Data-driven Constitutive Modelling of Expanded Polystyrene Foams

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Agenda

- Background & Motivation
- Methodology
- Results & Discussion
- Conclusions & Outlook

Background & Motivation

Motivation

- EPS-foams are used for energy absorption in many applications
  - Packaging
  - Head protective gear
- Helmets are traditionally tested linearly
  - Compression dominated loading
  - Material models are calibrated using pure compression experiments
- More realistic scenarios is oblique impacts
  - Compression *and* shear
- The FEM-revolutions has not yet come to the head protective gear industry
  - Confidence in virtual experiments require good models
  - Limited by the lack of accurate prediction of mechanical response

Motivation

- Concurrently, many fields of science and engineering have started adopting ML-methods
- Artificial Neural Networks have shown some promise when it comes to capturing complex material behaviour
- Naive application of neural networks usually suffer from
  - Needs lots of data to generalise well
  - May result in non-physical behaviour
- Some researchers have proposed solutions to these two problems by through the architecture ensuring that the model obeys physical laws we hold to be true
- In this project I have applied such a machine learning model which satisfies many basic laws of material mechanics

Background

- In 2023 Linka & Kuhl proposed their machine learning framework for hyperelastic materials *Constitutive Artificial Neural Networks* (CANN)
- Neural network approximating the Helmholtz free energy as a function of invariants of $\boldsymbol{C}$
- A priori satisfaction of
  - Isotropy
  - Material symmetry
  - Stress free reference configuration
  - Thermodynamic consistency
  - Polyconvexity

$$\psi(\boldsymbol{C}) = \psi_1(\tilde{I}_1 - 3) + \psi_2(\tilde{I}_2 - 3) + \psi_3(I_3 - 1)$$

$$\boldsymbol{P} = 2\boldsymbol{F}\frac{\partial \psi}{\partial \boldsymbol{C}}$$

Background

- A priori satisfaction of
    - Isotropy
    - Material symmetry
    - Stress free reference configuration
    - Thermodynamic consistency
    - Polyconvexity
- Achieved by additive split so that the network is not fully connected and special activation functions, which preserve convexity properties
- Each $\psi_k : \mathbb{R} \to \mathbb{R}$ is
    - Convex
    - Non-negative
    - Zero at the origin

$$\psi(\boldsymbol{C}) = \psi_1(\tilde{\boldsymbol{I}}_1 - \mathbf{3}) + \psi_2(\tilde{\boldsymbol{I}}_2 - \mathbf{3}) + \psi_3(\boldsymbol{I}_3 - \mathbf{1})$$

$$\boldsymbol{P} = \mathbf{2}\boldsymbol{F}\frac{\partial \psi}{\partial \boldsymbol{C}}$$

Background

- Holthusen et al. extended the CANN framework to inelastic effects, through recurrent architecture (iCANN)
- Initially adapted for viscoelasticity, Holthusen et al. introduced a pseudo-potential governing the inelastic flow
- Multiplicative split of deformation tensor
- Subpotentials ψ_* designed according to CANN
- The pseudo potential g should satisfy
  - Convex
  - Non-negative
  - Zero at the origin

$$\psi(\bar{\boldsymbol{C}}_e, \boldsymbol{C}_i) = \psi_e(\bar{\boldsymbol{C}}_e) + \psi_i(\boldsymbol{C}_i)$$

$$\boldsymbol{S} = 2\boldsymbol{U}_i^{-1}\frac{\partial\psi}{\partial\bar{\boldsymbol{C}}_e}\boldsymbol{U}_i^{-1}$$

$$\bar{\boldsymbol{\Gamma}} = 2\bar{\boldsymbol{C}}_e\frac{\partial\psi}{\partial\bar{\boldsymbol{C}}_e} - 2\frac{\partial\psi}{\partial\boldsymbol{C}_i}\boldsymbol{C}_i$$

$$g(\bar{\boldsymbol{\Gamma}}) = g_1(I_1) + g_2(J_2) + g_3(J_3)$$

$$\dot{\boldsymbol{C}}_i = 2\boldsymbol{U}_i\frac{\partial g}{\partial\bar{\boldsymbol{\Gamma}}}\boldsymbol{U}_i$$

Background

- Boes et al. adapted the iCANN structure to plasticity
- Uses the pseudo-potential as a yield function $\Phi(\bar{\mathbf{\Gamma}}) = g(\bar{\mathbf{\Gamma}}) - 1$
- Newton iterations for plastic multiplier $\Delta\lambda$ inside the network structure to solve $\Phi = 0$ when needed

$$\psi(\bar{\boldsymbol{C}}_e, \boldsymbol{C}_i) = \psi_e(\bar{\boldsymbol{C}}_e) + \psi_e(\boldsymbol{C}_i)$$

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$$g(\bar{\mathbf{\Gamma}}) = g_1(I_1) + g_2(J_2) + g_3(J_3)$$

$$\bar{\boldsymbol{D}} = \frac{\partial\Phi}{\partial\bar{\mathbf{\Gamma}}}$$

$$\boldsymbol{C}_{i,n+1} = \boldsymbol{U}_{i,n}\exp(2\Delta\lambda\bar{\boldsymbol{D}})\boldsymbol{U}_{i,n}$$

Methodology

Network Architecture

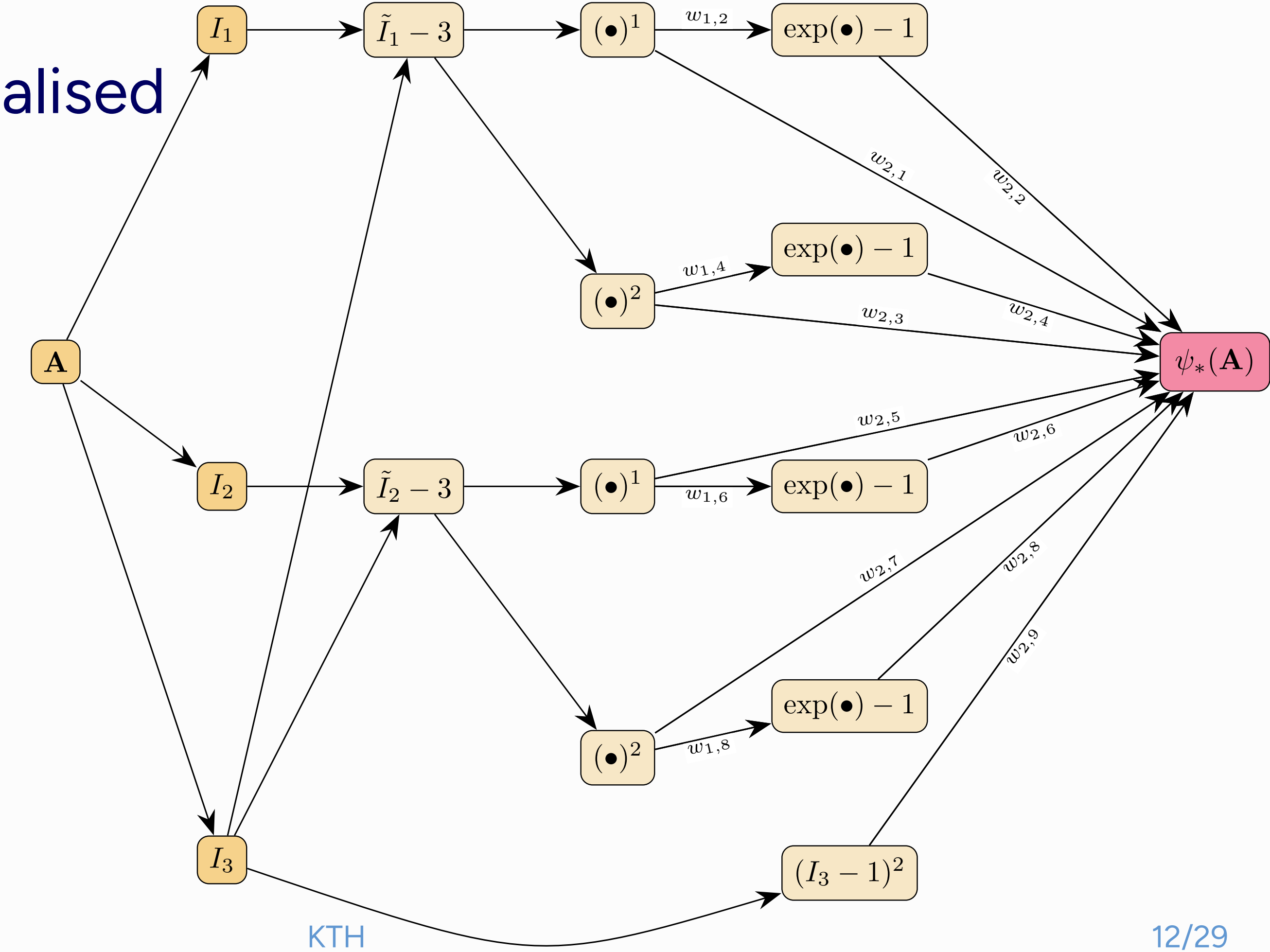
- Implementation of the associated plasticity iCANN by Boes et al.
- The construction of the pseudo-potential by Boes et al. and Holthusen et al. enforces symmetric yielding
- Introduction of arbitrary convex polynomial into the architecture enables asymmetric behaviour
- Corrected in order to preserve
    - $g(0) = 0$ and $g \geq 0$
    - $\left.\frac{\partial g}{\partial \bar{\Gamma}}\right|_{\bar{\Gamma}=0} = 0$

$$p(x) = \sum_{n=1}^{N} a_n (x + b_n)^{2n}$$

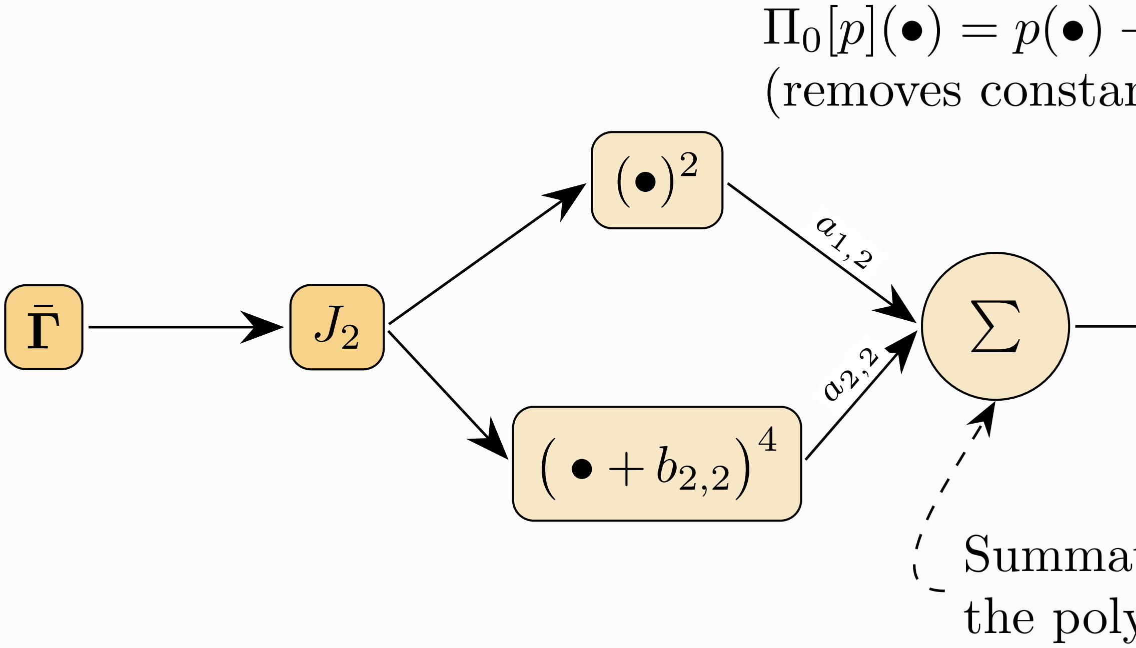
$$q(x) = p(x) - x p'(0) - p(0)$$

Network Visualised

Minor change to the volumetric term removes the condition that ensures $\psi \to \infty$ as $\det \boldsymbol{C} \to 0$.



Network Visualised



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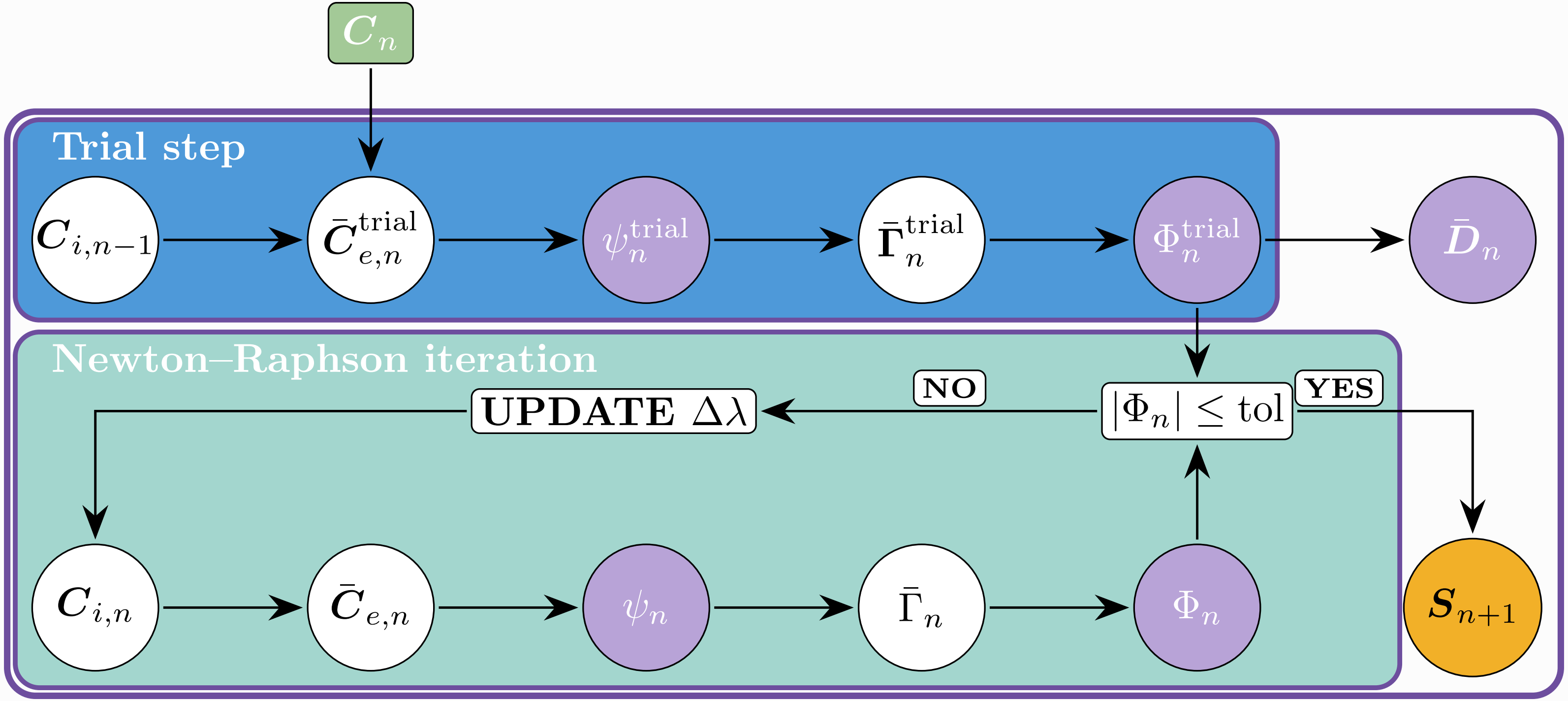
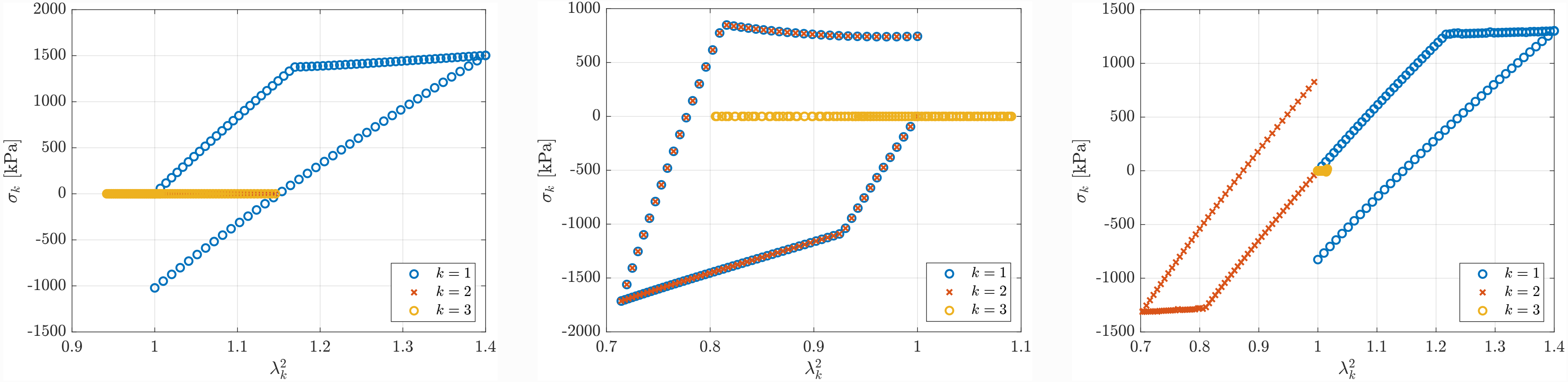
Network Visualised



Methodology

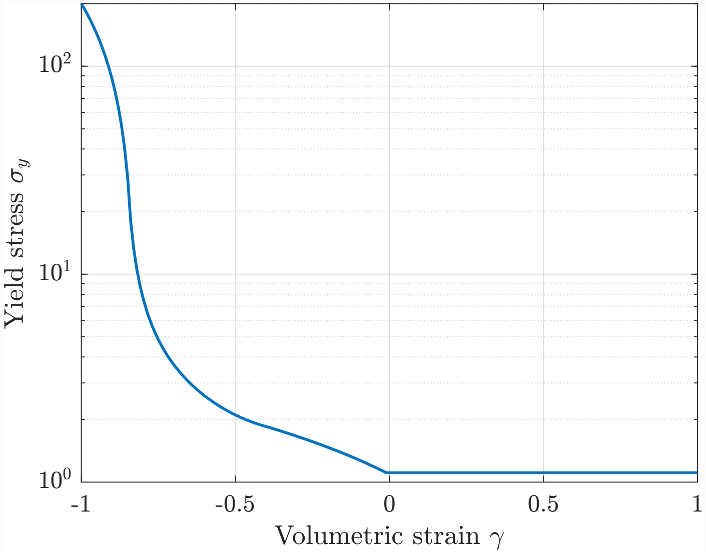
Artificial Data Generation

In order to demonstrate the expressiveness of the architecture data is generated using a dummy model with asymmetric yielding.



EPS-like Data Generation

- We investigate the suitability of the network architecture for EPS-foams, we try to reproduce behaviour in certain load cases from an existing model for EPS-foams. OpenRadioss' LAW33.
- No Poisson's effect and essentially independent flow along the principal stress directions, where the yield stress depends only on the volumetric strain.
- Typical yield curve supplied by Mips



Results & Discussion

Reproduction of Dummy Model

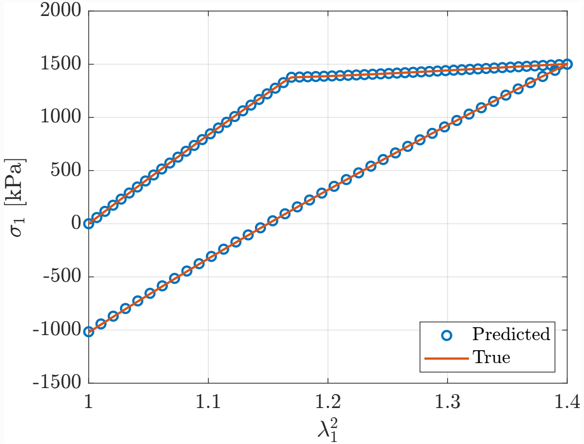
- Through sparsity promoting regularisation, the correct parameters were identified to be non-zero
- Notice that there is systematic underestimation of the parameters
- This is a result of the regularisation incentivising smaller parameter values

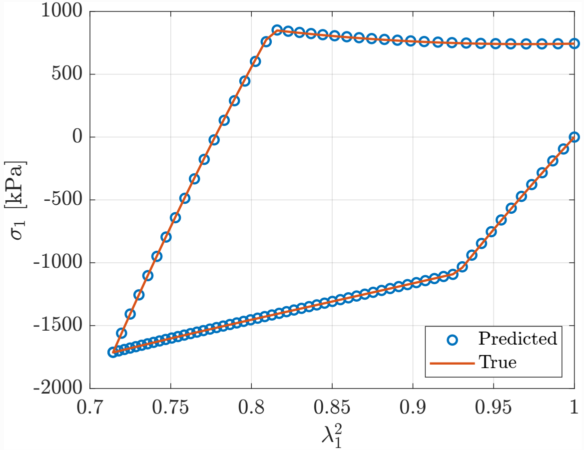
Table: Learned weights for the Helmholtz free energy on artificial data.

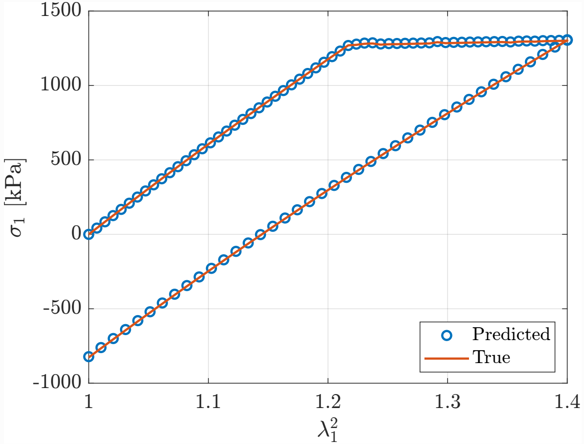
	Value	True Value	Unit
$w^e_{2,1}$	6244.23	6250	kPa
$w^e_{9,1}$	6195.94	6250	kPa
$w^i_{2,1}$	201.75	208.333	kPa
$w^i_{9,1}$	202.14	208.333	kPa
$a_{2,1}$	0.06228	0.0625	MPa^{-4}
$b_{2,1}$	399.63	400	kPa
$w_{1,2}$	0.09244	0.09375	MPa^{-4}

Reproduction of Dummy Model

Excellent agreement with the true data

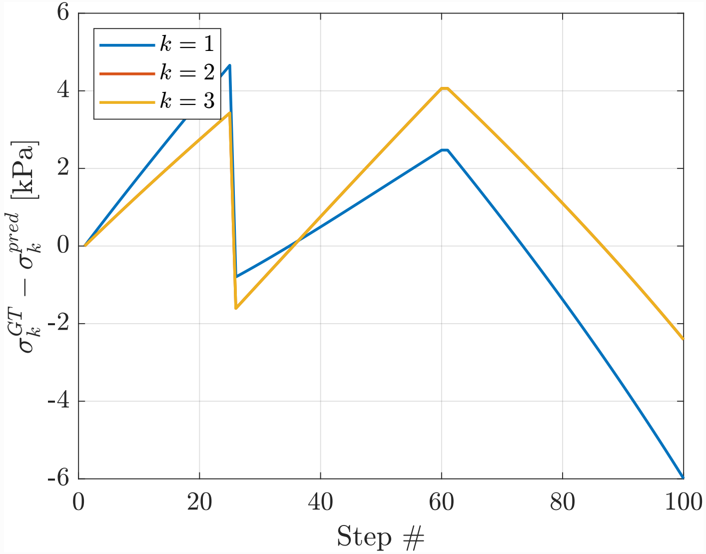


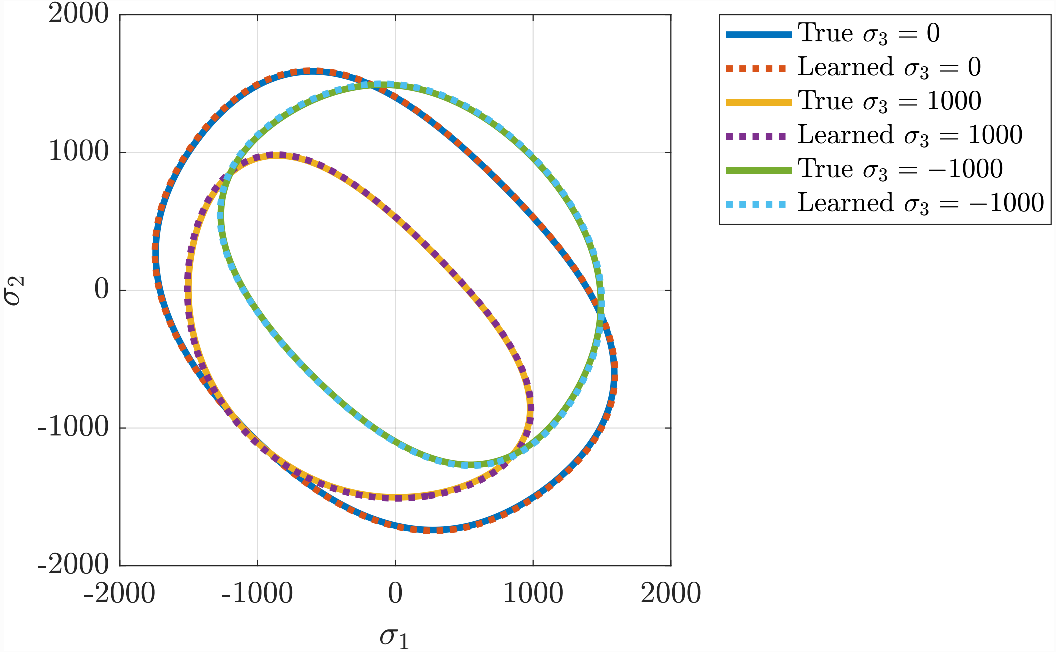




Reproduction of Dummy Model

Effect of parameter underestimation

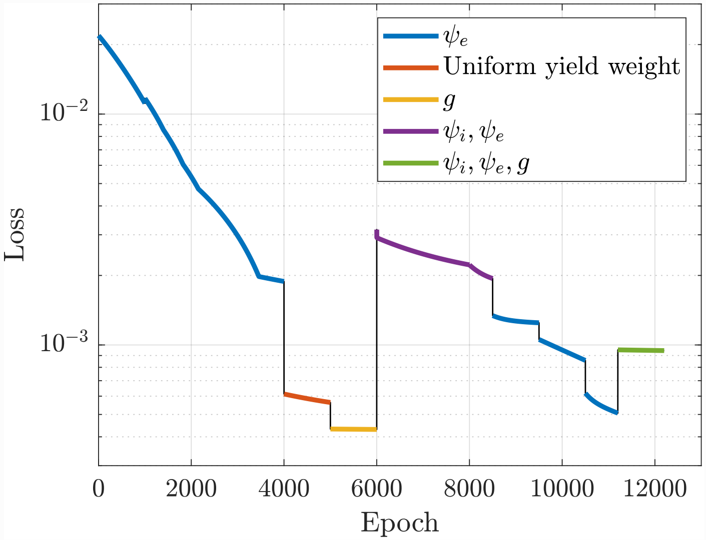




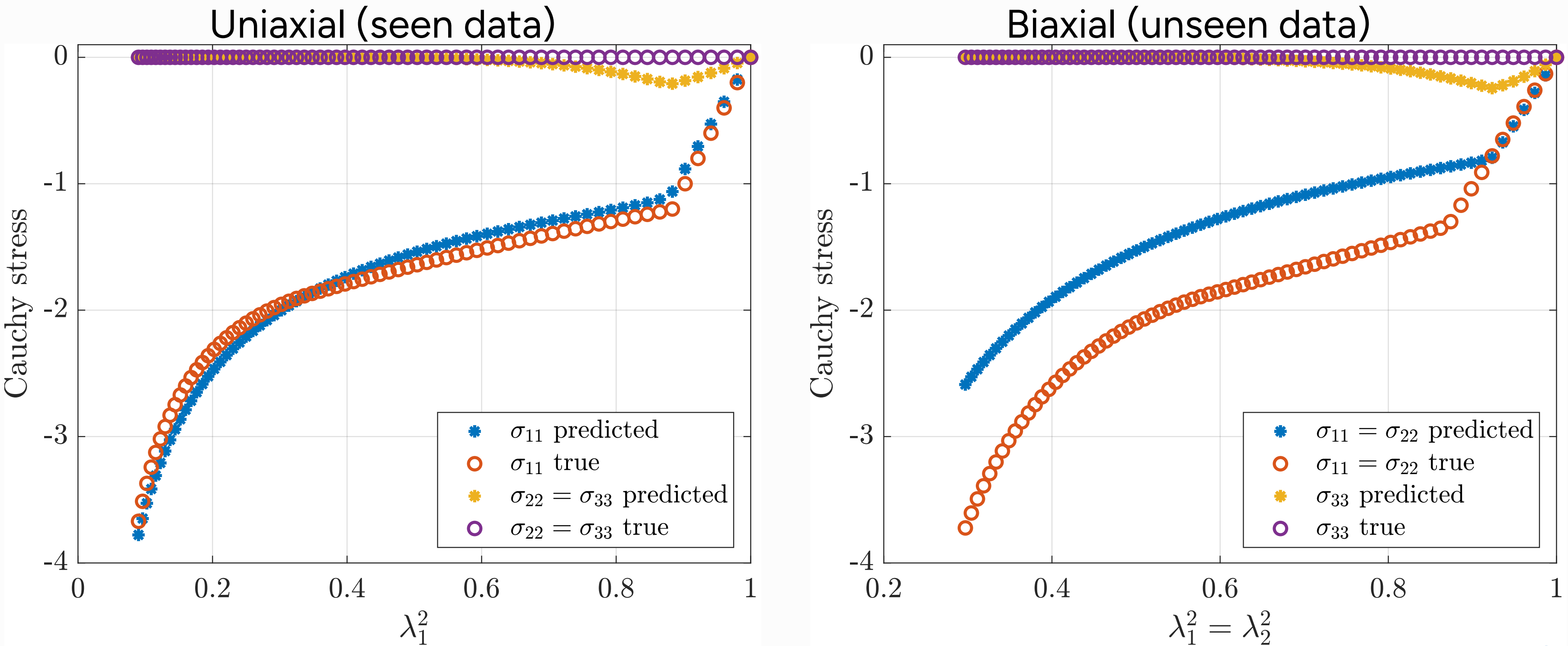
Results & Discussion

Training on Foam-like Data

- Numerical issues with stability etc. lead to a modified training regimen
- Training only on uniaxial data
- No regularisation on the pseudo-potential as it would always lead to inelastic inactivation
- Staged training with only a few networks active at a time, with different amount of data



Results on Foam-like Data



Results & Discussion

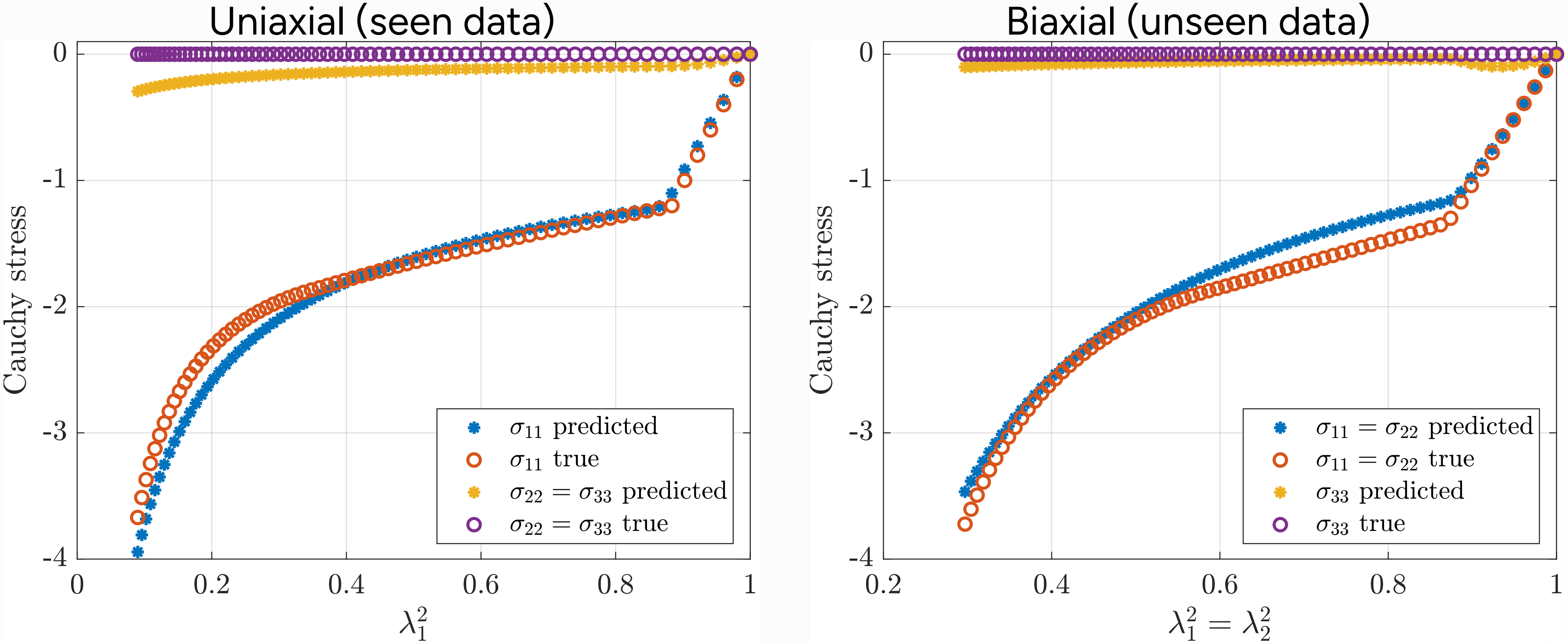
Foam-like Data – Modified model

- LAW33 has independent plastic flow along each principal stress direction
- This is tough to achieve when expressed using the invariants
- Thus, a modified pseudo-potential was tried

$$g(\bar{\boldsymbol{\Gamma}}) = a\left[\gamma_1^{16} + \gamma_2^{16} + \gamma_3^{16}\right]^{1/16}$$

- This makes the yield surface into what is essentially a cube with rounded corners in the principal stress space

Results on Foam-like Data – Modified model



From Learned Model to FEM-implementation

- In order to facilitate the use of learned iCANN models in FEA-software, a procedure for porting the model into Fortran was devised
- Python script exports the learned parameters to a Fortran module
- A second Fortran module builds the Helmholtz free energy and the pseudo potential from the model parameters
- A Fortran subroutine implements the material law by
    - Numerically differentiating the potentials ψ and g, and
    - Solving for the plastic multiplier using the secant method
- By importing the iCANN subroutine, the learned model is easily implemented for explicit computation in FEA-software like LS-Dyna and OpenRadioss, simply `call piCANN_mat_model(C, history, sigma, nElem)` in each time step

Conclusions & Outlook

Conclusions

- A minimal extension to the existing iCANN framework was proposed, enabling asymmetric yielding behaviour
- Numerical issues and unstable training process limited the training to be done on one time-series at a time
- Despite this, the performance of the model is good on the uniaxial test, and the hardening behaviour in the biaxial case is fairly similar, ignoring the early yield
- The cube-like yield surface improves the performance on the biaxial data as the cube is the largest possible yield surface uniaxial yield stress and flow direction has been prescribed

Outlook

- Future work on machine learning models for EPS foams should carefully consider which phenomena are needed to capture
- In order to capture the rate effects displayed by EPS foams under high-speed impacts, a viscoelastic iCANN should be considered
- A viscoelastic formulation might also be numerically more stable, as the yield condition $\Phi = 0$ is a discrete check, and the Newton-Raphson loop leads to complicated gradient computation
- If using an elastoplastic model, non-associated flow should be attempted, this however would reduce the robustness of the learned model and increase the data requirements as inferring a surface from only points is harder than inferring it from points and normals

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