DATA-DRIVEN CONSTITUTIVE LAWS FOR HYPERELASTICITY IN PRINCIPAL SPACE USING SYMBOLIC REPRESENTATIONS OF PYTORCH ANNS IN FENICS

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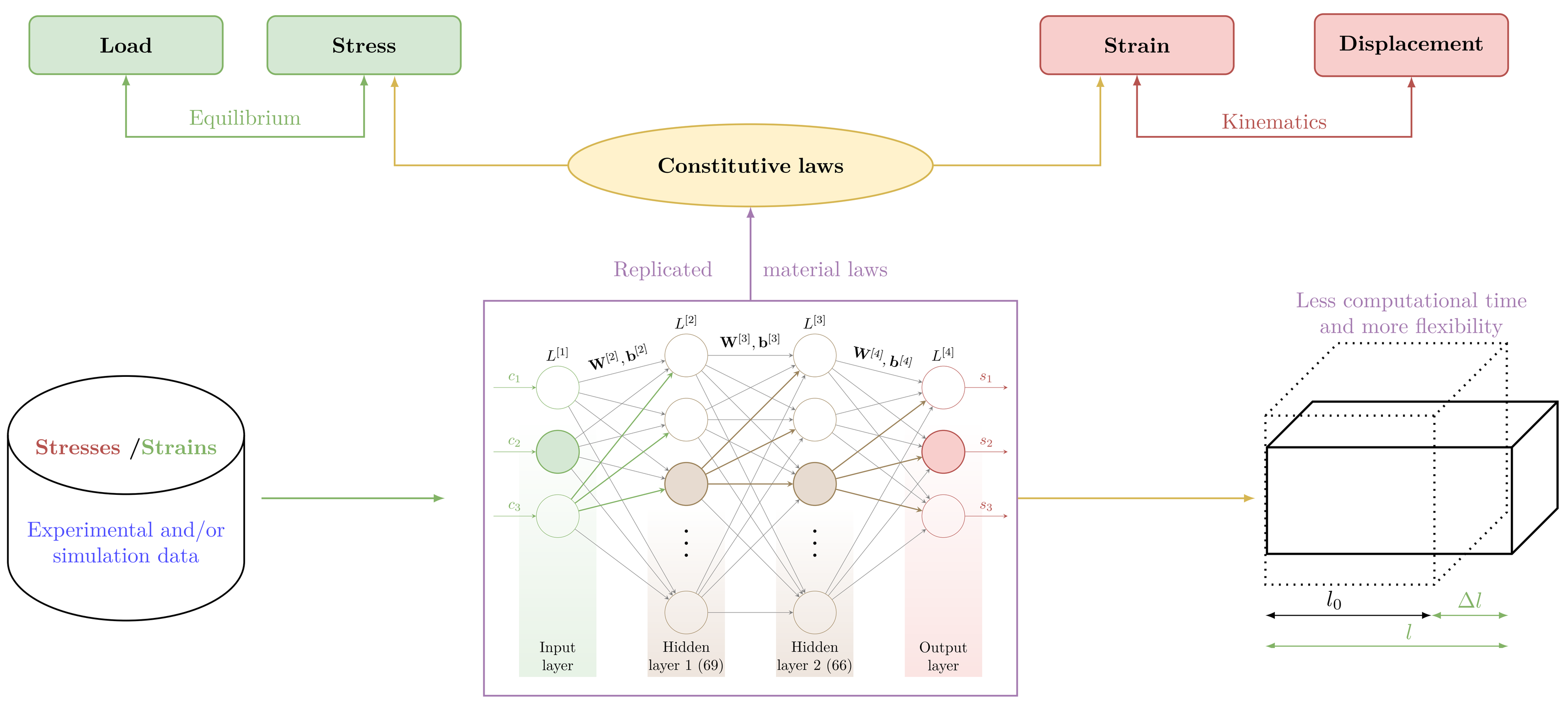
HIGHLIGHTS

- Hyperelastic material laws are learnt from strain-stress datasets in principal space using Artificial Neural Network (ANN).
- Construction of symbolic ANN which can be differentiated symbolically via FEniCS.
- The ANN expression is then used within the FEniCS framework for numerical prediction of the displacement fields.
- For the first time, ANN-based and stretch based hyperelastic models (e.g., Ogden model) are implemented in native FEniCS.

INTRODUCTION

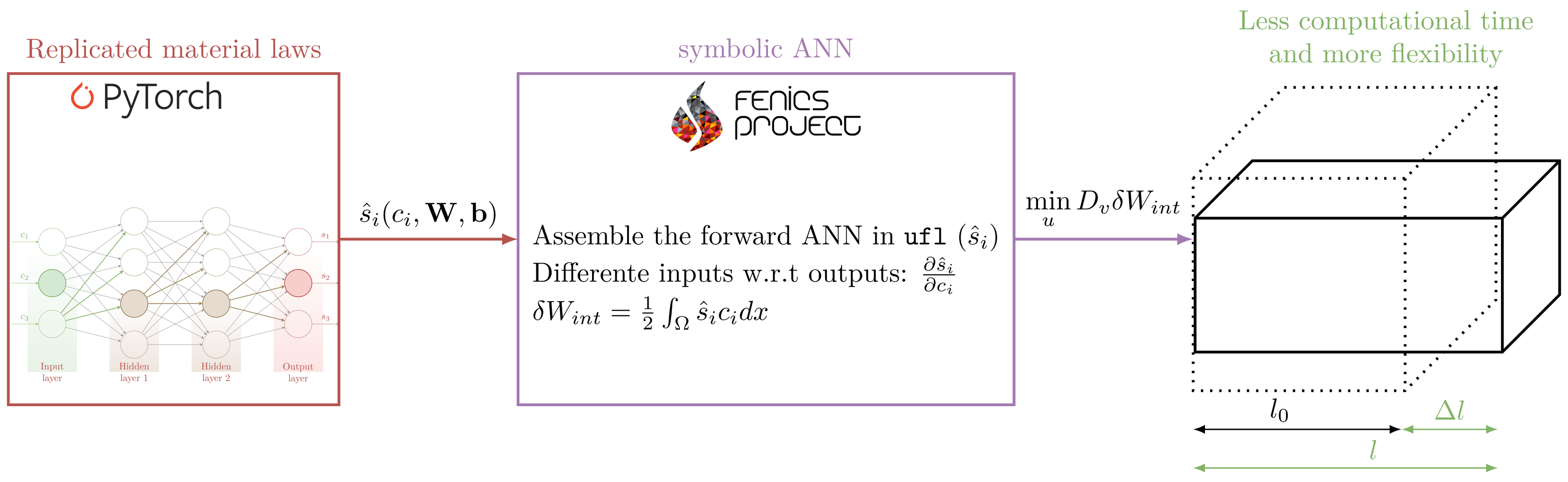
This work focuses on developing a framework for modelling the behaviours of advanced materials using symbolic representations of ANN inside the FEniCS framework [1] providing a flexible and computationally efficient data-driven toolchain for materials characterisation.



The concept of materials laws: material responses are unique with respect to applied loads. This relationship can be described using model-based constitutive equations or model-free ANNs.

HOW IT WORKS

The stretch-stress datasets are fed into the Pytorch framework [2] for training the ANN with suitable modifications of the loss function to ensure the physical constraints. Subsequently, the underlying symbolic version of the ANN is expressed in UFL and provided to FEniCS, such that the tangent operator can be obtained automatically. Finally, the computational results of the trained material laws are presented in terms of the deformation behaviour of arbitrary specimens of that same material subject to arbitrary boundary conditions (and load paths).



DATA COLLECTION

These synthetic training data are acquired from evaluation of randomised assumed deformation states at the material point, $\mathcal{N}(\mu,\,\sigma^2)$, from which the square of the principal stretch state ($\mathbf{c}$) is computed (as input) and the associated principal stress state ($\mathbf{s}$ as output) results from a known phenomenological material law.

$$\mathbf{F} = \mathbf{I} + \mathcal{N}(\mu,\,\sigma^2)$$ Deformation gradient

$$\mathbf{C} = \mathbf{F}^\top\mathbf{F},$$ Right Cauchy-Green strain tensor

$$\mathbf{C} = \sum_{i=1}^{3} c_i \mathbf{N}_i \otimes \mathbf{N}_i,$$ Spectral decomposition

$$\mathbf{c} = \{c_1, c_2, c_3\}.$$ Inputs vectors

$$\mathbf{S} = \sum_{i=1}^{3} s_i(\mathbf{c})\mathbf{n}_i \otimes \mathbf{n}_i = \sum_{i=1}^{3} s_i(c_1, c_2, c_3)\mathbf{N}_i \otimes \mathbf{N}_i.$$ Stress tensor (Isotropic case)

$$\mathbf{s} = \{s_1, s_2, s_3\}.$$ Outputs vectors

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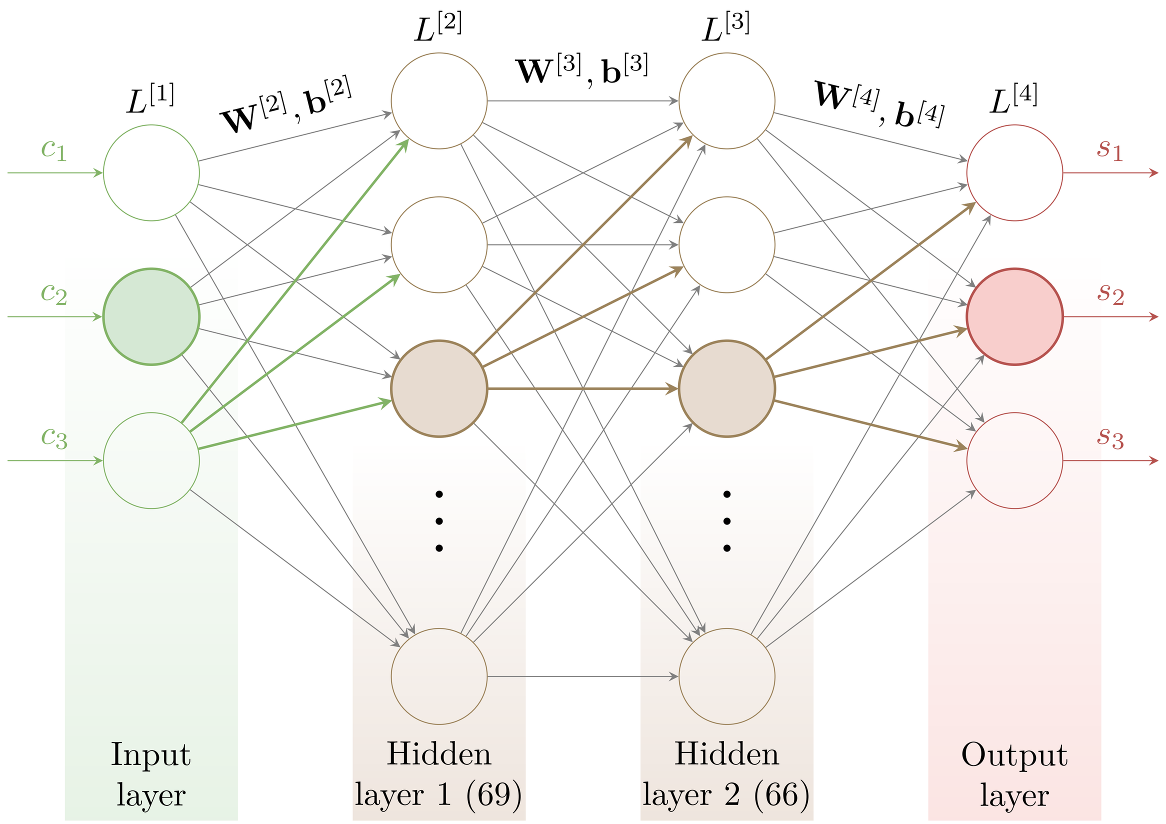
ANN ARCHITECTURE



The architecture of the ANN used as surrogate material law. It is optimized based on the strain-stress training dataset using the Optuna framework. Activation function: ***Swish****.*

Loss function:

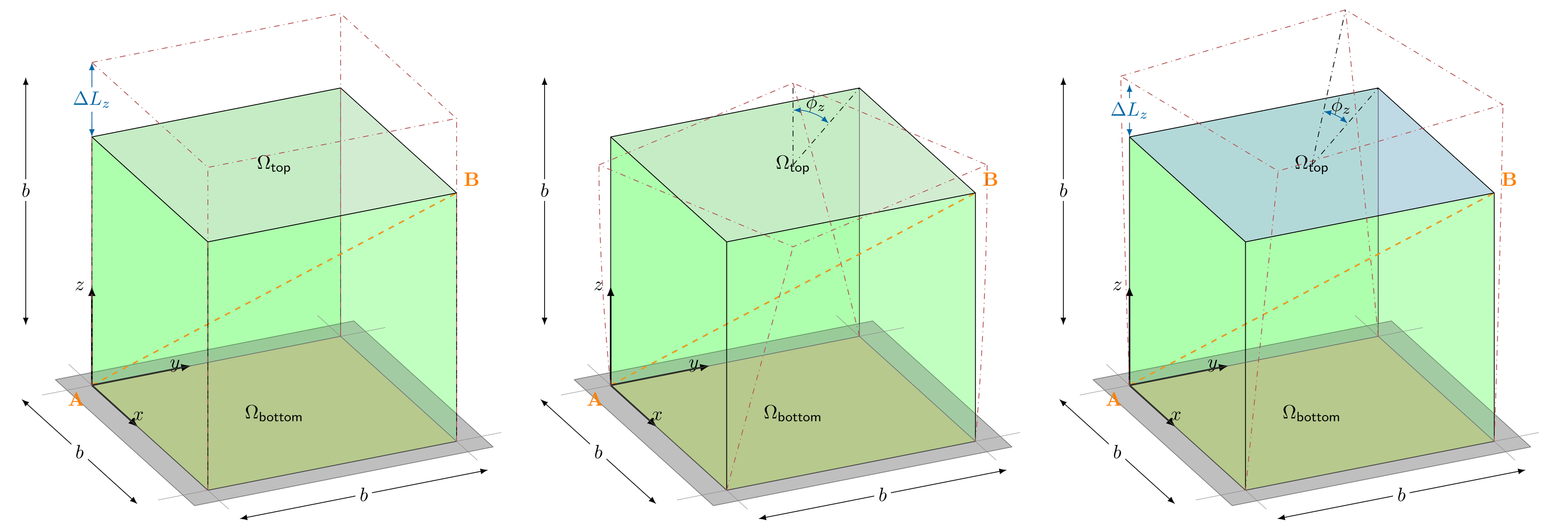
$$\mathcal{L}_{total} = \frac{1}{N}\sum_{i=1}^{N}\left(\left\|\mathbf{s}-\hat{\mathbf{s}}\right\|_2^2\right) + \alpha\left\|\mathbf{s}(\mathbf{c}=\mathbf{1}) - \hat{\mathbf{s}}(\mathbf{c}=\mathbf{1})\right\|_2^2,$$

where α is a tuneable weight of the physical constraint.

TEST CASES

We use the UFL version of ANN to predict numerically the mechanical response of a unit cuboid specimen subjected to 3 different tests: uniaxial extension, torsion, and combination of both uniaxial extension and torsion simultaneously. The performance of the data-driven model is measured using Mean Absolute Percentage Error (MAPE).

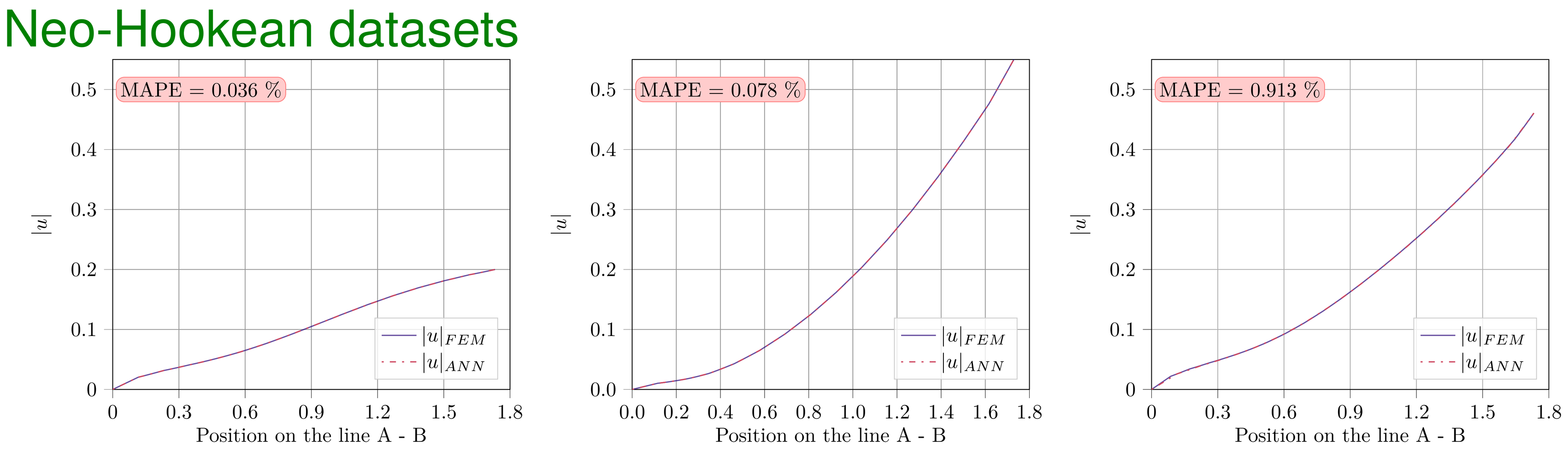
Geometry and boundary conditions



Case 1: Uniaxial extension *Case 2: Torsion* *Case 3: Combine both 1 & 2*

Dirichlet boundary conditions applied on the top of a unit cube specimen, and the bottom is fixed.

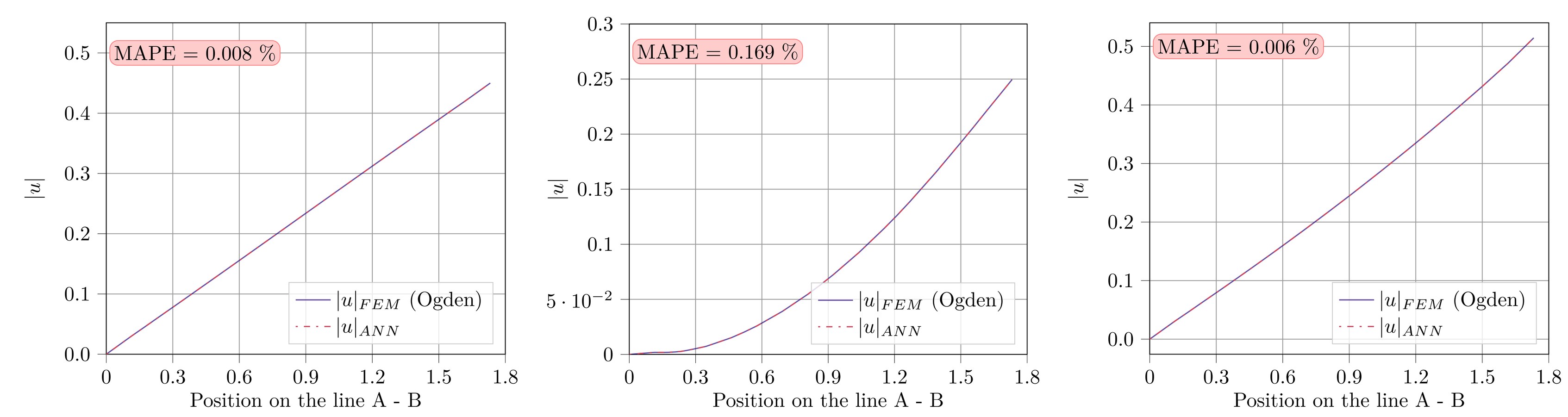
Neo-Hookean datasets



Case 1: Uniaxial extension *Case 2: Torsion* *Case 3: Combine both 1 & 2*

Comparison of the magnitude of displacements over line A - B between Neo-Hookean FEM and ANN-based material laws on the unit cube

Ogden [3] datasets



Case 1: Uniaxial extension *Case 2: Torsion* *Case 3: Combine both 1 & 2*

Comparison of the magnitude of displacements over line A - B between Ogden FEM and ANN-based material laws on the unit cube

SUPERVISORY TEAM

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[1] Anders Logg and Garth N. Wells. "DOLFIN: Automated Finite Element Computing". In: *ACM Trans. Math. Softw.* 37.2 (Apr. 2010), 20:1–20:28. ISSN: 0098-3500. DOI: 10.1145/1731022.1731030.

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