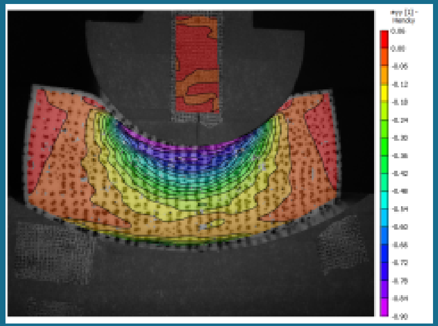
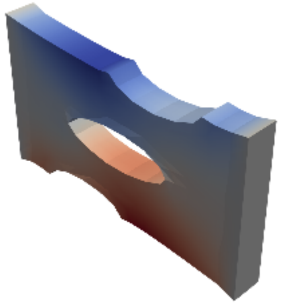
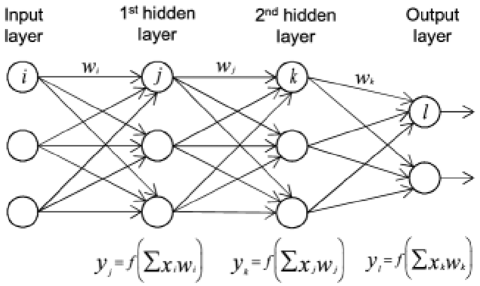
SAND2022-7724C

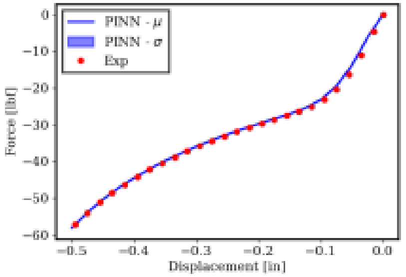
Sandia National Laboratories

Novel Physics-Informed Neural Network Approach for Large-Deformation Mechanics Constitutive Model Calibration









Craig Hamel, Sharlotte Kramer, and Kevin Long

15 June 2022

2022 SEM Annual Conference

Data Science in Constitutive Models Session; Paper 13355

U.S. DEPARTMENT OF ENERGY NNSA

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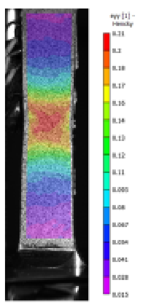
Constitutive model calibration can require fewer tests when using full-field data, but current inverse methods for such calibration have several drawbacks.

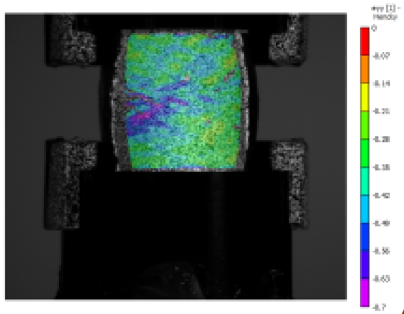
Experimental Data Requirements

Simple Tests



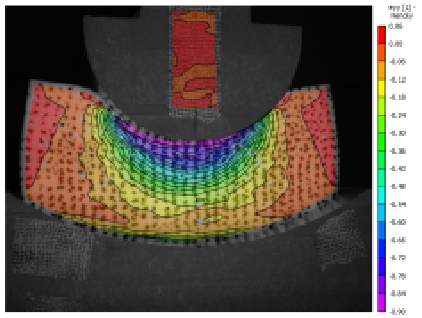
Tension

Notched Tension

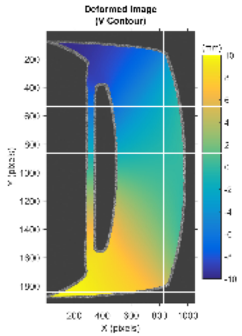


Compression

Complex Heterogeneous Tests



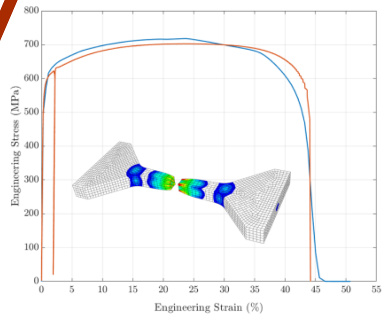
Impact with Round Indenter



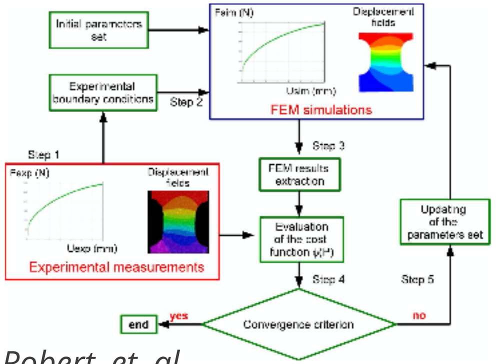
Tension of "D" Shaped Sheet

Example Inverse Methods

Finite Element Method Updating (FEMU):

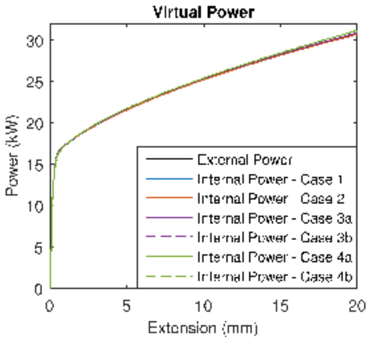


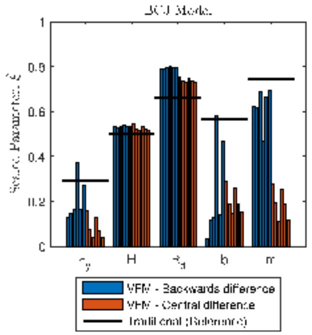
Kramer, et. al., IJF, 2019



Robert, et. al., J. Strain Anal. Engr. Design, 2012

Virtual Fields Method (VFM):





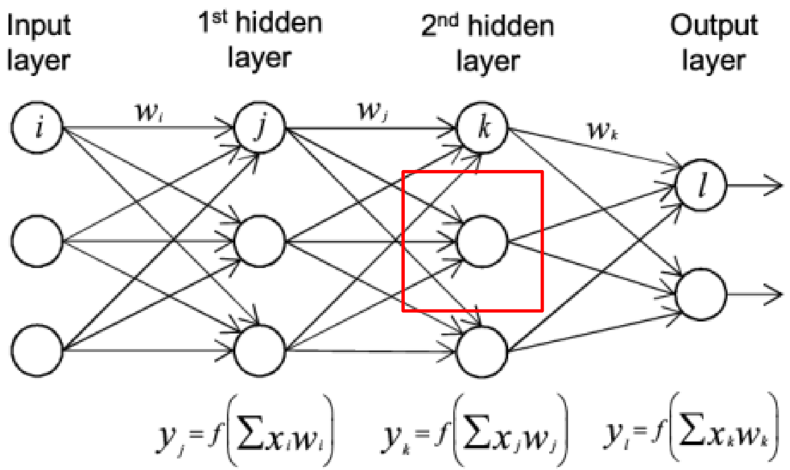
Jones, et. al., Sandia Report SAND2018-10635, 2018

Issues:

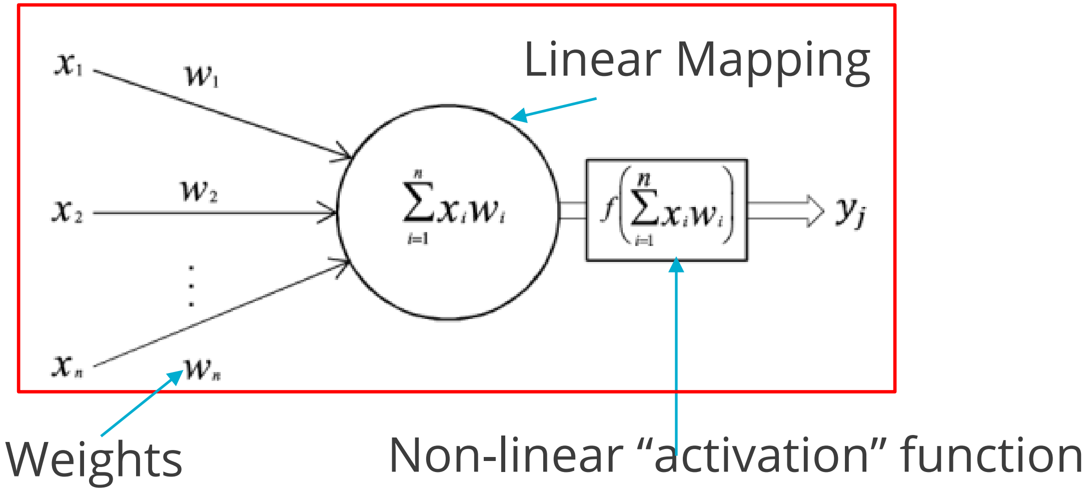
- **Expensive and slow**
- **Hard to map surface data to FEM mesh**
- **Hard to use more than one experiment**
- **(VFM) Need volumetric strain data or plane-stress / sheet-material only limitation**

Physics-informed neural networks (PINNs) offer a new paradigm for constitutive model calibration with full-field data.
But what are PINNs?

Neural Network (NN) With Several Layers



Perceptron – Bioinspired-model of neurons in the brain



Loss Function: Error between Training Data and Output to NN

$$L = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}$$

PINN Loss Function: Error between Training Data and Output to NN and Physics Constraints

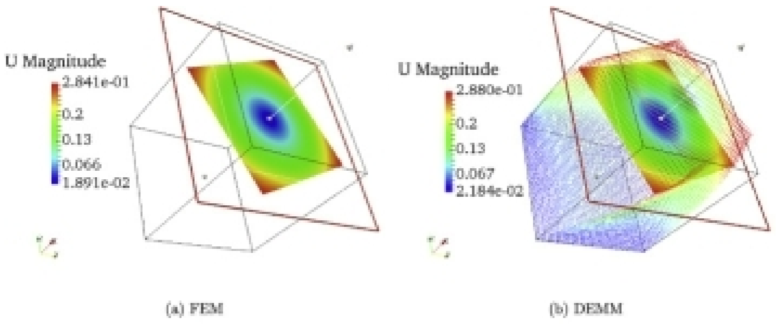
$$L = \alpha \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n} + \beta \Pi_N$$

PINNs for solid mechanics is a recent advancement.

Deep Energy Method for Finite-Strain Hyperelasticity

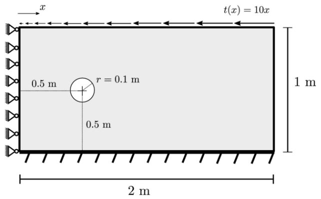
Nguyen-Thanh et. al., *Euro. J. Mechanics A*, 2020

Forward-Only Approach: U_x Field for Twisted Cuboid



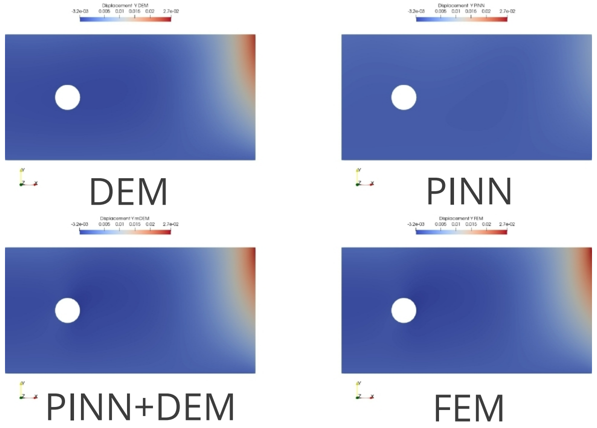
PINNs + Deep Energy Method to Resolve Stress Concentrations in Finite-Strain Hyperelasticity

Fuhg and Bouklas, *J. Comp. Phys.*, 2022



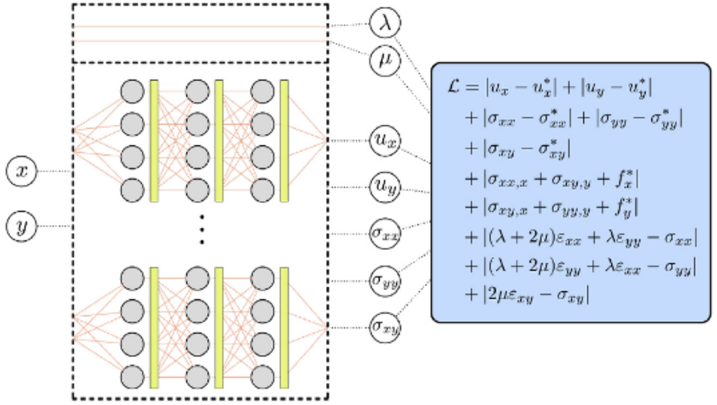
Beam with Deflection

Forward-Only Approach: U_x Field



PINNs for Inverse Method for 2D Problems

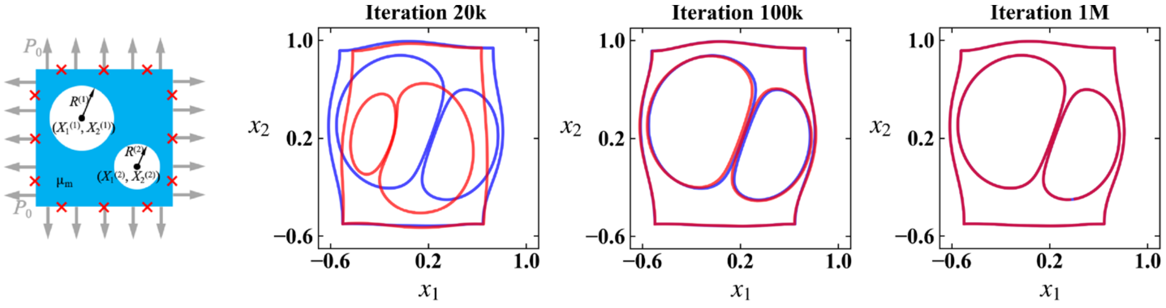
Haghighat et. al., *CMAME* 2021



Separate PINN for each component of 2D stress and displacement

PINNs for Geometry Defect and Material Property Identification in 2D

Zhang et. al. *Science*, 2022

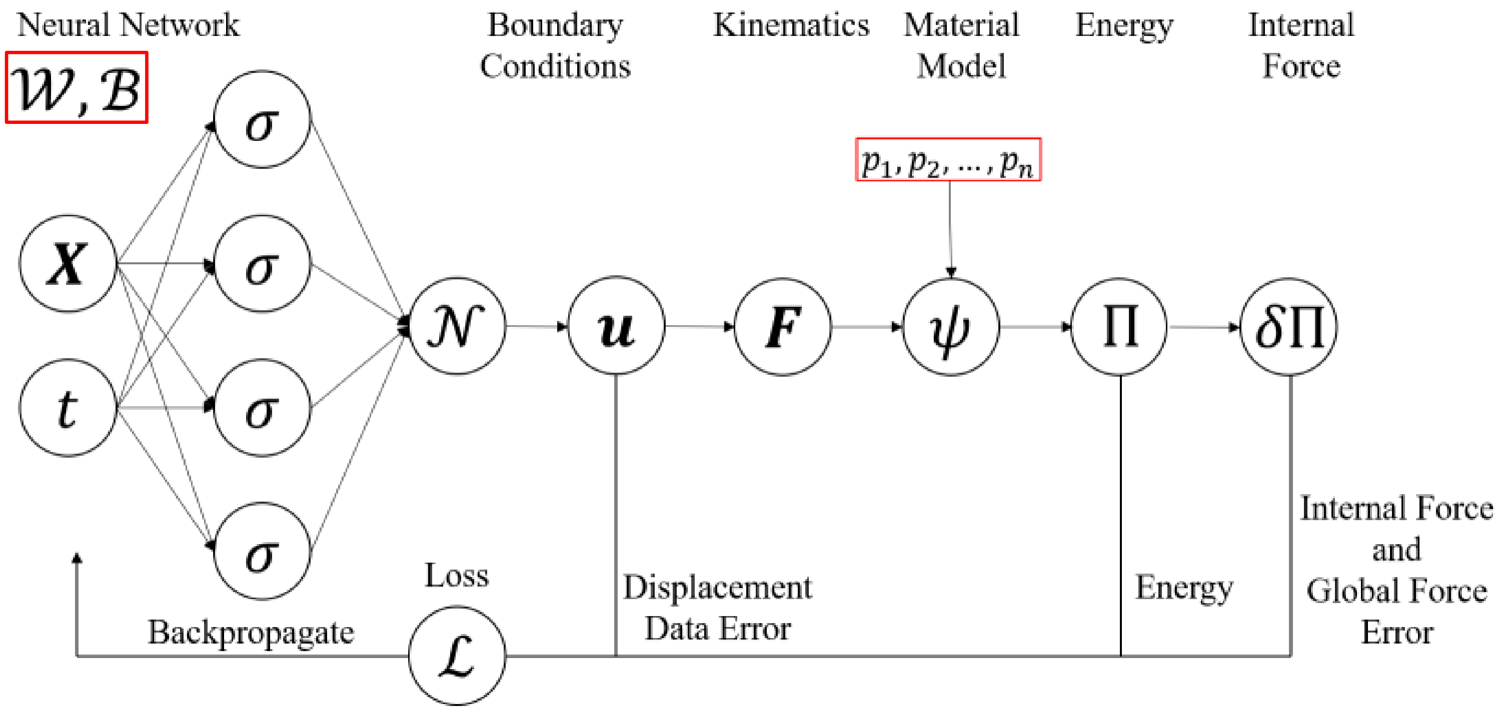


Shape estimation of PINN (red) vs. FEM (blue) for a hyperelastic material with increasing level of PINNs training

Our current PINNs approach uses an energy formulation, allowing us to **calibrate material models with energy potentials**.

Strain energy — Energy due to body forces — Energy due to surface tractions

$$\min_{\mathbf{u}\in H^1(\mathcal{B}_0)} \Pi(\mathbf{u}) \longrightarrow \delta\Pi = \int_{\mathcal{B}_0} \delta\psi(\mathbf{E})\, dv - \int_{\mathcal{B}_0} \mathbf{b}\cdot\delta\mathbf{u} dv - \int_{\partial\mathcal{B}_0^{\mathbf{t}}} \tilde{\mathbf{t}}\cdot\delta\mathbf{u} da = 0,$$



Trainable parameters

Craig Hamel, Kevin Long, and Sharlotte Kramer, "Calibrating Constitutive Models with Full Field Data via Physics Informed Neural Networks" (Submitted to *Strain*) https://arxiv.org/abs/2203.16577

Our PINNs approach to material model calibration utilizes heterogenous full-field data and global force data.

Kinematics

Displacement BC — Neural network

$$\mathbf{u}_{\mathcal{N}}(\mathbf{X},t) \approx \tilde{\mathbf{u}}(\mathbf{X},t) + f(\mathbf{X})\mathcal{N}(\mathbf{X},t)$$

$$\mathbf{F}^e_{\mathcal{N}} = \mathbf{I} + \nabla_{\mathbf{X}}\mathbf{u}^e_{\mathcal{N}}$$

$$\nabla_{\mathbf{X}}\mathbf{u}^e_{\mathcal{N}} = \sum_{I=1}^{N_{nodes}} \mathbf{u}^I_{\mathcal{N}} \otimes \nabla_{\mathbf{X}} N^I$$

Standard shape functions for Hex8 elements

Total potential energy for time step n

$$\Pi^n_{\mathcal{N}} = \sum_{e=1}^{N_e}\sum_{q=1}^{N_q} w_q \left(\det \mathbf{J}^e\right) \psi^e\left(\mathbf{F}^e_{\mathcal{N}}\right)$$

Internal Force Vector

$$\mathbf{f}_{\mathcal{N}} = \delta\Pi_{\mathcal{N}} = \frac{\partial \Pi_{\mathcal{N}}}{\partial \mathbf{u}_{\mathcal{N}}}$$

Total loss function $\mathcal{L} = \beta\mathcal{L}_r + \gamma\mathcal{L}_{\mathbf{u}} + \delta\mathcal{L}_f$

Loss function for potential energy $\mathcal{L}_r = \Pi_{\mathcal{N}} + \alpha\|\delta\Pi_{\mathcal{N}}\|^2_{free}$

For inverse problems we have the additional error terms for experimental data

Surface Displacements

$$\mathcal{L}_{\mathbf{u}} = \frac{1}{N_{\mathbf{u}}}\sum_{i=1}^{N_{\mathbf{u}}} \|\mathbf{u}_{\mathcal{N}}\left(\mathbf{X}^*_i, t^*_i\right) - \mathbf{u}^*_i\left(\mathbf{X}^*_i, t^*_i\right)\|^2$$

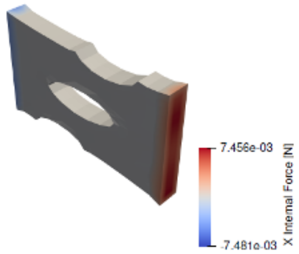
Global Force

$$\mathcal{L}_f = \frac{1}{N_t}\sum_{n=1}^{N_t} \|f_{net}(t_n) - f^*_{net}(t_n)\|^2$$

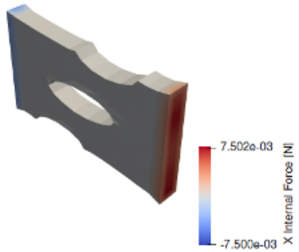
As a validation exercise, our PINNs architecture used in the forward problem reasonably approximates forces in the large-deformation of hyperelastic models as compared to FEM.

Forward problem code-to-code V&V using Gent constitutive model

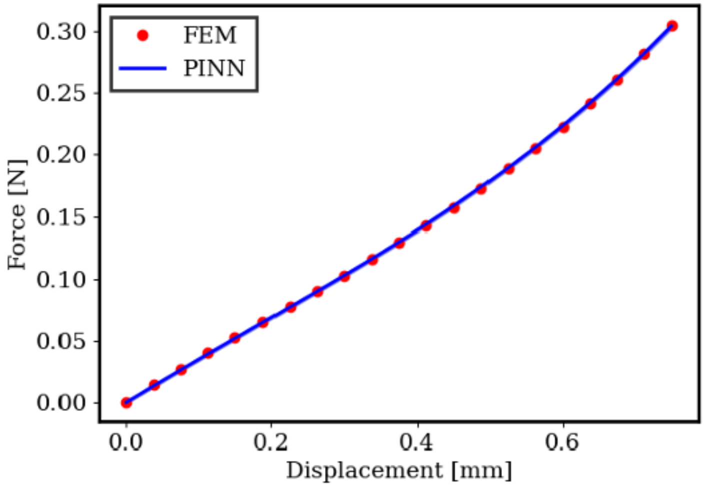
Internal force f_x



(a) FEM f_x



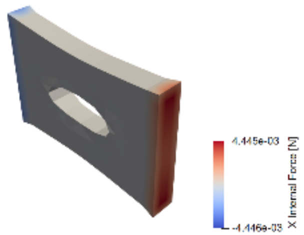
(d) PINN f_x



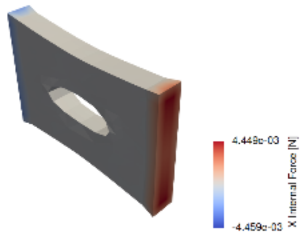
$$\psi\left(\mathbf{C}\right) = \frac{1}{2}K\left[\frac{1}{2}\left(J^2-1\right) - \ln J\right] - \frac{1}{2}\mu J_m \ln\left(1 - \frac{\bar{I}_1 - 3}{J_m}\right)$$

Forward problem code-to-code V&V using Neo-Hookean constitutive model

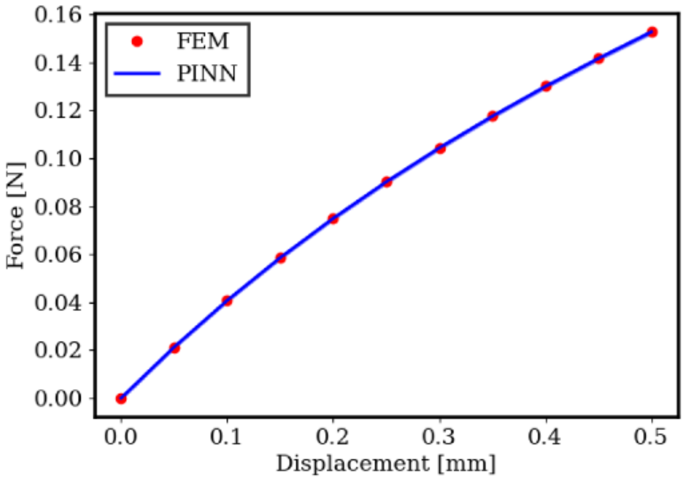
Internal force f_x



(a) FEM f_x



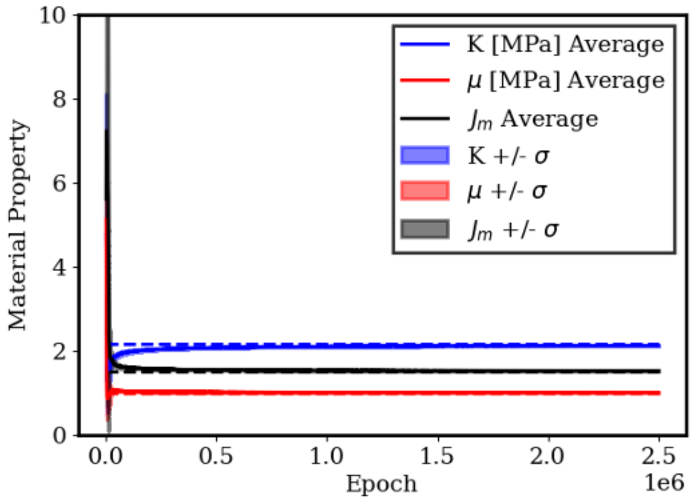
(d) PINN f_x



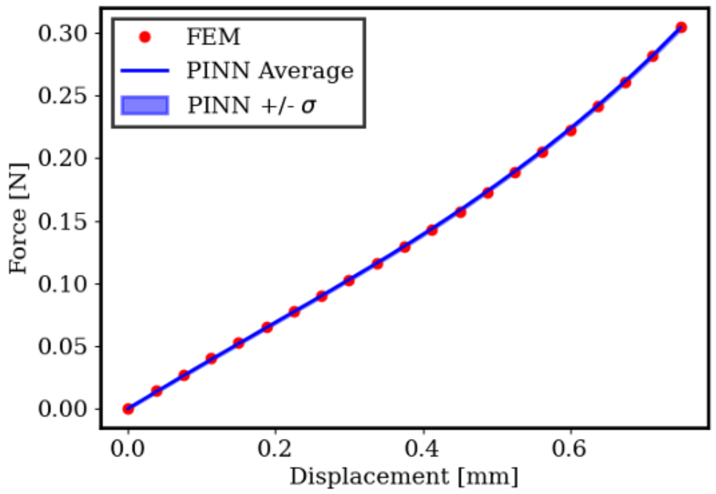
$$\psi\left(\mathbf{C}\right) = \frac{1}{2}K\left[\frac{1}{2}\left(J^2-1\right) - \ln J\right] + \frac{1}{2}\mu\left(\bar{I}_1 - 3\right)$$

Our PINNs inverse method can calibrate polymer models, demonstrated by using synthetic **heterogeneous full-field surface data of large deformation in multiple material models**.

Demonstration of Calibrating Gent Model

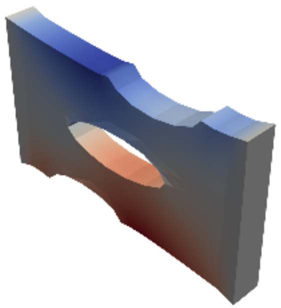


Elastomer in tension



DIC-Like Data Used

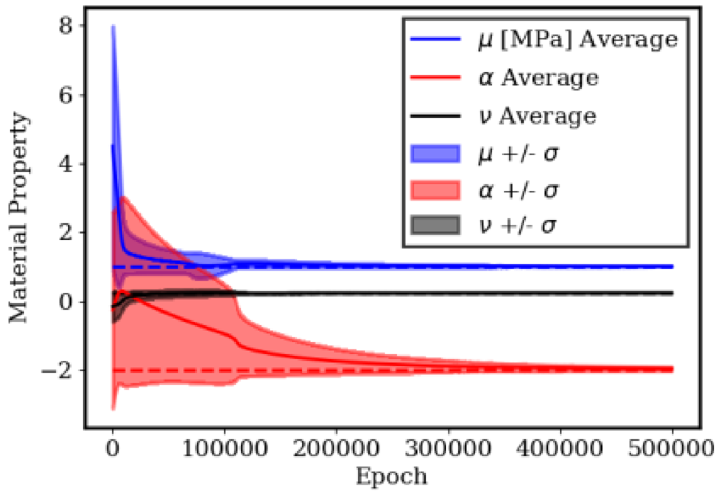
- Specimen is strained to 75% in tension with 600 finite elements.
- **DIC-Like Data: The surface displacement (front face) and global force** are extracted from FE simulations.
- Three parameters corresponding to the material properties are added to the PINN optimizer.
- **The goal is to “learn” the three parameters for the Gent constitutive model.**



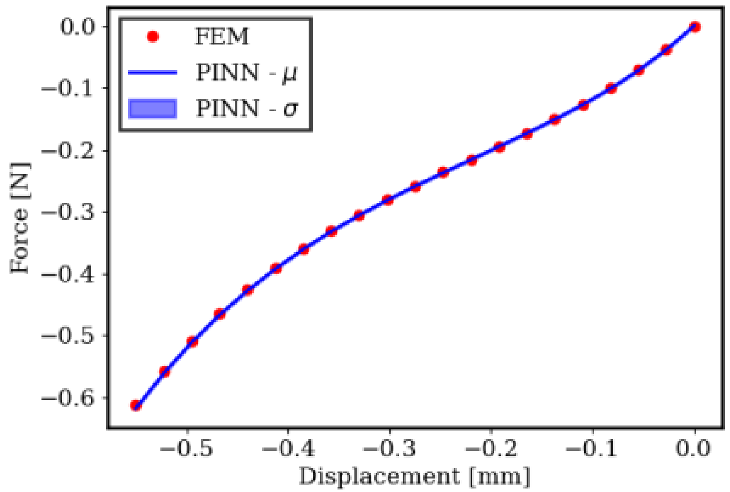
$$\psi(\mathbf{C}) = \frac{1}{2}K\left[\frac{1}{2}\left(J^2-1\right)-\ln J\right] - \frac{1}{2}\mu J_m \ln\left(1-\frac{\bar{I}_1-3}{J_m}\right)$$

Our PINNs inverse method can calibrate polymer models, demonstrated by using synthetic heterogeneous full-field surface data of large deformation in multiple material models.

Demonstration of Calibrating Hyperfoam Model

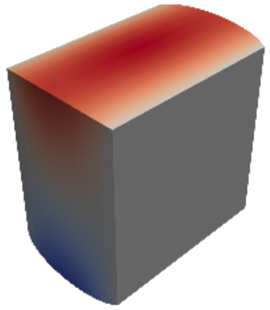


Foam in compression



DIC-Like Data Used

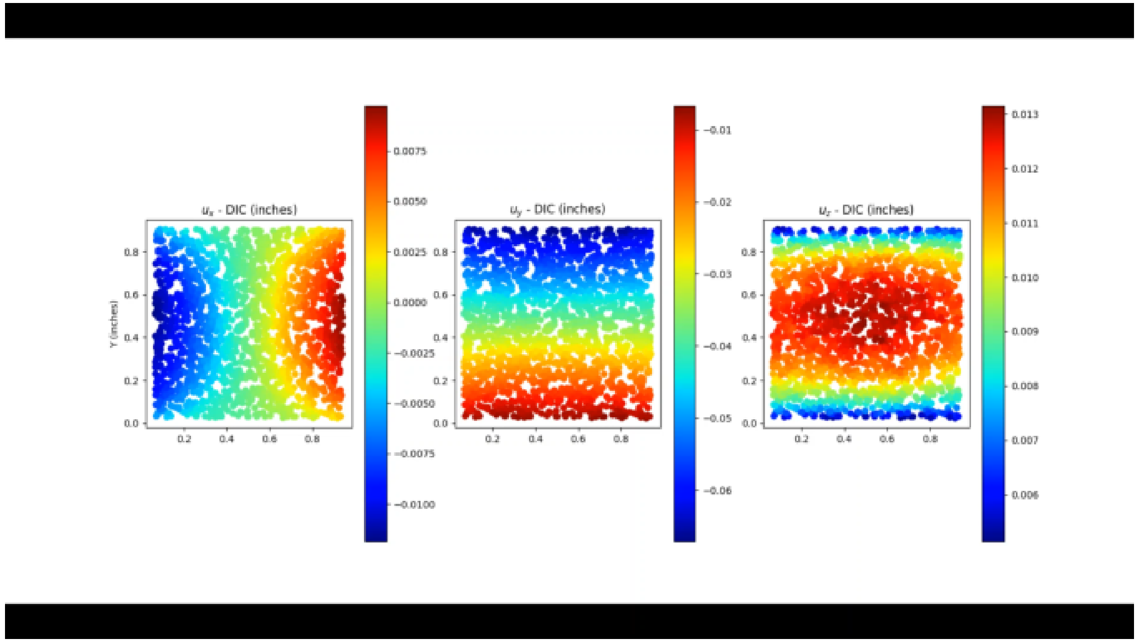
- Specimen is strained to -55% in tension with 1000 finite elements.
- **The surface displacement (front face) and global force are extracted from FE simulations.**
- Three parameters corresponding to the material properties are added to the PINN optimizer.
- **The goal is to “learn” the three parameters for the Hyperfoam constitutive model.**



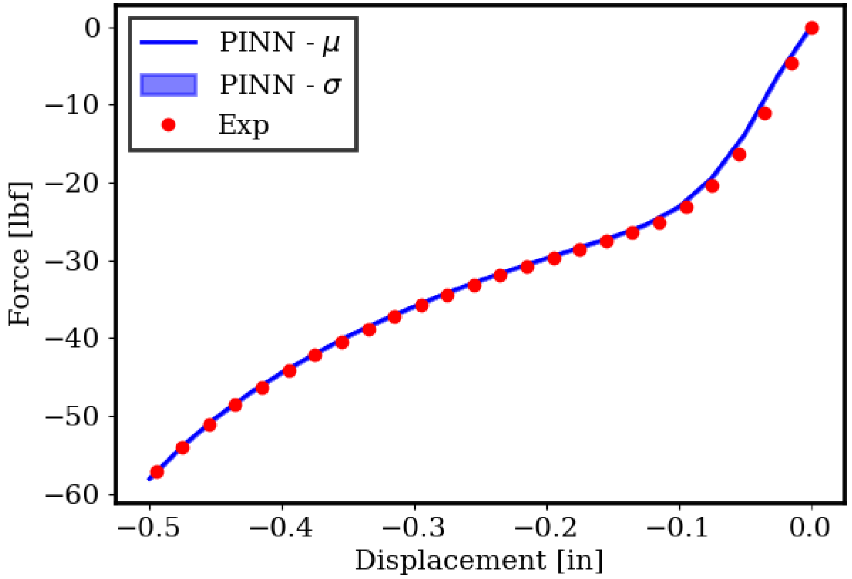
$$\psi^{eq}\left(\lambda_1, \lambda_2, \lambda_3\right) = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2}\left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}\left(J^{-\alpha_i\beta_i} - 1\right)\right]$$

Our PINNs inverse method has shown promise to calibrate a large-deformation Hyperfoam model using experimental data.

Displacement Data



Global Force Data



Here, **~5% of the correlated DIC points are picked at random for each image** and fed into the PINN along with the global force data.

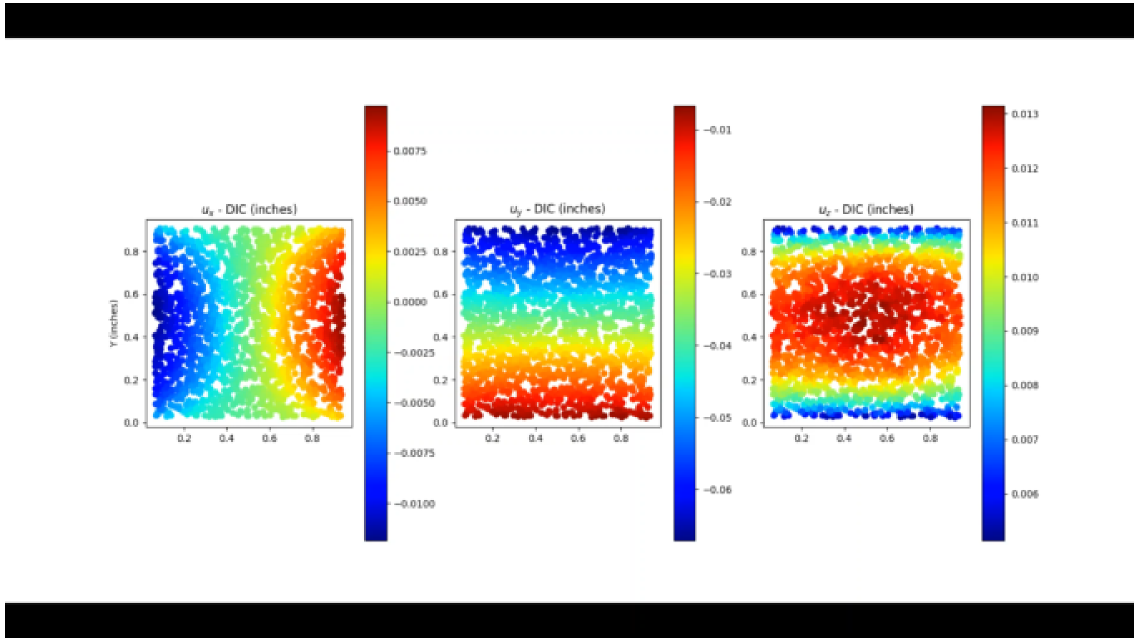
No interpolation was necessary onto the computational grid, and larger/smaller amounts of data is not an issue.

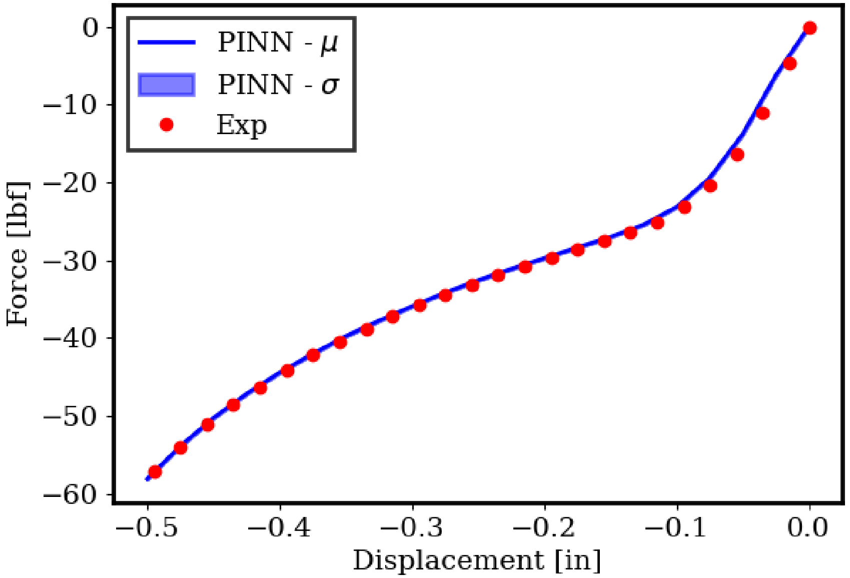
$$\psi^{eq}\left(\lambda_1, \lambda_2, \lambda_3\right) = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2}\left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}\left(J^{-\alpha_i \beta_i} - 1\right)\right]$$

Our PINNs inverse method approach for material model calibration overcomes shortcomings of current inverse methods that use full-field experimental data.

FEMU and VFM	PINNs
Issues	**Merits**
Computationally expensive and slow	Moderate computational expense
Hard to map surface data to mesh	No need to map surface data to mesh
Hard to use more than one experiment	Extensible to use multiple experiments simultaneously
(VFM) Need volumetric strain data or sheet-material only limitation	Variable amount of full-field data acceptable
Restricted to known model forms	Extensible to data-driven models
Difficult to incorporate experimental uncertainty quantification (UQ)	Readily addresses experimental UQ using Bayesian PINNs

Questions?


u_x - DIC (inches)
u_y - DIC (inches)
u_z - DIC (inches)
Y (inches)


PINN - μ
PINN - σ
Exp
Force [lbf]
Displacement [in]