Data-Driven Anisotropic Finite Viscoelasticity with Neural ODEs

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Introduction

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Viscoelastic materials

- Most biological tissues are viscoelastic
- Soft tissues contain water that *flows* when the tissue is loaded
- Polymers such as rubber - realignment of polymer chains
- Personalized surgery and soft robotics require accurate material models

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- Arbitrary states of stress
- 3D
- *Physics-constrained* $\Longrightarrow$ 2^{nd} law of Thermodynamics

Previous work on modeling hyperelasticity with Neural ODEs (NODE):

V. Tac, F. S. Costabal, and A. B. Tepole, "Data-driven tissue mechanics with polyconvex neural ordinary differential equations," *Computer Methods in Applied Mechanics and Engineering*, vol. 398, p. 18, 2022, doi: 10.1016/j.cma.2022.115248.

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- NODEs are *monotonic* $\implies$ can be used to construct convex functions
- NODE architecture can be tweaked to ensure:
  - Non-decreasing/Non-increasing
  - Non-negative
  - Pass through the origin, i.e. include $(0, 0)$
  - $\cdots$

Variational finite viscoelasticity

Multiplicative split of the deformation gradient

$$\mathbf{F} = \mathbf{F}_e^M \mathbf{F}_i^M = \mathbf{F}_e^F \mathbf{F}_i^F$$

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Additive split of the Helmholtz free energy function

$$\Psi = \Psi_{EQ}^M(\mathbf{C}) + \Psi_{EQ}^F(\mathbf{C}) + \Psi_{NEQ}^M(\mathbf{C}_e^M) + \Psi_{NEQ}^F(\mathbf{C}_e^F) \quad (1)$$

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Dissipation Inequality:

$$\frac{1}{2}\mathbf{S} : \dot{\mathbf{C}} - \dot{\Psi} \geq 0 \tag{2}$$

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Substitute from (1) to (2) to get

$$\underbrace{-2\frac{\partial \Psi}{\partial \mathbf{C}_i^M} : \frac{1}{2}\dot{\mathbf{C}}_i^M}_{\text{Energy diss. in matrix}} \quad \underbrace{-2\frac{\partial \Psi}{\partial \mathbf{C}_i^F} : \frac{1}{2}\dot{\mathbf{C}}_i^F}_{\text{Energy diss. in fibers}} \geq 0 \tag{3}$$

Variational finite viscoelasticity

Require that the two terms independently satisfy the inequality,

$$-2\frac{\partial\Psi}{\partial\mathbf{C}_i^M}:\frac{1}{2}\dot{\mathbf{C}}_i^M \geq 0 \qquad \text{(Matrix dissipation inequality)} \tag{4}$$

$$-2\frac{\partial\Psi}{\partial\mathbf{C}_i^F}:\frac{1}{2}\dot{\mathbf{C}}_i^F \geq 0 \qquad \text{(Fiber dissipation inequality)} \tag{5}$$

Dissipation of energy in the matrix

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$$-2\frac{\partial \Psi}{\partial \mathbf{C}_i^M} : \frac{1}{2}\dot{\mathbf{C}}_i^M \geq 0 \quad \xrightarrow{\text{Push forward}} \quad -\tau_{NEQ}^M : \underbrace{\frac{1}{2}(\mathscr{L}\mathbf{b}_e^M)(\mathbf{b}_e^M)^{-1}}_{?} \geq 0 \tag{6}$$

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Creep potential

$$-\frac{1}{2}(\mathscr{L}\mathbf{b}_e^M)\mathbf{b}_e^{M^{-1}} = \frac{\partial \Phi}{\partial \tau_{NEQ}^M}$$

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1. Φ is a convex function of τ_{NEQ}^M

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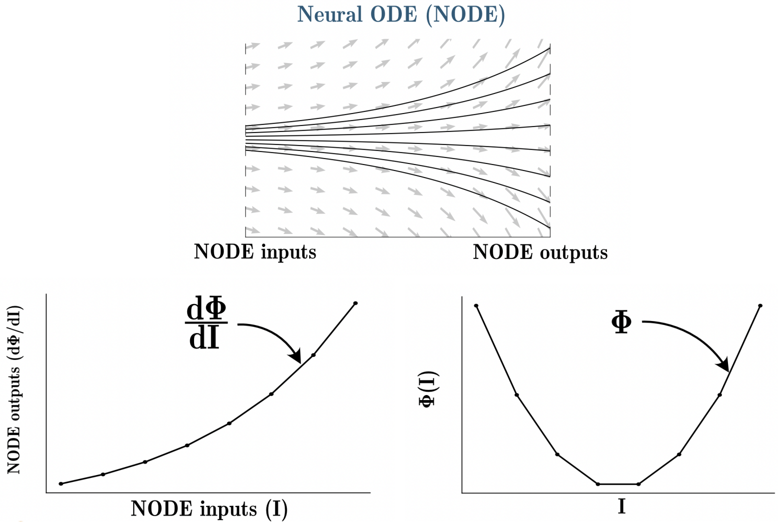
1. Φ is a convex function of τ_{NEQ}^M
2. $\arg\min_{\tau_{NEQ}^M}\Phi=\mathbf{0}$

Proposed creep potential:

$$\Phi(\tau_{NEQ}^M)=\hat{\Phi}_1(I_1^\tau)+\hat{\Phi}_2((I_1^\tau)^2)+\hat{\Phi}_3((I_1^\tau)^2-3I_2^\tau)$$

NODEs, convexity & monotonicity



Dissipation of energy in the matrix

NODE-based creep potential:

$$\Phi = \hat{\Phi}_1(\underbrace{I_1^\tau}_{\xi_1}) + \hat{\Phi}_2(\underbrace{(I_1^\tau)^2}_{\xi_2}) + \hat{\Phi}_3(\underbrace{(I_1^\tau)^2 - 3I_2^\tau}_{\xi_3})$$

$$\frac{\partial \hat{\Phi}_1}{\partial \xi_1} = \mathcal{N}_1(\xi_1), \qquad \frac{\partial \hat{\Phi}_2}{\partial \xi_2} = \mathcal{N}_2(\xi_2), \qquad \frac{\partial \hat{\Phi}_3}{\partial \xi_3} = \mathcal{N}_3(\xi_3)$$

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Typical closed form creep potential used in the literature:

$$\Phi_{RG} = \frac{1}{9\eta_V}\xi_2 + \frac{1}{3\eta_D}\xi_3 \,.$$

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$\Longrightarrow$ Highly flexible data-driven creep potential that satisfies the 2nd law of Thermodynamics *exactly*.

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Substitute the free energy function

$$\Psi = \Psi^M_{EQ}(\mathbf{C}) + \Psi^F_{EQ}(\mathbf{C}) + \Psi^M_{NEQ}(\mathbf{C}^M_e) + \Psi^F_{NEQ}(\mathbf{C}^F_e) \tag{7}$$

into the fiber dissipation inequality

$$-2\frac{\partial \Psi}{\partial \mathbf{C}^F_i} : \frac{1}{2}\dot{\mathbf{C}}^F_i \geq 0 \tag{8}$$

to get

$$\underbrace{2I^F_{4e}\frac{\partial \Psi^F_{NEQ}}{\partial I^F_{4e}}}_{\tau^F_{NEQ}} \frac{\mathbf{M}}{\mathbf{C}^F_i : \mathbf{M}} : \frac{1}{2}\dot{\mathbf{C}}^F_i \geq 0 \tag{9}$$

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In terms of stretches:

$$\tau_{NEQ}^F \left(\frac{\dot{\lambda}_i^F}{\lambda_i^F} \right) \geq 0 \tag{10}$$

Dissipation of energy in the fiber

NODE-based evolution equation for the fiber:

$$\left(\frac{\dot{\lambda}_i^F}{\lambda_i^F}\right) = \mathcal{N}(\tau_{NEQ}^F) \tag{11}$$

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Note: Monotonicity of NODE ($\mathcal{N}$) implies:

- $\mathcal{N}(\tau_{NEQ}^F) > 0$ when $\tau_{NEQ}^F > 0$
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$\implies \tau_{NEQ}^F \left(\frac{\dot{\lambda}_i^F}{\lambda_i^F}\right) \geq 0$

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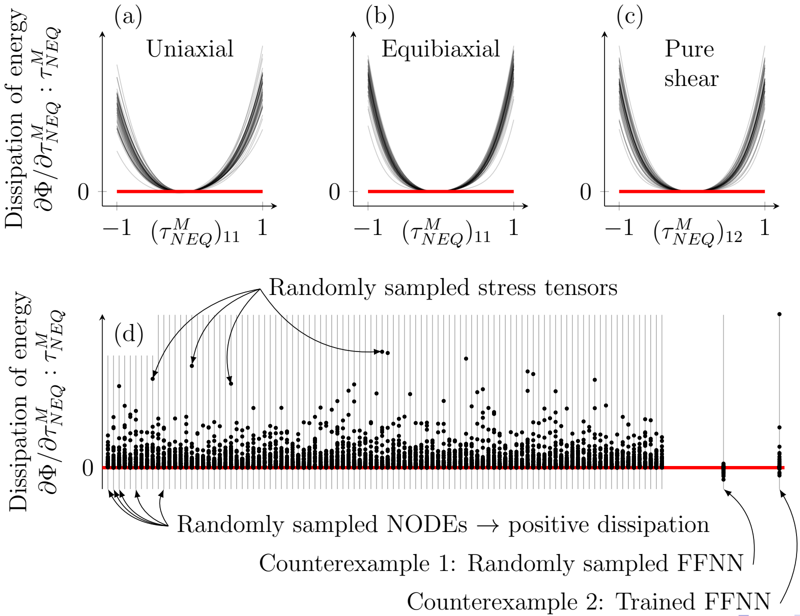
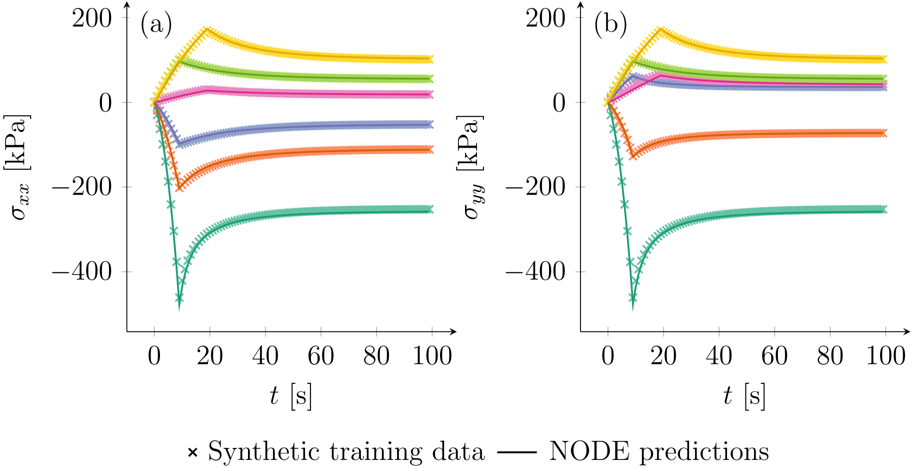
$\implies \tau_{NEQ}^F \left(\frac{\dot{\lambda}_i^F}{\lambda_i^F}\right) \geq 0$

$\implies$ Highly flexible data-driven evolution equation that satisfies the 2nd law of Thermodynamics *exactly*.

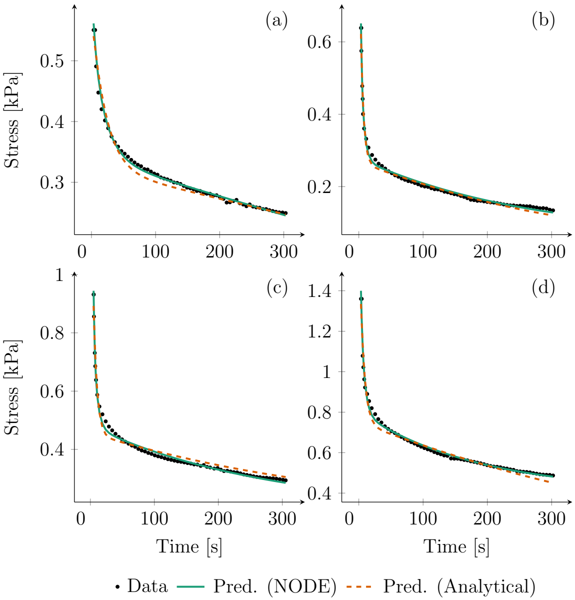
Guaranteed positive dissipation



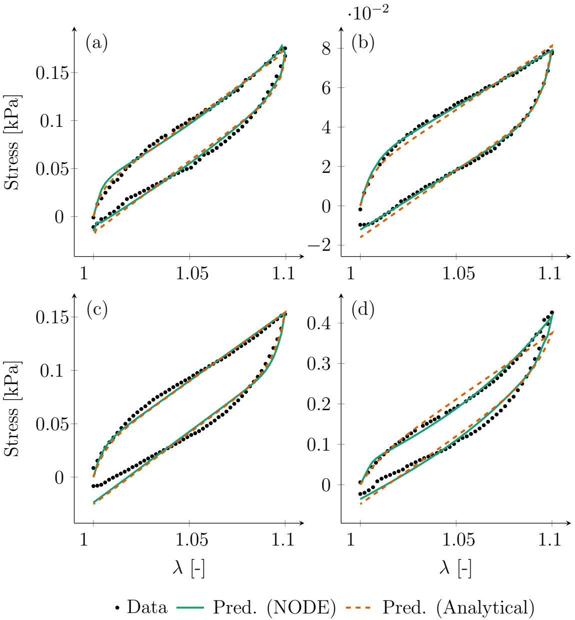
Training with synthetic data



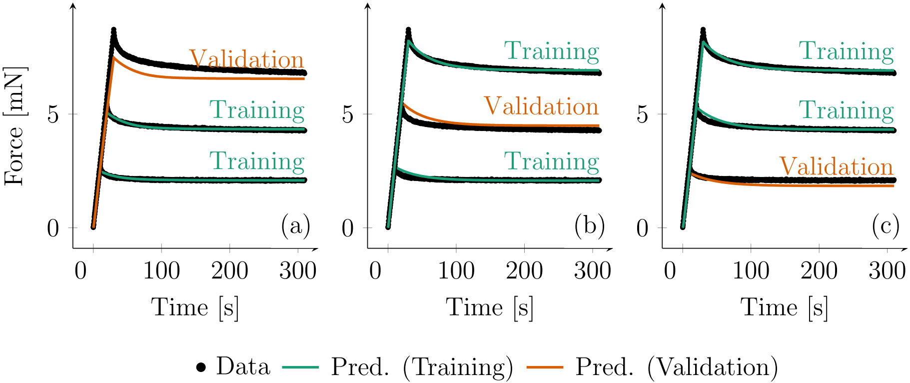
Training with data from human brain



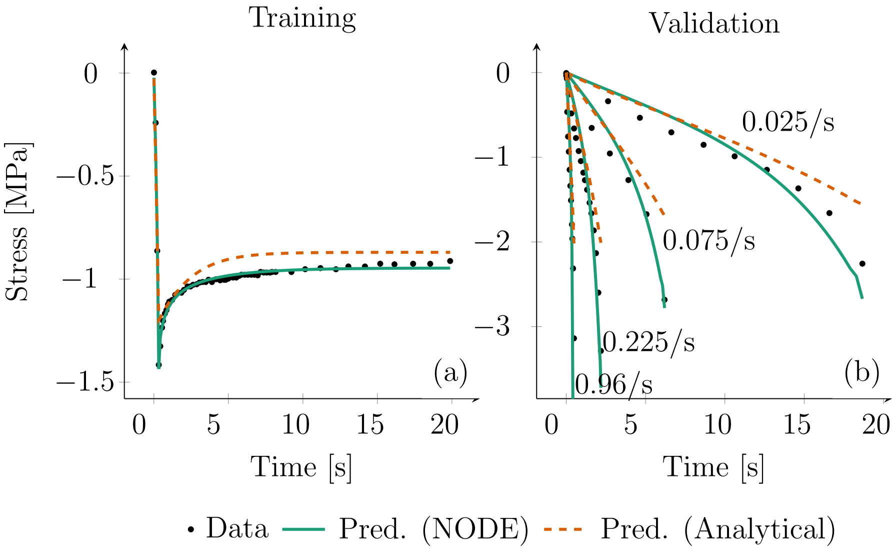
Training with *cyclic* data from human brain



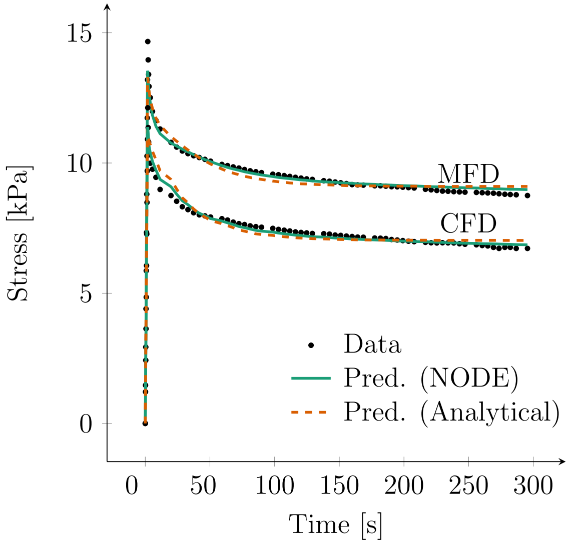
Training with blood clot data



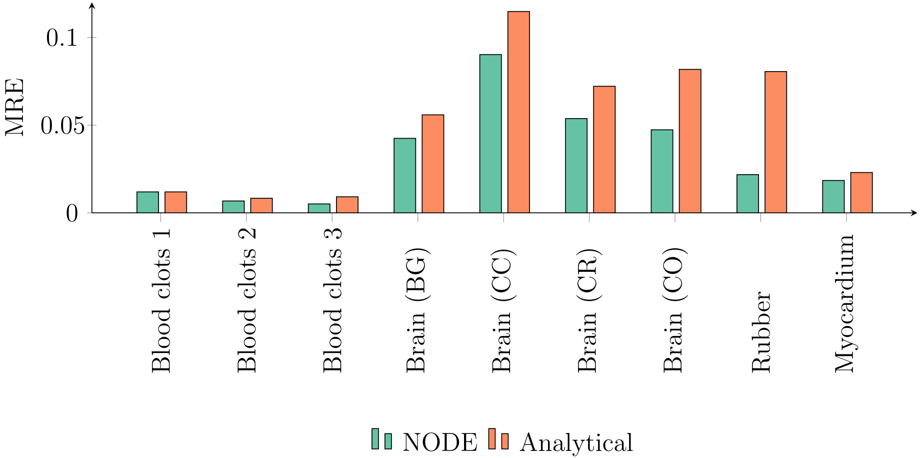
Training with rubber data



Training with data from human myocardium (anisotropic)



Summary of all training cases



Conclusions

- We developed a fully data-driven model of finite viscoelasticity
  - Anisotropic
  - Physics-constrained
  - Arbitrary deformations and stresses
  - Large deformations and large deviations from the Thermodynamic equilibrium
  - Extremely flexible
- First such model to the best of our knowledge
- Trained and tested with experimental data from biological *and* man-made materials
  - Rubber
  - Blood clots
  - Human brain
  - Human myocardium
- Under different loading conditions
  - Stress relaxation
  - Cyclic loading
  - Monotonic compression
- Outperforms the benchmark closed-form model in all cases!

Thank you!