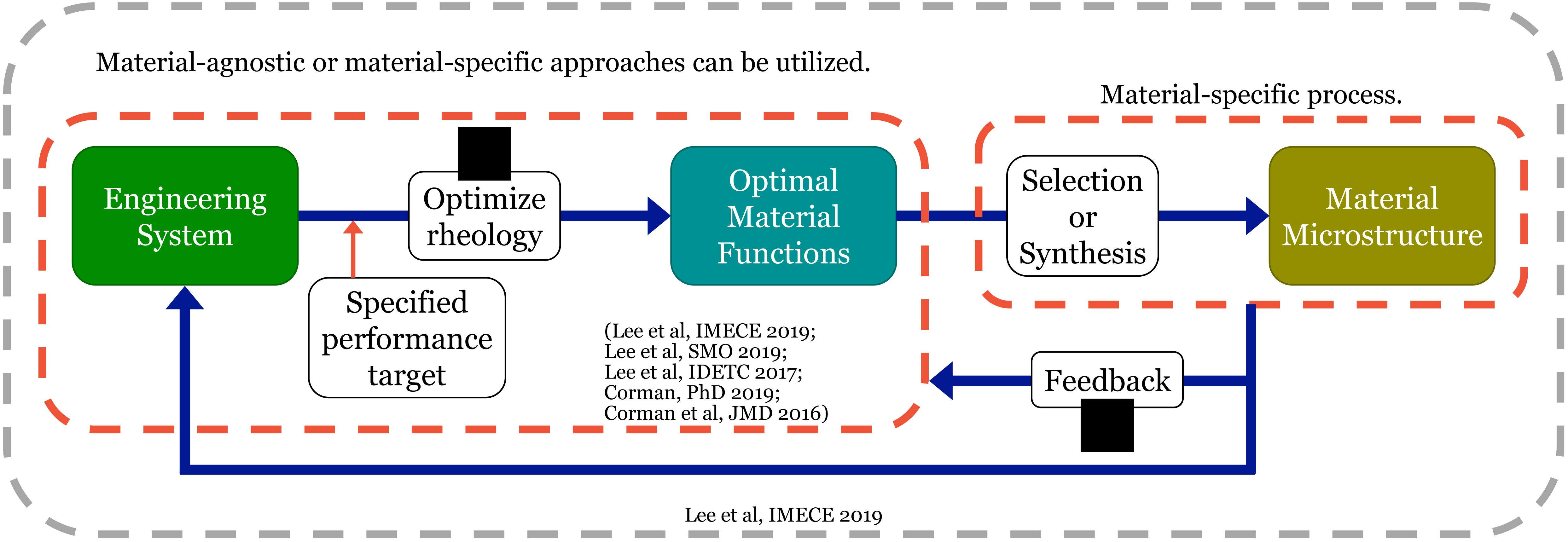


VDI: Viscoelastic Damping Isolator
(Huang et al, 2015)

ILLINOIS

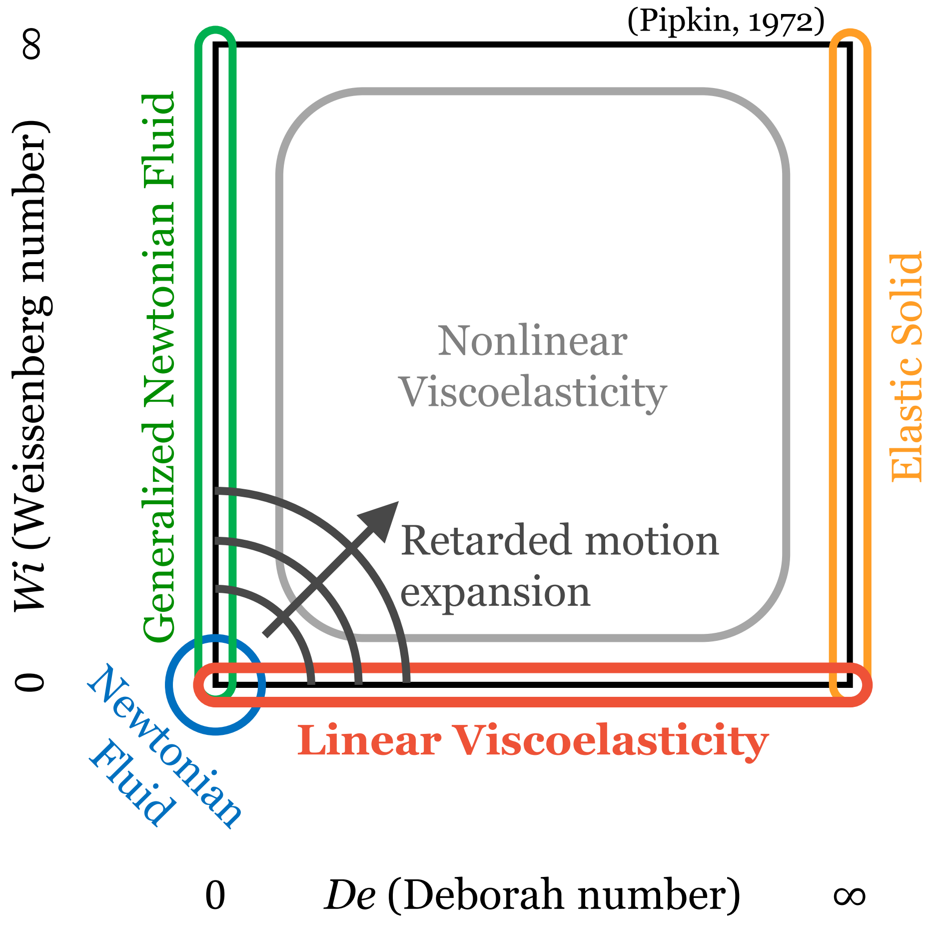
Engineering Design With Material Functions

- Design procedure **with** and **of** rheological materials



Mapping Linear Viscoelasticity (LVE) For Engineering Design

Pipkin Space



- Many equivalent representations, e.g.,
  - relaxation modulus, $G(t)$
  - creep compliance, $J(t)$
  - complex moduli, $G'(t)$, $G''(t)$

(Corman et al., JMD 2016)

- Not all representations are design-appropriate,

  e.g., $G'(t)$, $G''(t)$ are related to each other and cannot be independently designed, (Bird et al., DPL1 1987; Mours & Winter, 2000)

  Kramers-Kronig relation: $\frac{G'(\omega)}{\omega^2} = \frac{2}{\pi}\int_0^\infty \frac{G''(x)}{\omega^2 - x^2}\frac{dx}{x}$

- Preferred characteristics for design representations
  - encompass the most general material behavior,
  - do **NOT** violate fundamental restrictions,
  - are directly measurable to facilitate development or selection of real materials.

MAP1: Continuous Relaxation Spectra Description For LVE Materials

Natural choices of material descriptions:

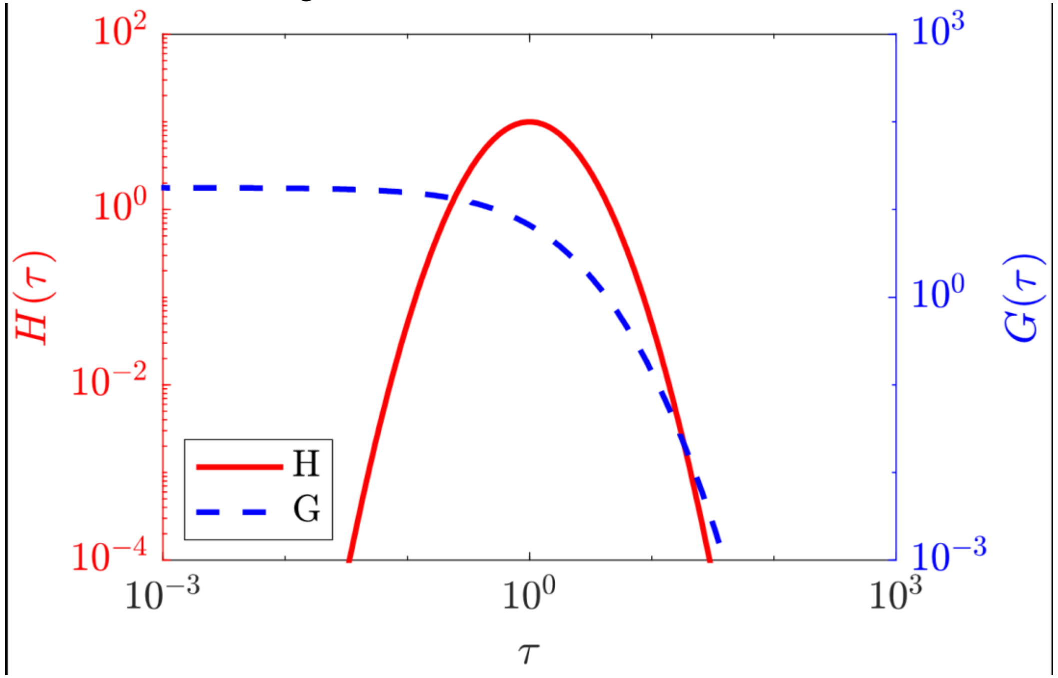
- Force/stress controlled load
  - Creep compliance $J(t)$
  - Retardation spectrum $L(\tau)$
- Deformation/strain controlled load
  - Relaxation modulus $G(t)$
  - Relaxation spectrum $H(\tau)$

Design of materials perspective:

- Connect to physical microstructural mechanisms and information.
- The relaxation spectra $H(\tau)$ is a useful design-appropriate material description.

- Definition of relaxation modulus

$$G(t) = \int_0^\infty \frac{H(\tau)}{\tau} e^{-t/\tau} d\tau$$
$$= \int_0^\infty H(\tau) e^{-t/\tau} d\ln\tau$$



Example: Continuous relaxation spectrum in Log-Normal distribution and corresponding relaxation modulus

MAP1: Continuous Relaxation Spectra Description For LVE Materials

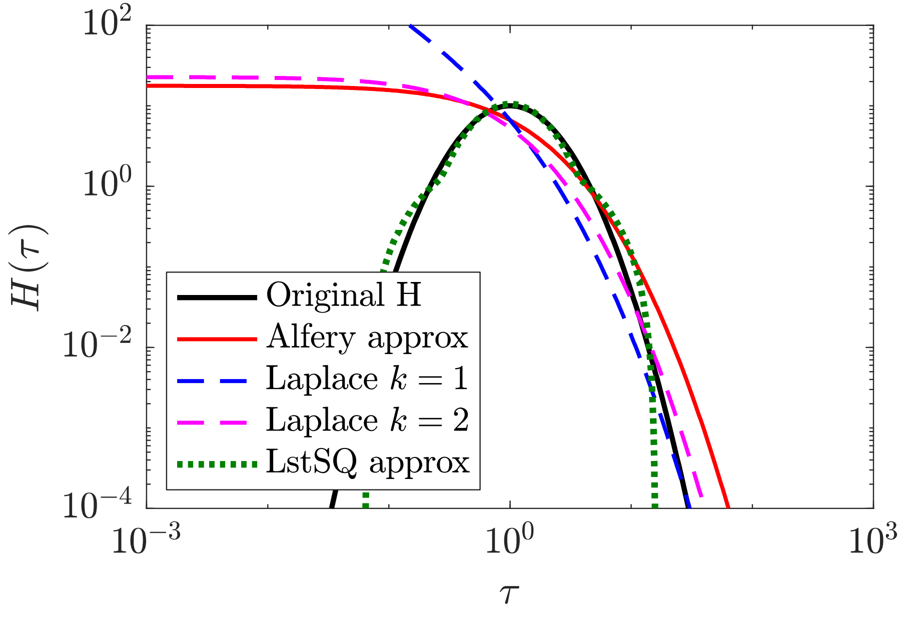
(Schwarzl and Staverman, 1952)

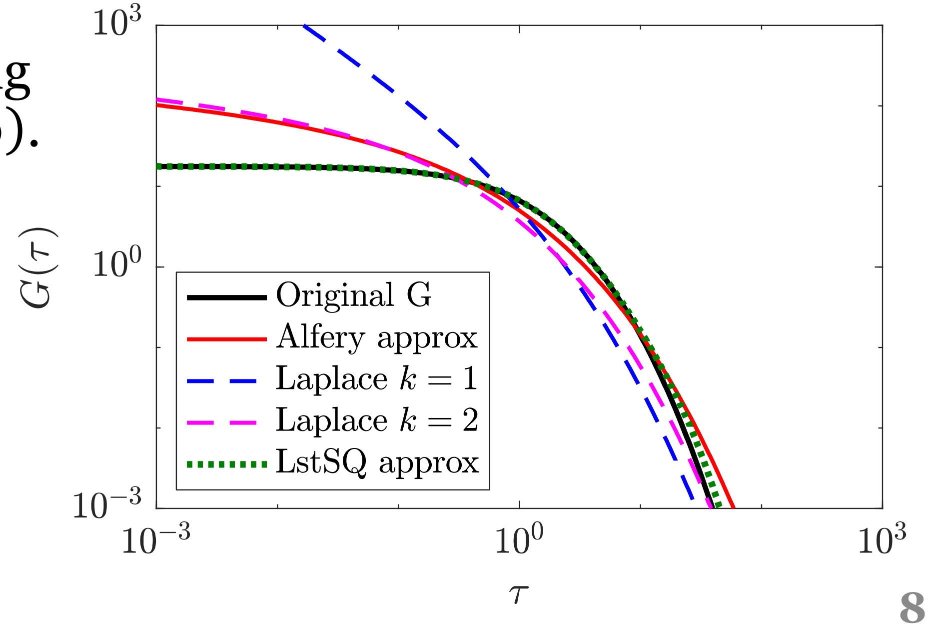
Conversion from modulus to spectrum
: mathematically ill-posed problem

- A small difference (error) in modulus, G, results in a large difference in spectrum, H.
- Alfrey approximation: $H(\tau) = -\left[\frac{dG(t)}{d\ln t}\right]_{t=\tau}$,
- Spectra approximation, Laplace approximation, etc
- Least square fitting of $G(t)$ using optimization algorithms: $\min_{\tilde{H}(\tau)} \int \left[\tilde{G}\left(\tilde{H}(\tau)\right) - G\left(H(\tau)\right)\right]^2 d\tau$, etc.
- Software, such as TRIOS (TA Instrument) can aid computing approximated $H(\tau)$ from complex modulus, $G'(\omega)$ and $G''(\omega)$.

Design process generally does not demand this sophisticated conversion:

- Design with relaxation spectrum
- Obtain molecular weight distribution from the spectrum
- Convert from spectrum to modulus (not difficult)





MAP1: Continuous Relaxation Spectra Description For LVE Materials

Shape of the spectrum

- Theoretically not constrained
- Generally parameterized to represent typical behaviors for real materials / Can be superposed
- Parameterizations
  - Log-Normal: glasses, noncovalent networks
  - Rouse model: polymer dynamics, bead-spring
  - Fractional Maxwell model: spring-pot
  - Fractional Zener: amorphous polymer
  - Critical Gel: polymer at point of gelation
  - BSW: entangled, narrowly-distributed polymer
  - Modified BSW: broadly-distributed polymer
  - Generalized Maxwell model: discrete timescales
  - Box Distribution, Wedge, Power Law, Asymmetric Lorentzian, etc.

Characteristics of the spectrum

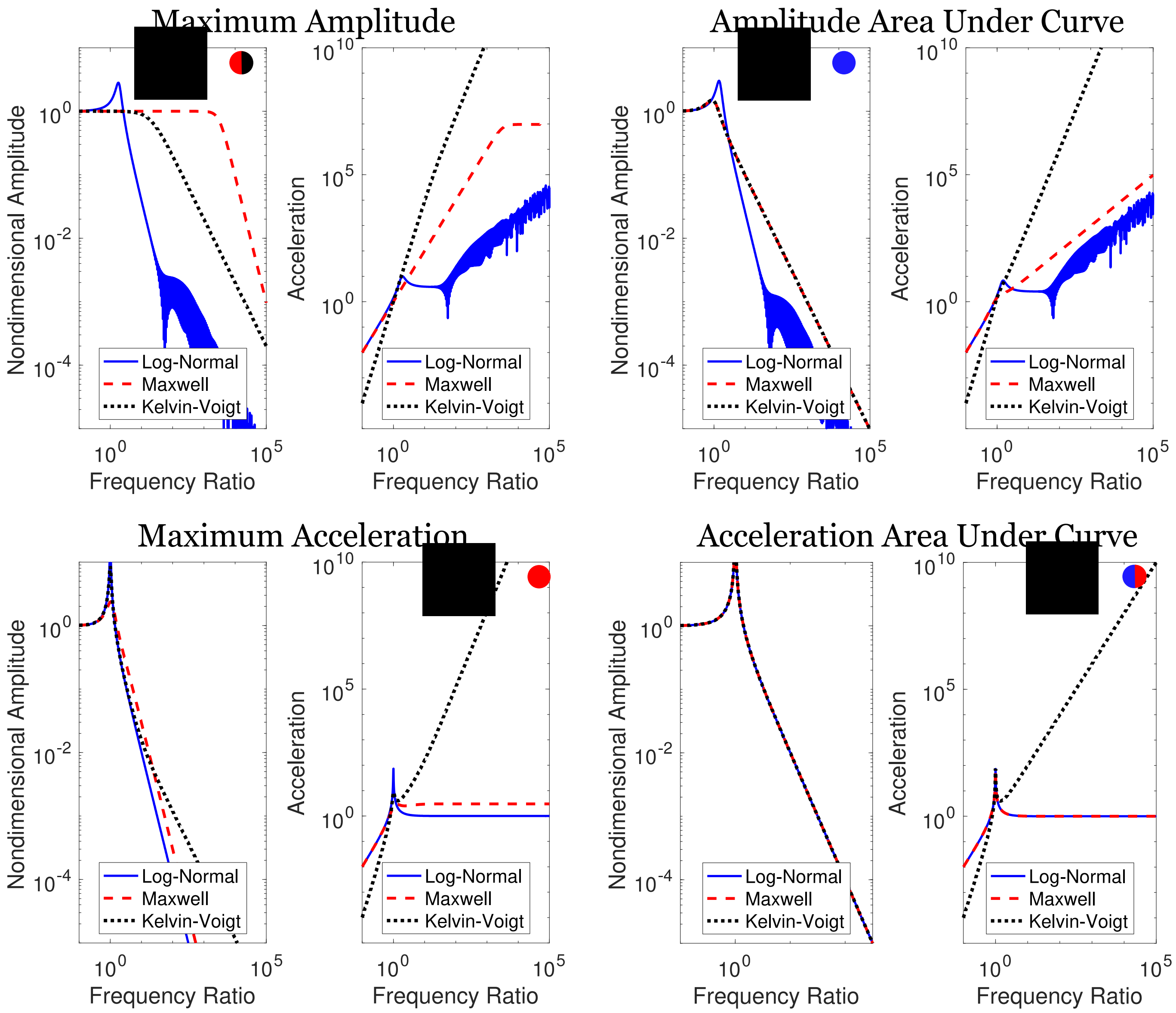
- Primary timescale, viscosity strength, and deviation of these properties describe the spectrum shape.
- Dispersity of the prominent time scale represents dispersity in the microstructure.
- Dispersity in the microstructure mechanism leads relaxation behavior.

(Ferry, 1980; Tschoegl, 1989; Baumgaertel, 1992; Martinetti, 2015; De Rosa, 1994)

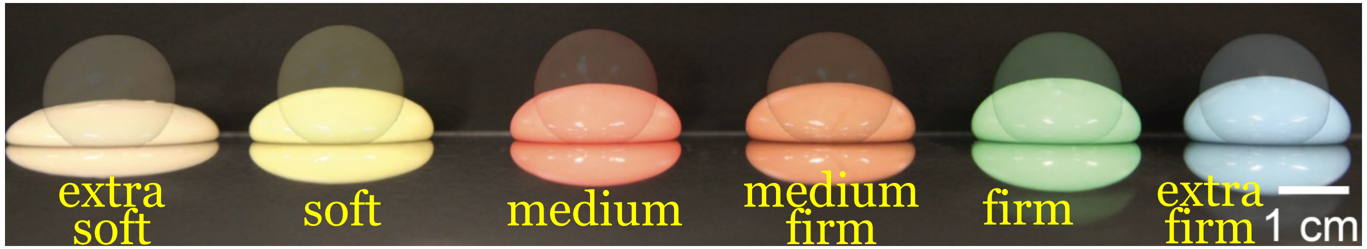
Case Study – 1D Viscoelastic Vibration Isolator Design

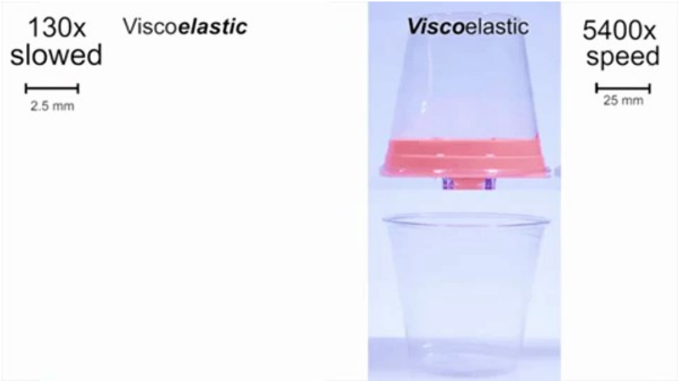
Problem: Design 1D viscoelastic vibration isolator under wide range of frequencies

- Log-Normal spectrum is successfully utilized for designing viscoelastic relaxation modulus.
- Different parameterizations for the continuous relaxation spectra could be easily implemented with this design framework.
- Obtained different optimal designs, meaning that each model has its own design space bounds.
- Direct optimization of shape of the relaxation spectrum may support more flexible design space exploration.



MAP2: Reduced-Dimensionality Description For LVE Materials



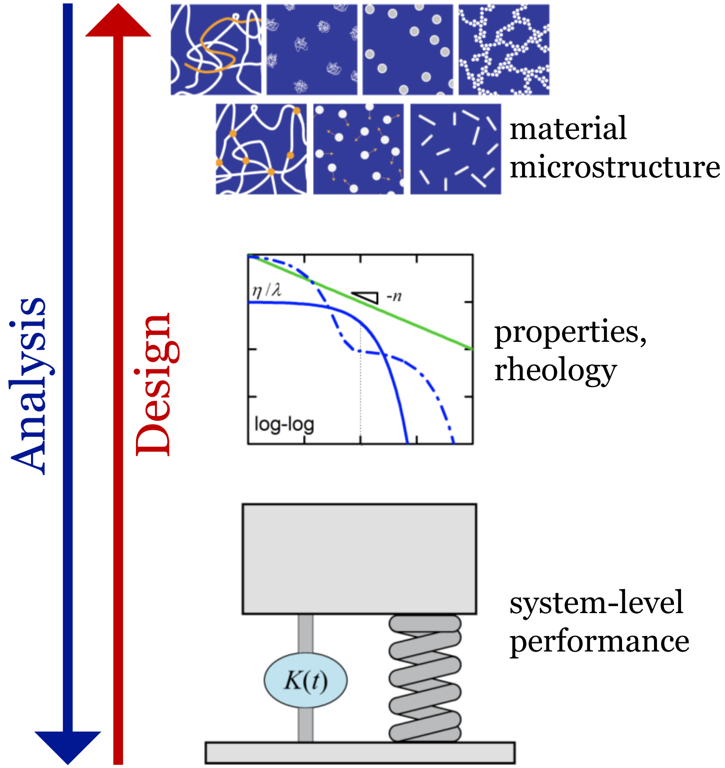


Intuition in design with/of materials is important

- Simplicity of describing materials by single value material properties gives greater insight.
  (e.g., density, viscosity, Young's modulus, yield stress/strain, etc.)
- Ashby diagrams, Materials databases, and the Materials genome help engineers to explore a wide range of materials.

Lack of such intuitive description for LVE

- Different putties have different material functions (e.g., relaxation modulus), but still this is in the shape of a function of a timescale.
- Most work in the rheology literature is analysis of materials, but design problems are the inverse of analysis.
- Materials descriptions motivated by design could provide improved intuition for designers.



MAP2: Reduced-Dimensionality Description For LVE Materials

- Low-dimensional viscoelastic constants
  - Describe viscoelastic qualities e.g., elasticity, viscosity, compliance
  - Computed from the integral moments of the spectrum (0th, 1st, 2nd moments)
  - Includes characteristic relaxation times

$$M_0 = \int_0^\infty Q(\tau)d\tau = \int_0^\infty \frac{H(\tau)}{\tau} d\tau = \boldsymbol{G_0} \text{ elasticity}$$

$$M_1 = \int_0^\infty \tau Q(\tau)d\tau = \int_0^\infty H(\tau)d\tau = \eta_0 \text{ viscosity}$$

$$M_2 = \int_0^\infty \tau^2 Q(\tau)d\tau = \int_0^\infty \tau H(\tau)d\tau = J_0\eta_0^2$$

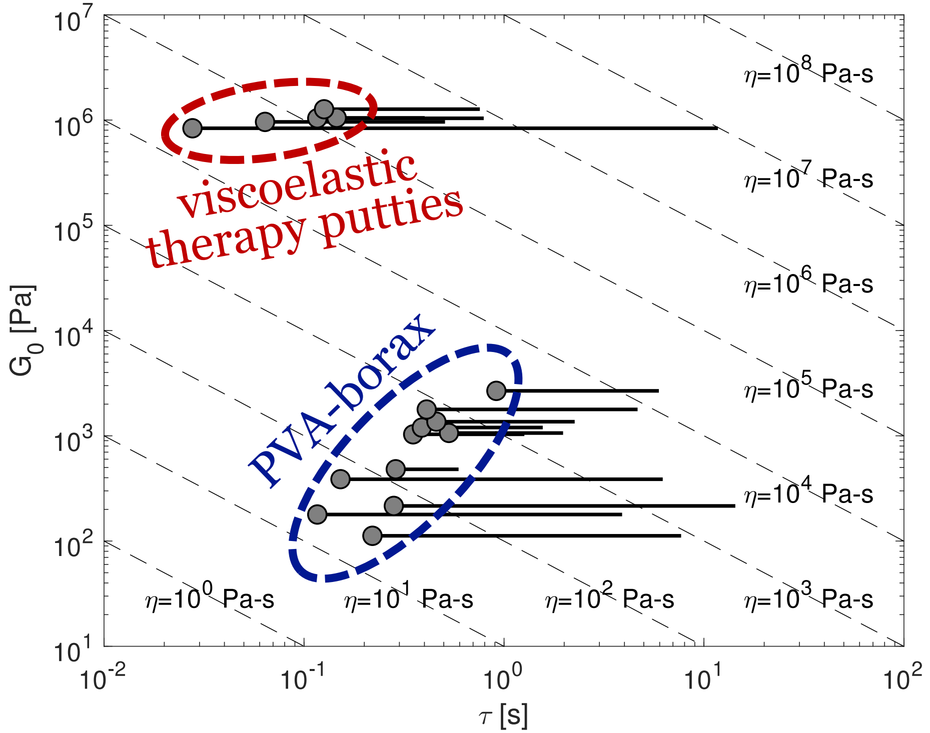
$$\boldsymbol{\tau_1} = \frac{M_1}{M_0} = \frac{\eta_0}{G_0} = \tau_n\text{:}$$ (mean relaxation time of the viscosity weighted spetrum)

$$\boldsymbol{\tau_2} = \frac{M_2}{M_1} = J_0\eta_0 = \tau_w\text{:}$$ (mean relaxation time of the modulus weighted spetrum)

- Timescale polydispersity index: PDI
  - deviation from dominant relaxation timescale
  - PDI can be interpreted as the distance between the timescales τ_1 and τ_2 in log scale

$$\text{PDI} = \tau_2/\tau_1$$

- LVE description visualized in an Ashby-like plot



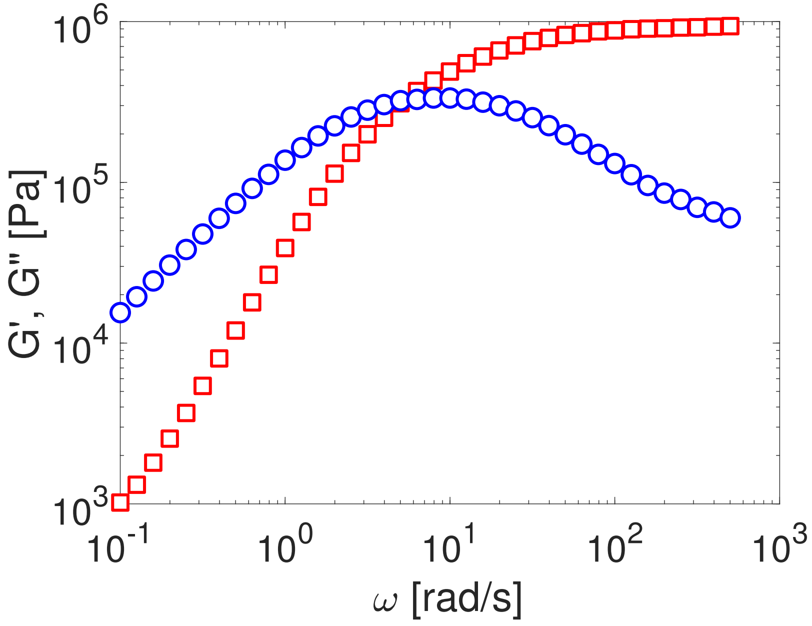
(Corman, PhD 2019)

Case Study – Experimental Measurement to Reduced-Dimensionality Description

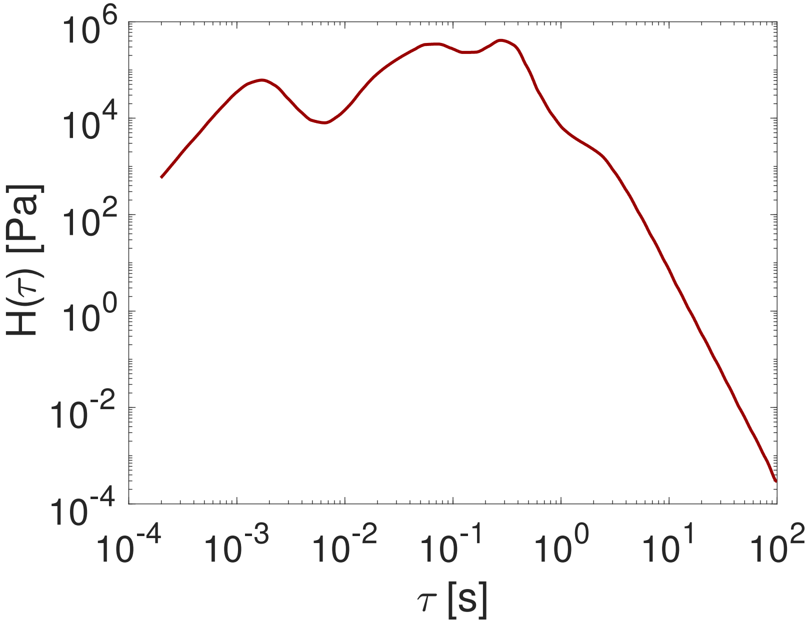
Experimental measurement of complex moduli (G', G'')

Extraction of relaxation spectrum
(using TA Instrument TRIOS)

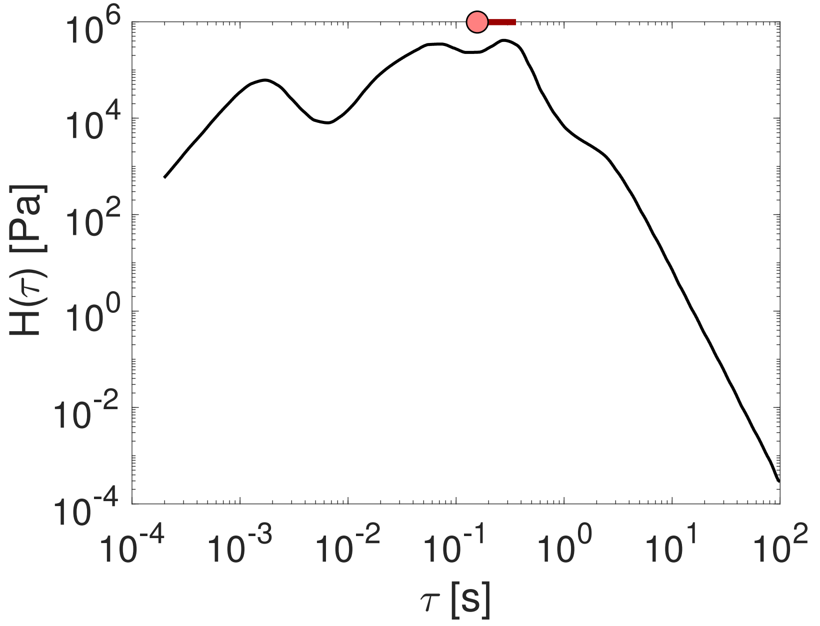
Computation of reduced-dimensionality description
$\tau_1 = 0.157, \tau_2 = 0.358, \; G_0 = 982245.6$



Experimental data

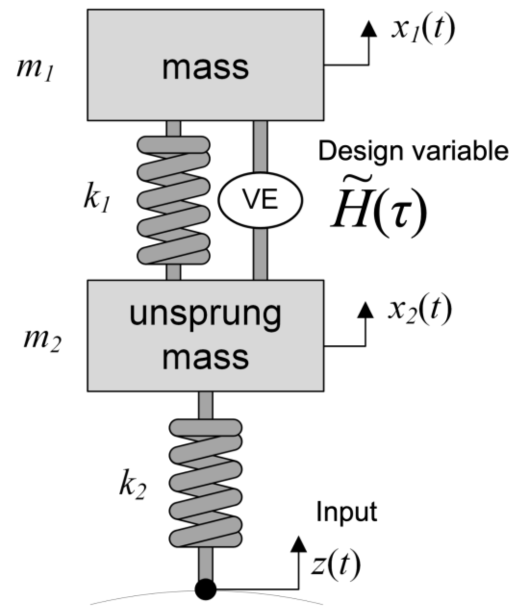


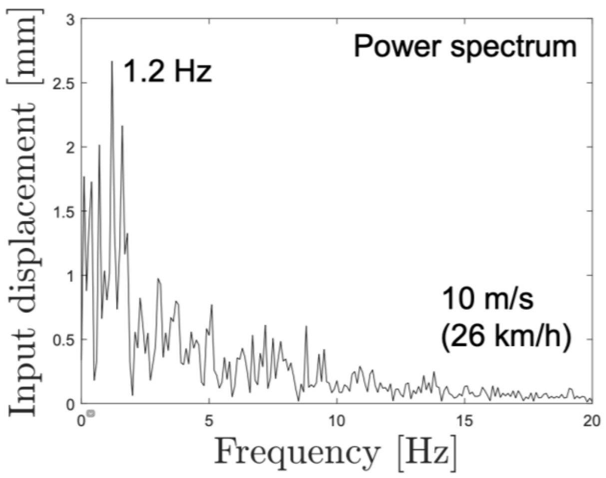
Relaxation spectrum

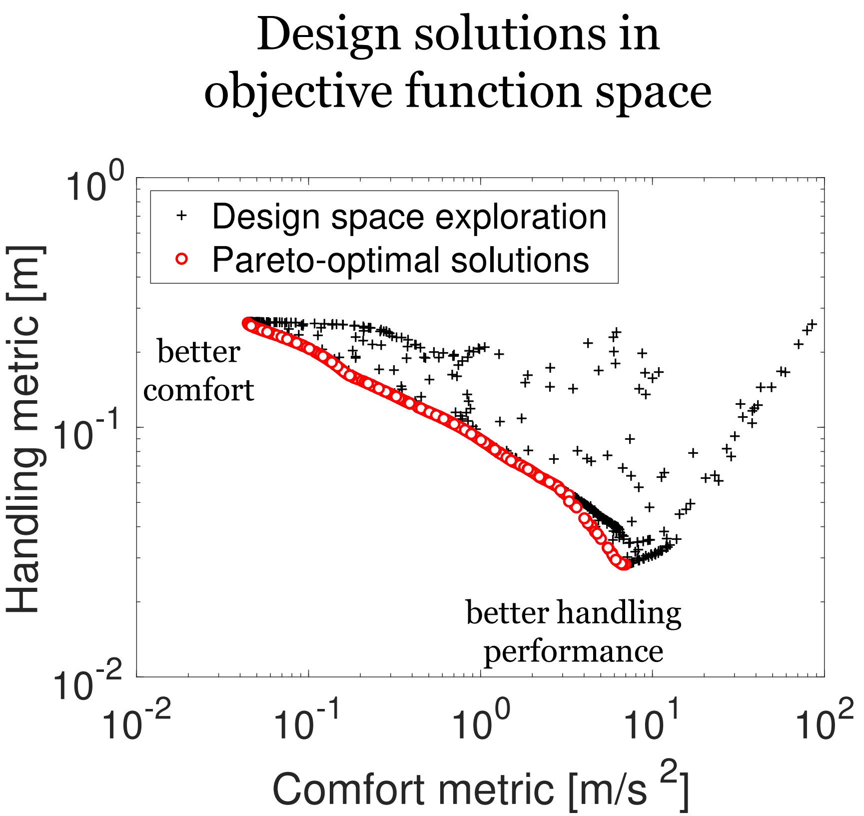


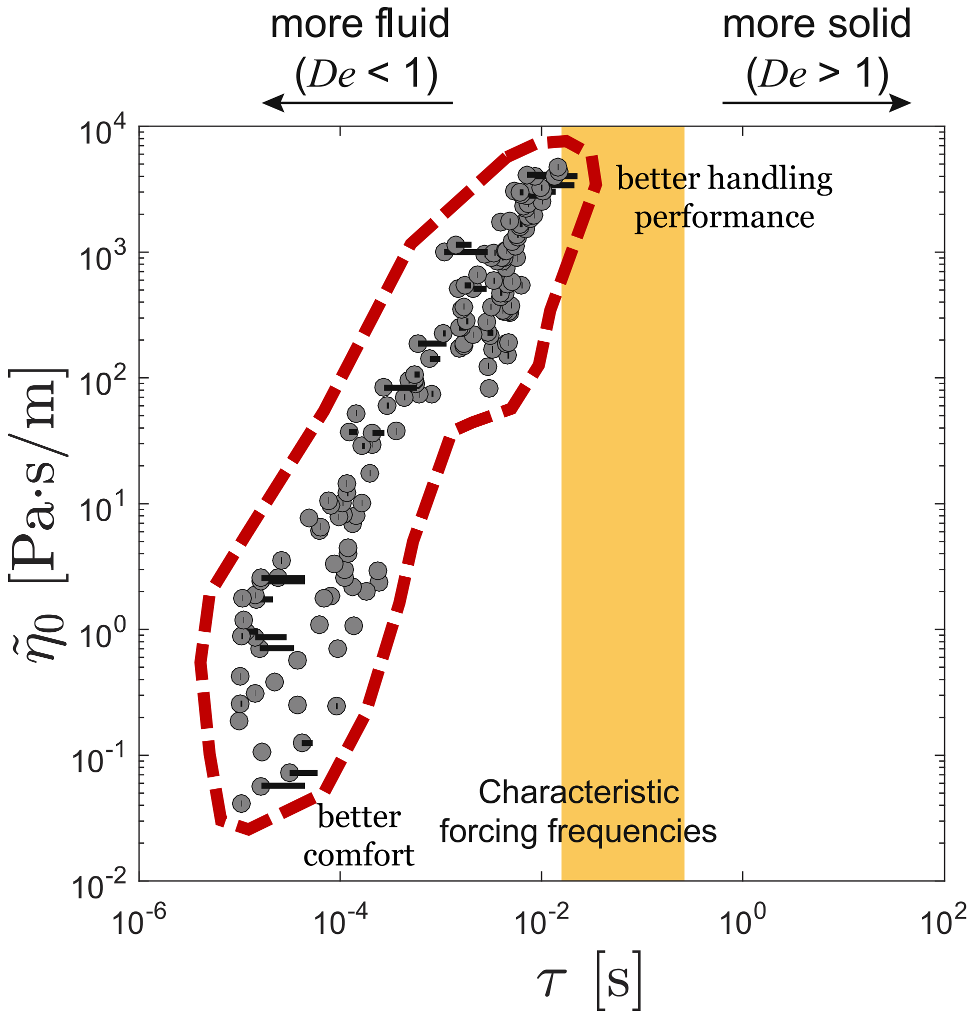
Reduced-dimensionality description

Case Study – Quarter Car Suspension Viscoelastic Damping Design









Conclusions and Future Works

- Design with/of nontrivial materials (e.g., soft, rheologically-complex materials) has the potential to achieve unprecedented design innovations.
- Characteristics of design-appropriate models are identified.
- Design appropriate LVE material descriptions are presented:
    - Continuous relaxation spectra, $H(\tau)$
    - Reduced-dimensionality description, $[G_0, \tau_1, \tau_2]$
- Limitations
    - Conversion between different material descriptions can be nontrivial.
    - Reduced-dimensionality description cannot uniquely map specific materials.
      (same value, but different material possible)
- Demonstrated with case studies: Vibration isolator, Experimental data process, Vehicle suspension

Conclusions and Future Works

- Regarding design appropriate modeling
  - Are design-appropriate models available for nonlinear viscoelasticity?
  - Is it possible to find material function constraints?
    e.g., Criminale-Eriksen-Filbey (CEF) fluid model has unbounded material functions.
  - Can a data-driven design approach be an effective resolution for this material function bounding problem?

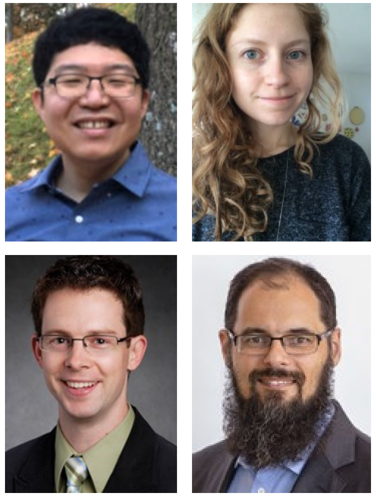
- Regarding the reduced dimensionality description
  - How large is the space of distinct materials that map to the same reduced model parameter values?
  - How to handle multiple spectrum peaks with simple representation?

References

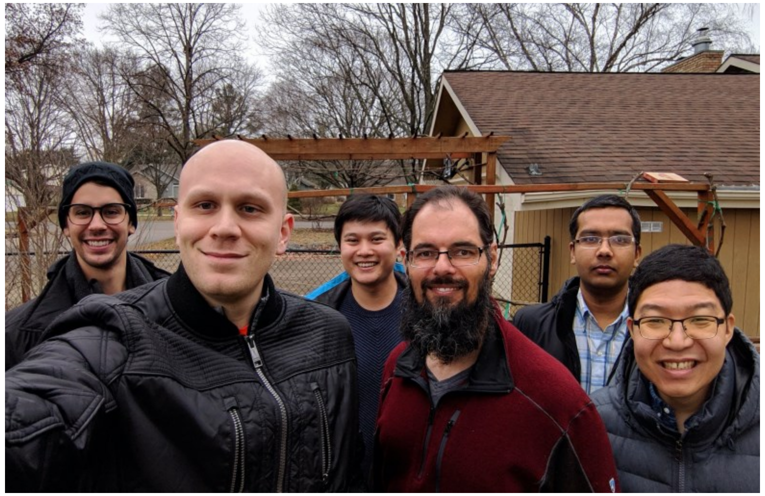
1. R.E. Corman, “Design tools for linear viscoelastic fluids,” Ph.D. Dissertation, University of Illinois at Urbana-Champaign, 2019.
2. R.E. Corman, et al., “Setting material function design targets for linear viscoelastic materials and structures,” *J. Mech. Des.*, 138(5):051402, 2016. doi:10.1115/1.4032698
3. B.W. Huang, et al., “Seismic analysis of a viscoelastic damping isolator,” *Adv. Mater. Sci. Eng.*, 2015:280625, 2015. doi:10.1155/2015/280625
4. Y.H. Lee, et al., “Simultaneous design of non-Newtonian lubricant and surface texture using surrogate-based multiobjective optimization,” *Struct. Multidiscip. O.*, 60(1):99-116, 2019. doi:10.1007/s00158-019-02201-1
5. Y.H. Lee, et al., “A multiobjective adaptive surrogate modeling-based optimization (MO-ASMO) framework using efficient sampling strategies,” In *ASME 2017 IDETC/CIE*, DETC2017-67541, Cleveland, OH, USA. doi:10.1115/DETC2017-67541
6. A.C. Pipkin, *Lectures on Viscoelasticity Theory*, Springer, New York, 1972.
7. R.B. Bird, et al., Dynamics of Polymeric Liquids, Vol.1 Fluid Mechanics, 2nd ed, Wiley, New York, 1987.
8. M. Mours and H.H.Winter, “Mechanical spectroscopy of polymers,” In T. Tanaka (eds) *Experimental Methods in Polymer Science*, Academic Press, San Diego, 2000.
9. F. Schwarzl and A.J. Staverman, “Higher approximations of relaxation spectra” *Physica*, 18(10):791-798, 1952. doi:10.1016/S0031-8914(52)80267-8
10. J.D. Ferry, Viscoelastic Properties of Polymers, 3rd ed, Wiley, New York, 1980.
11. N.W. Tschoegl, *The Phenomenological Theory of Linear Viscoelastic Behavior*, Springer, Berlin, 1989.
12. M. Baumgaertel and H.H. Winter, “Interrelation between continuous and discrete relaxation time spectra,” J. Non-Newton. Fluid., 44:15-36, 1992. doi:10.1016/0377-0257(92)80043-W
13. L. Martinetti, “Uniaxial extensional behavior of A-B-A thermoplastic elastomers: structure-properties relationship and modeling,” Ph.D. Dissertation, University of Minnesota, 2015.
14. M.E. De Rosa and H.H. Winter, “The effect of entanglements on the rheological behavior of polybutadiene critical gels,” *Rheol. Acta*, 33:220-237, 1994. doi: 10.1007/BF00437307

Thank you.

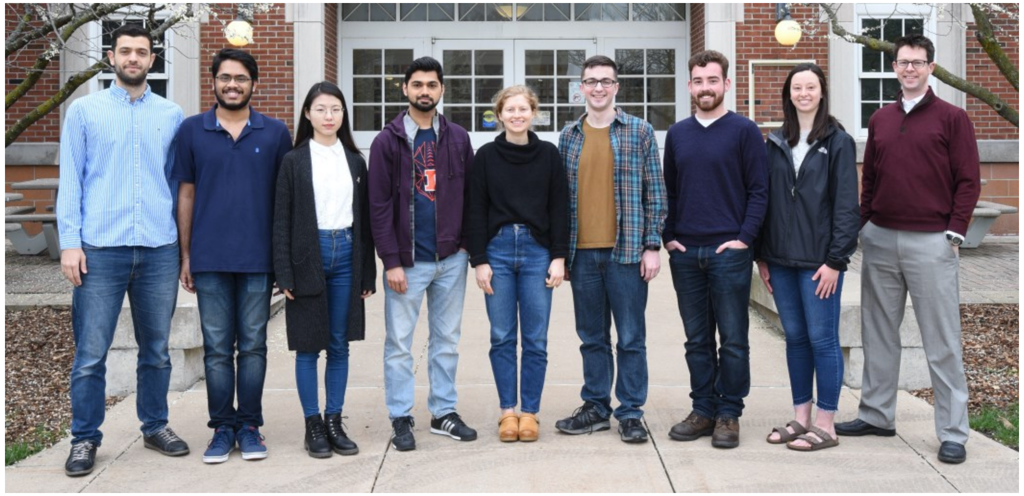
This material is partially based upon work supported by the National Science Foundation under Grant No. CMMI-1463203.



Authors



Engineering System Design Laboratory



Ewoldt Research Group