Data-driven constitutive modelling

learning from Material Testing 2.0

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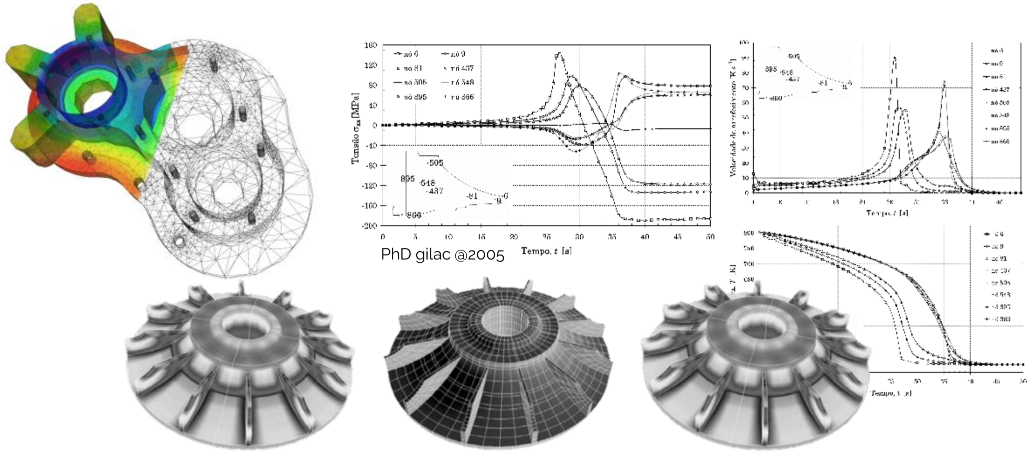
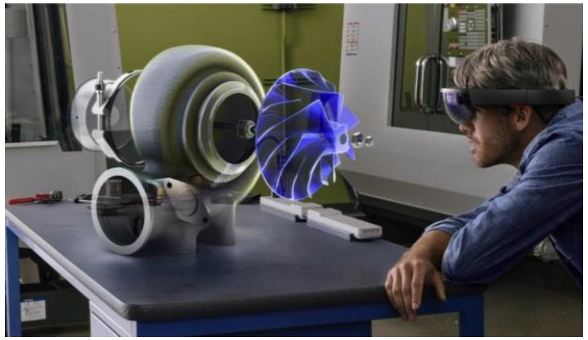
VForm-xSteels

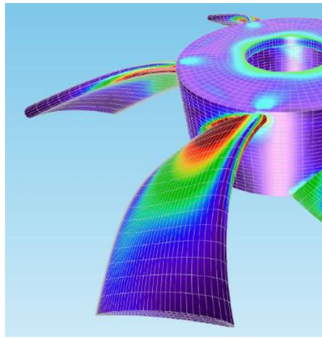
This project has received funding from the Research Fund for Coal and Steel under grant agreement No 888153

Introduction

- FEA modelling for predictive purposes;







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Introduction

- FEA modelling for predictive purposes;
- Material behaviour is generally made using differential constitutive equations;

Explicit formulation

$$\mathbf{Z}(t) = \mathbf{H}(\mathbf{x}, t)$$

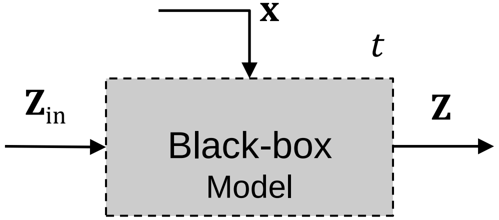
Observed/measurable variables

Differential formulation

$$\mathbf{Z}(t) = \mathbf{G}(\mathbf{Y}, \mathbf{x}, t)$$

$$\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}t} = \mathbf{F}(\mathbf{Z}_{\mathrm{in}}, \mathbf{Y}, \mathbf{x}, t) \quad \text{with} \quad \mathbf{Y}(t_0) = \mathbf{Y}_0$$

Black-box formulation



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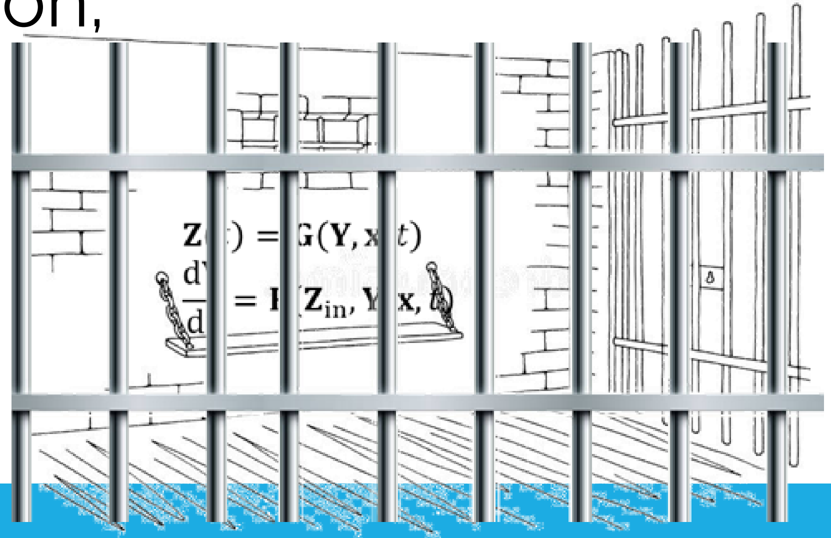
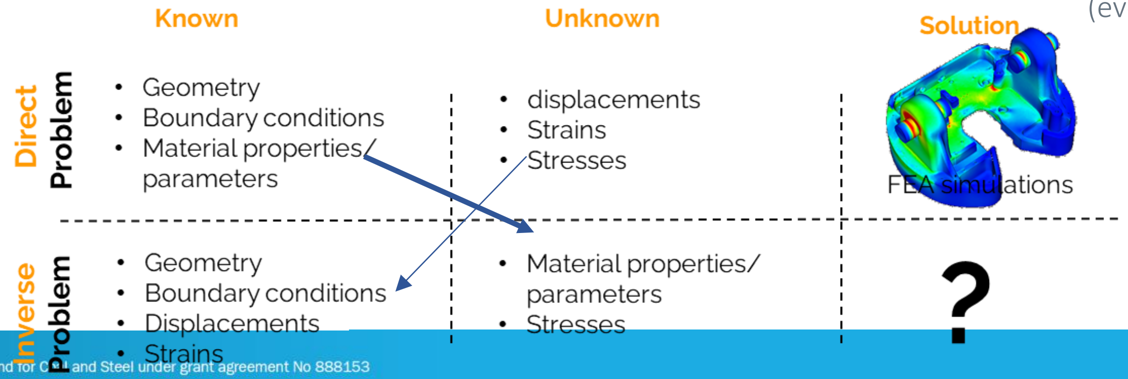


Introduction

- FEA modelling for predictive purposes;
- Material behaviour is generally made using differential constitutive equations;
- These models are constrained by their mathematical formulation;
- These models require painful calibration;

(even using dedicated software)



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Introduction

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Challenges for successful (precise) modelling?

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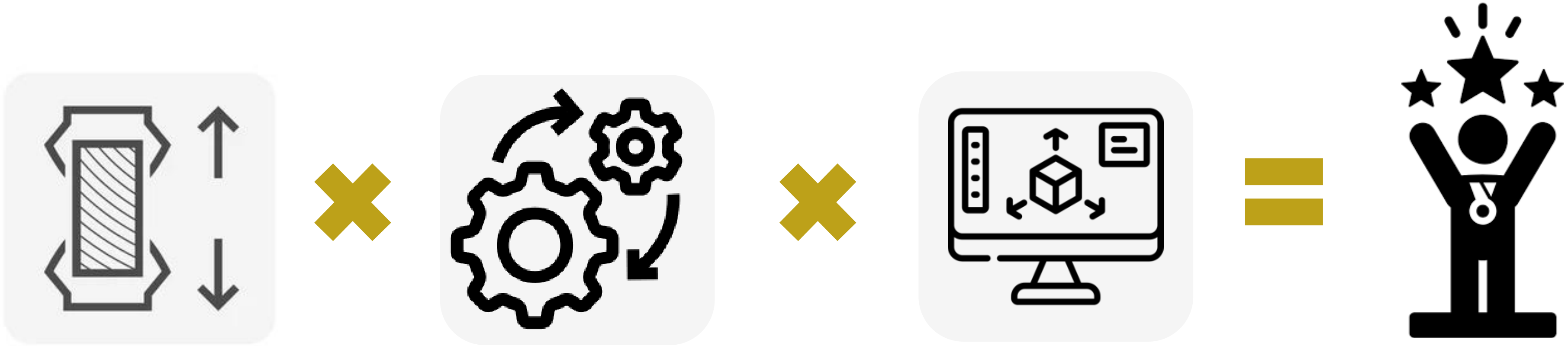
Introduction: success of the material modelling

- Introduction
- Success of the material modelling



Quality/quantity of the reference (observ. experimental) × Inverse methodology (calibration process) × Constitutive model (formulation) = Success

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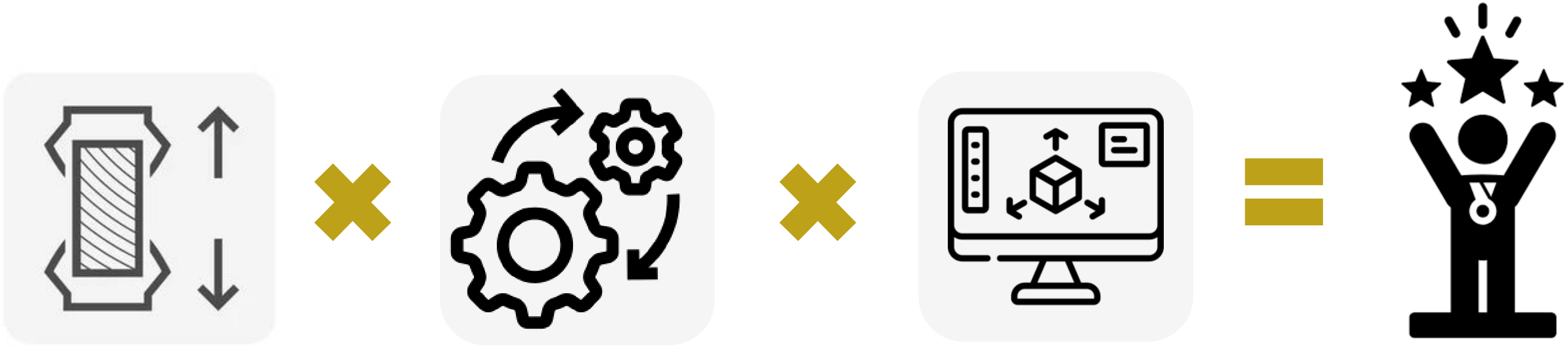
Introduction: can AI approaches contribute?



Quality/quantity of the reference (observ. experimental) | Inverse methodology (calibration process) | Constitutive model (formulation) | Success

Challenges for AI in material modelling?

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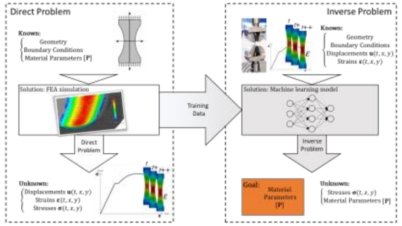
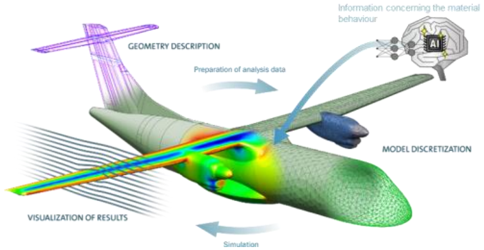
Opportunities of ML in material modelling

VForm-xSteels

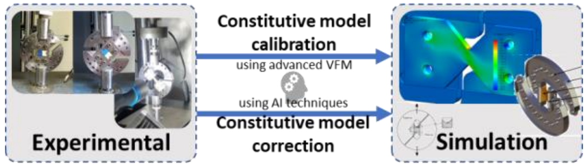
Parameter identification
create the inverse model



Fully implicit ML material model
ML fully replaces analytical models



Constitutive model corrector
enhancing known knowledge



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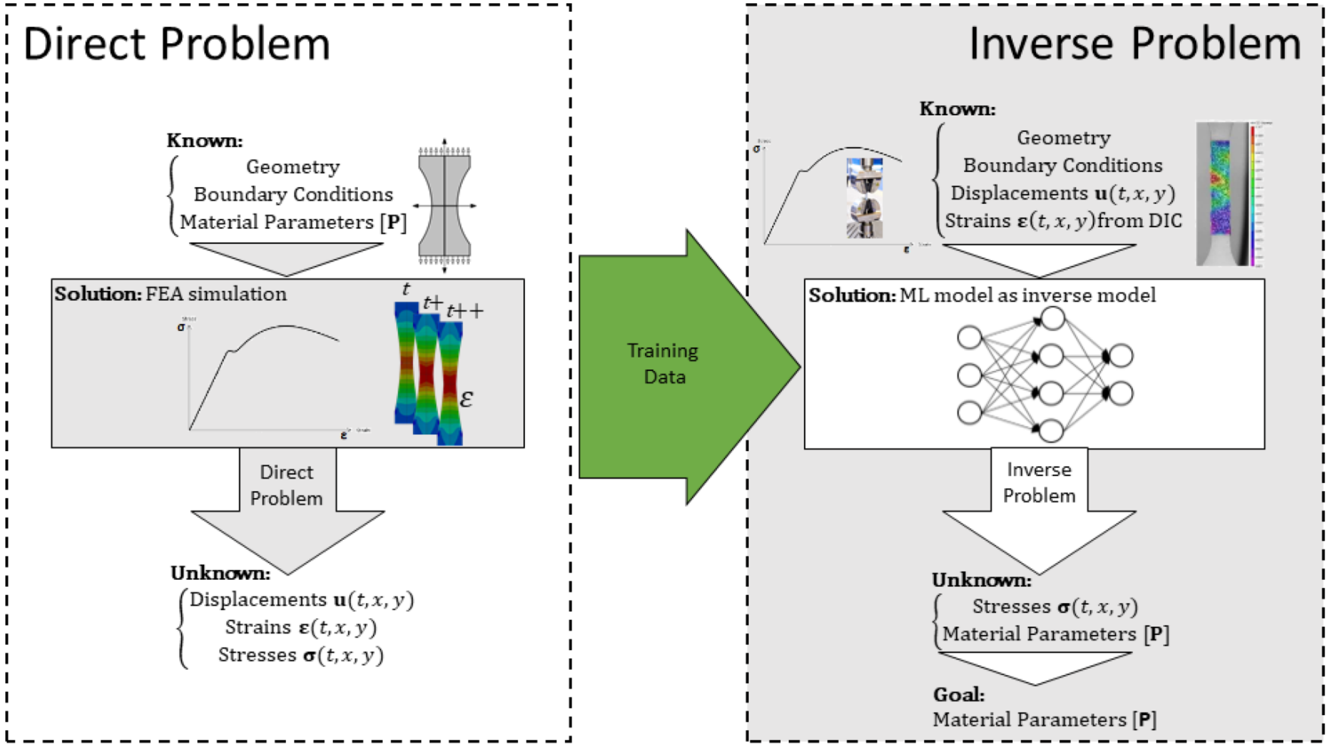
Opportunities of ML in material modelling

- Parameter identification: create the inverse model



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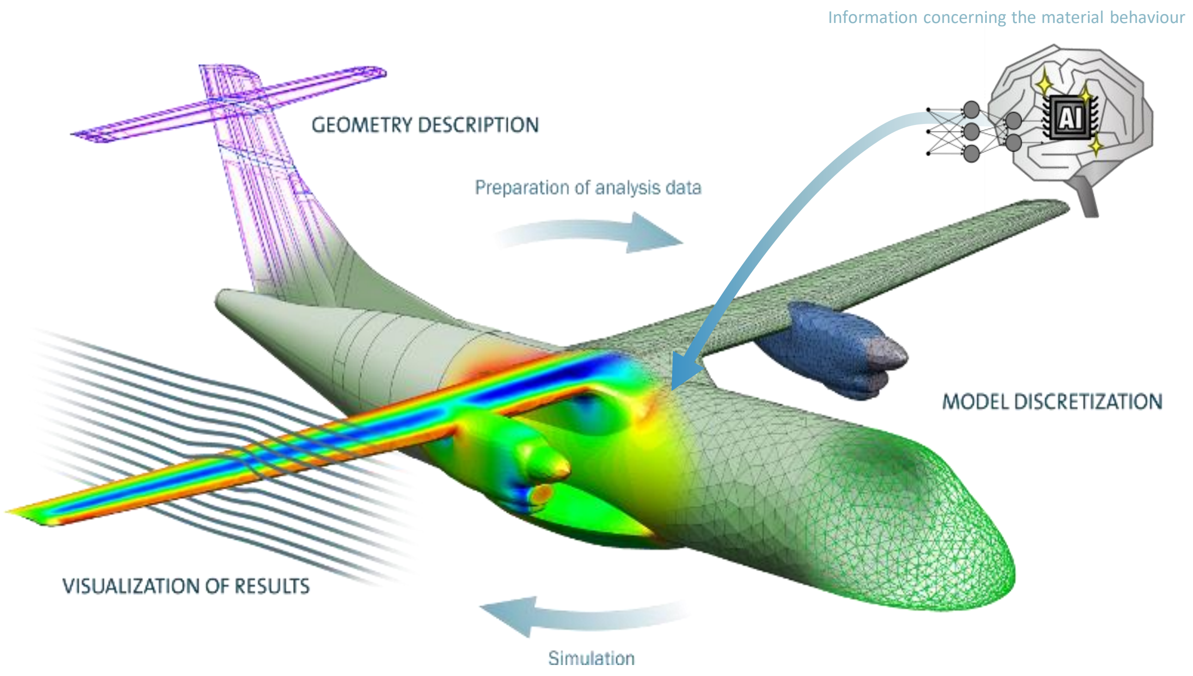
Opportunities of ML in material modelling

- Fully implicit ML material model: ML fully replaces analytical models



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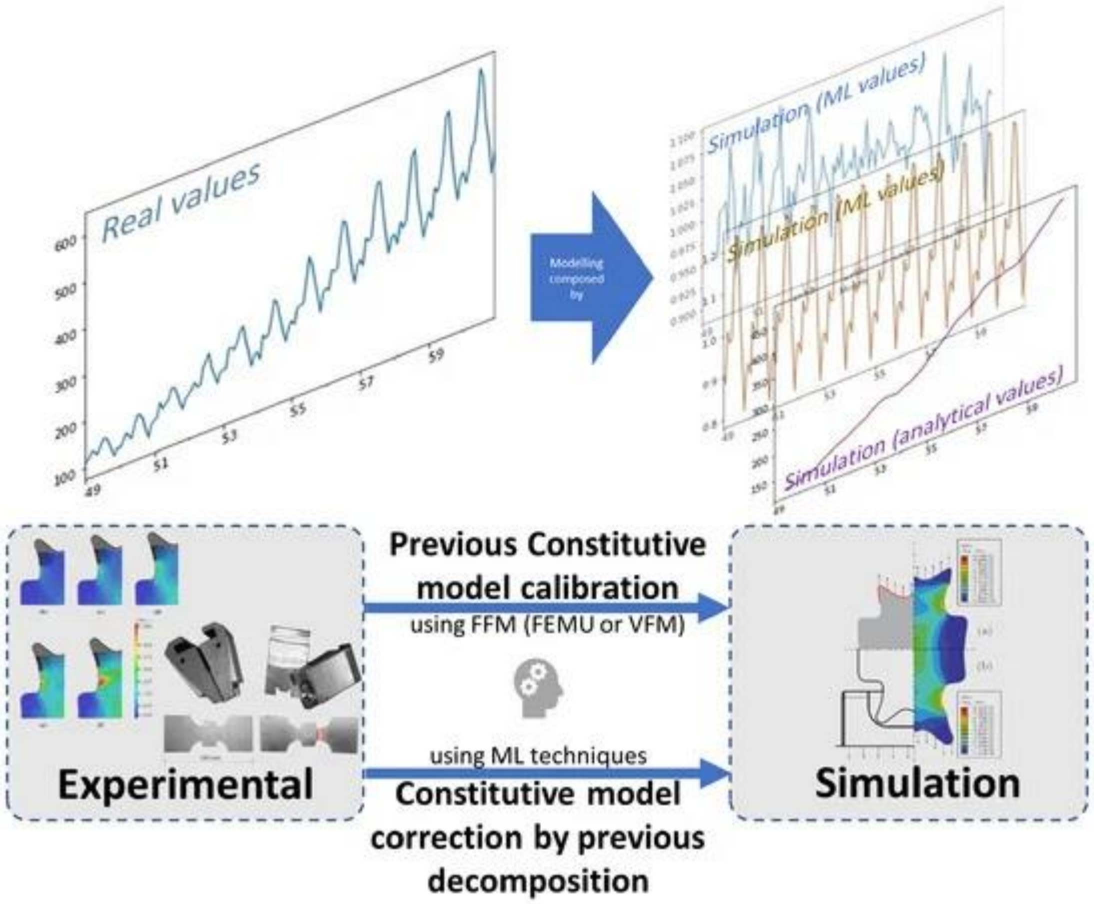
Opportunities of ML in material modelling

- Constitutive model corrector: enhancing known knowledge



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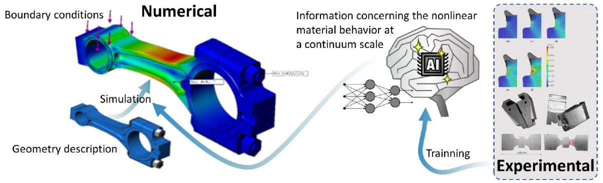
Data-driven material model

Fully implicit ML material model:

Can a ML fully replace analytical models?



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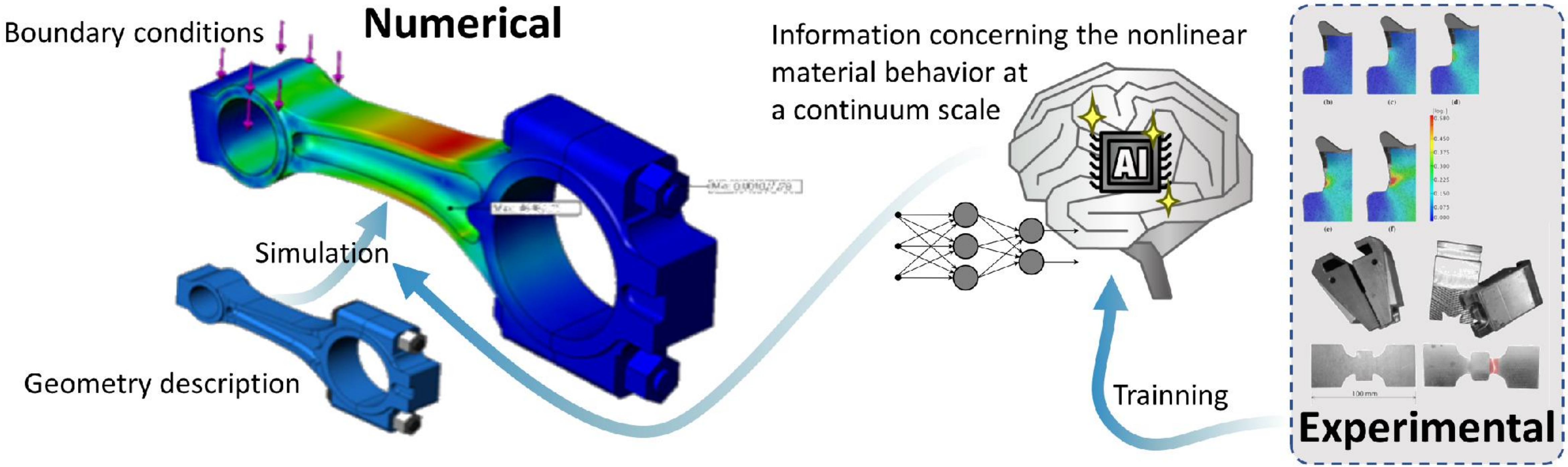
ML fully replaces analytical models

Non-constrained by their mathematical formulation



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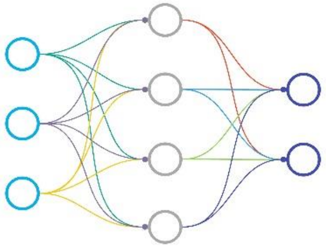
Material models: are data-driven models the solution?

Hybrid models

Flexibility dealing larger volumes of information

Hybrid models enhance/correct well-known existing models



$$\sigma = E(\varepsilon^{t} - \varepsilon^{vp})$$

$$\dot{\varepsilon}^{vp} = \left(\frac{|\sigma - \chi| - R}{K}\right) \cdot sgn(\sigma - \chi)$$

$$\dot{\chi} = H \cdot \dot{\varepsilon}^{vp} - D \cdot \chi |\dot{\varepsilon}^{vp}|$$

$$\dot{R} = h \cdot |\dot{\varepsilon}^{vp}| - d \cdot R |\dot{\varepsilon}^{vp}|$$

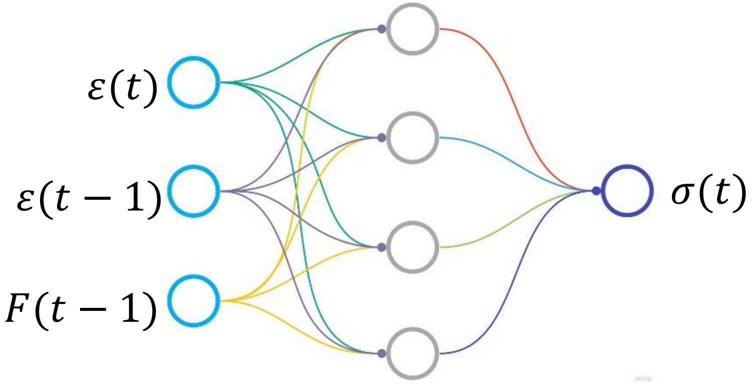
ANNs provide a radically different approach to the field:

- powerful function approximators
- implicitly learn constitutive relations from data
- no assumptions on mathematical formulation
- fast computation times

Implicit models

Neural networks partially/fully replace the material constitutive model

Predictions directly from data; no prior assumptions on yield criteria, hardening law, etc.



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ANNs: main issues in material modelling

- **Interpretability**:
  - ANNs are black-boxes:
    - ***How does the model arrive at such predictions?***
    - ***What's the relationship between the inputs and outputs?***
    - ***Does this relationship hold on a physical sense?***

- **Wide solution space**:
  - Large number of possible solutions
  - Spurious predictions that do not comply with fundamental physical laws
- **ANN and other ML models are hungry for data**:
  - A large set of data is generally required for a precise training
- **ANN are made for labelling data training**:
  - However, the output of a model is not an observable feature

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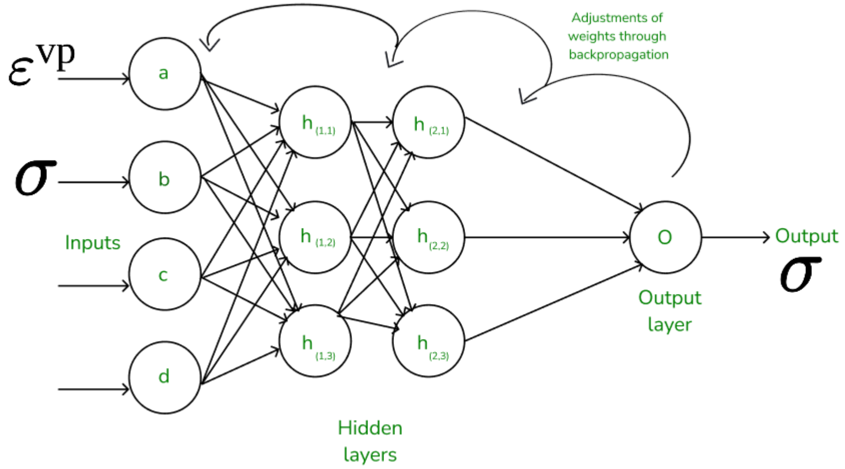
ANNs – main issues in material modelling

- The vast majority of the approaches documented in the literature for implicit (data-driven) constitutive modelling consists of feeding the ANN with paired data (usually, stress and strain) during the training process in order to assimilate the material behavior.



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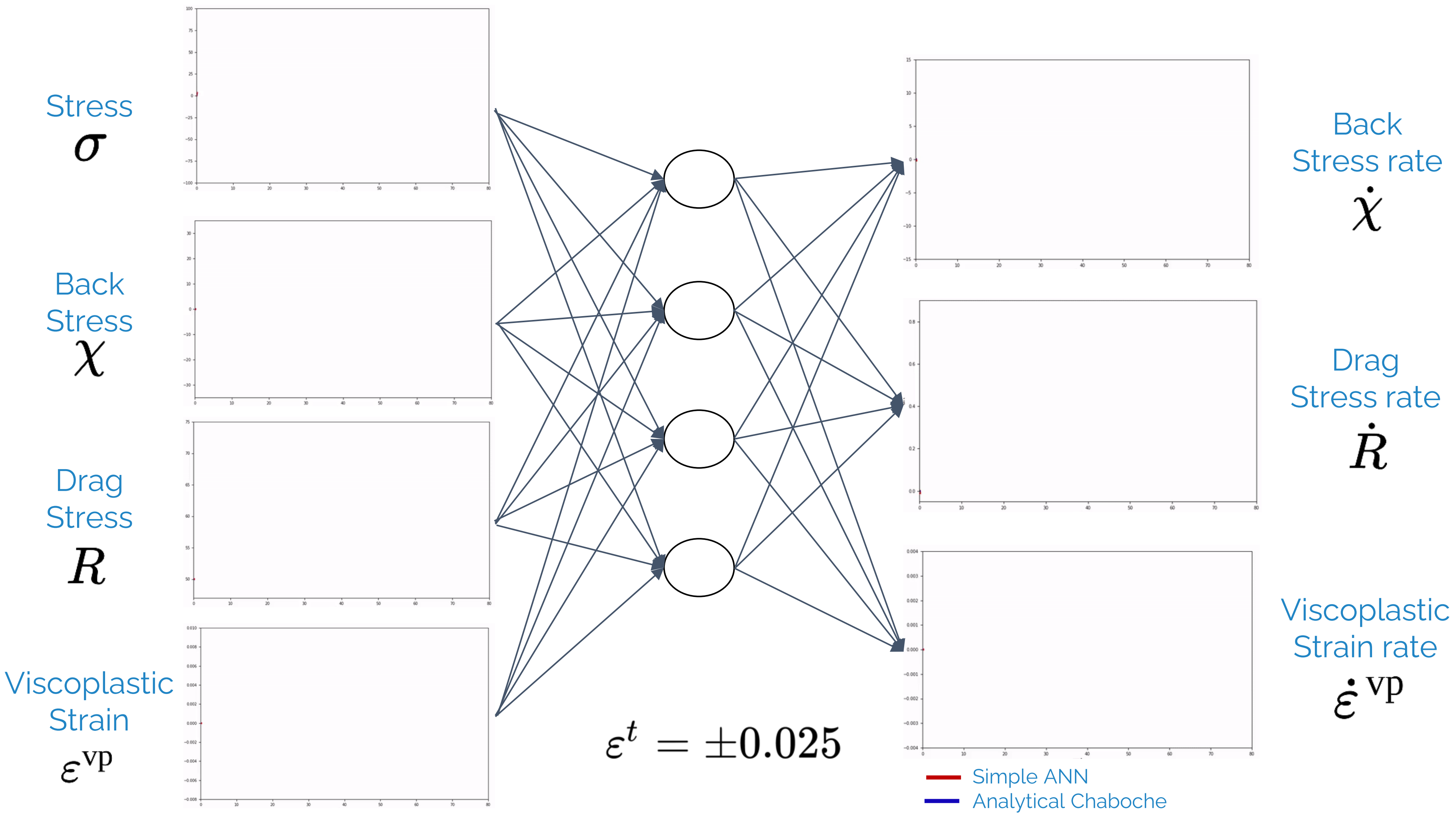
Feeding the ANN with paired labelled data



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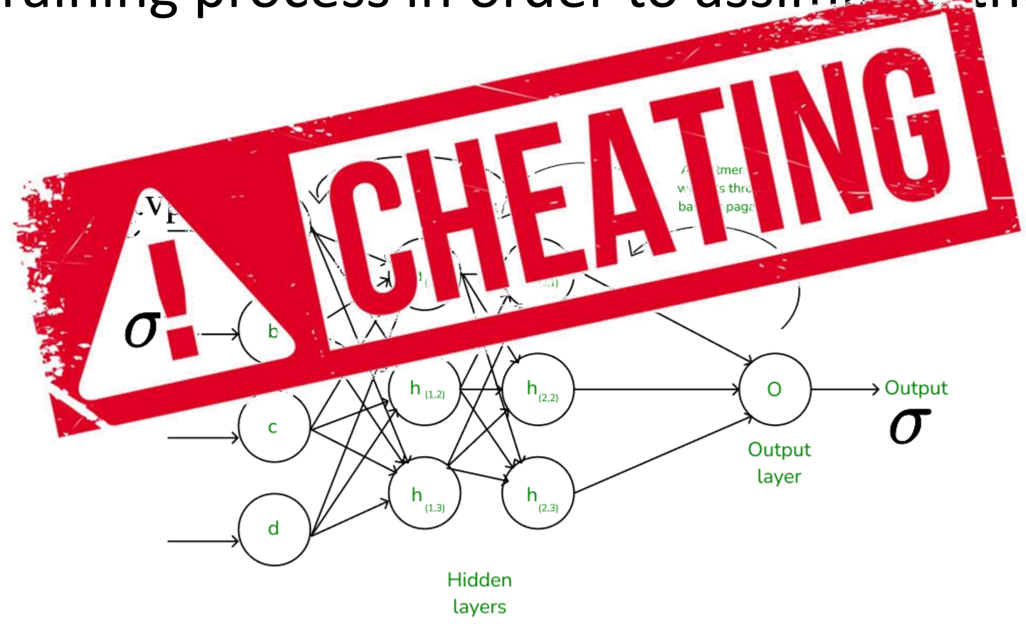

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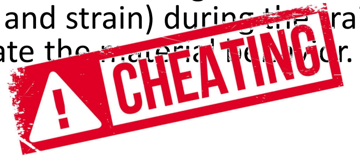
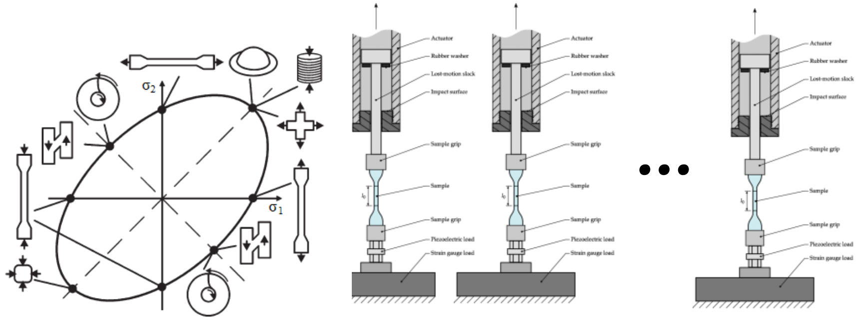
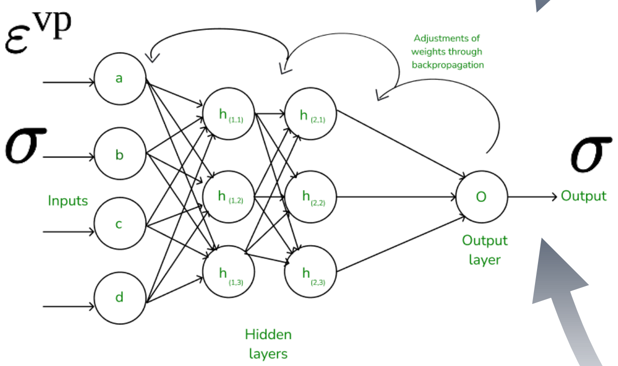
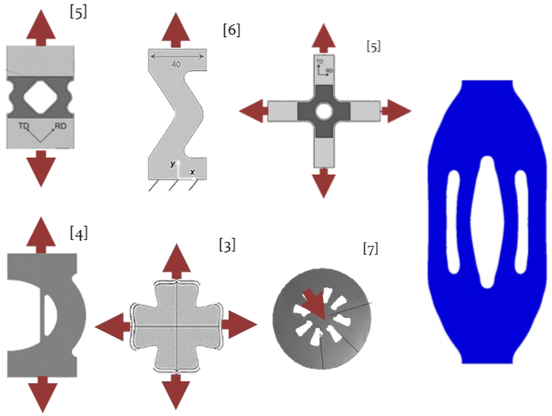




The process requires copious amounts of data, and obtaining comprehensive stress-strain relationships while relying on the standard simple mechanical tests poses a great challenge.





DIC technique can provide large amount of data, however, stress is not provided (the output of labelled data).

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Implicit data-driven constitutive modelling

Direct training

- Common approach in the literature
- Data numerically generated
- Labelled data pairs (stress-strain)
- **Easy to train** with a ground-truth value
- **Variables not always obtainable in a real experimental setting**

Indirect training

- Not widely used
- Numeric or full-field data
- Relies only on measurable data (e.g., displacements, global force)
- Variable to predict is indirectly obtained from measurable or intermediate variables
- **Harder to train**

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Solution: learning from Material testing 2.0

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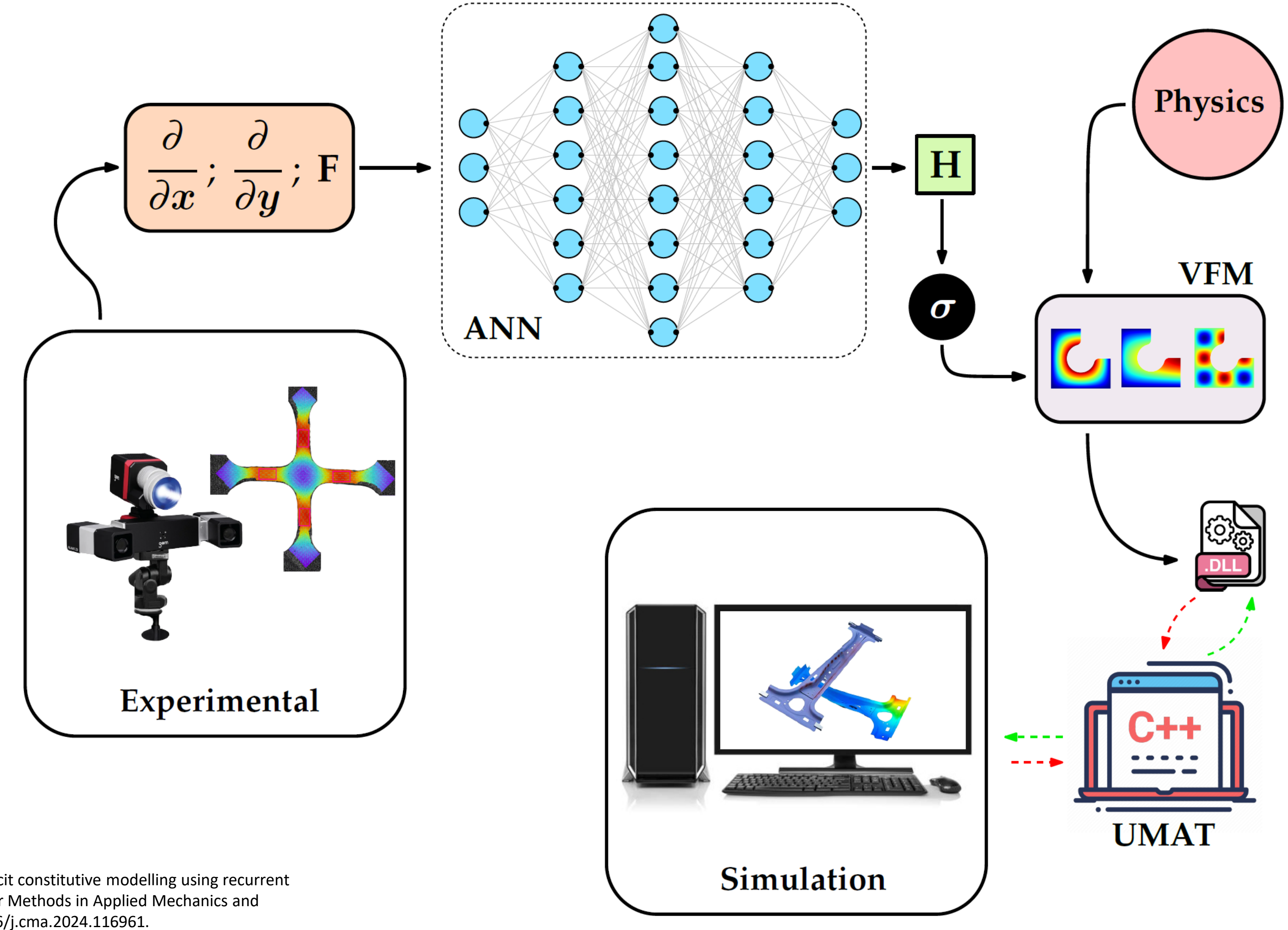
Implicit data-driven constitutive modelling



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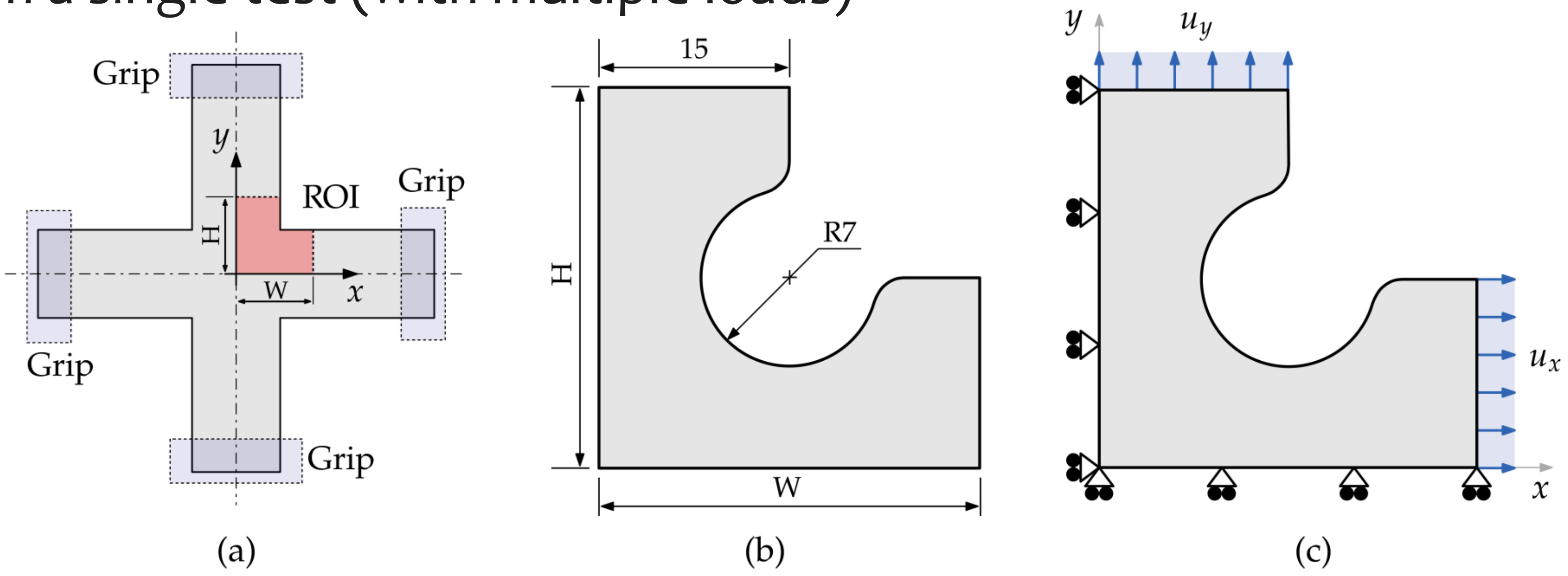
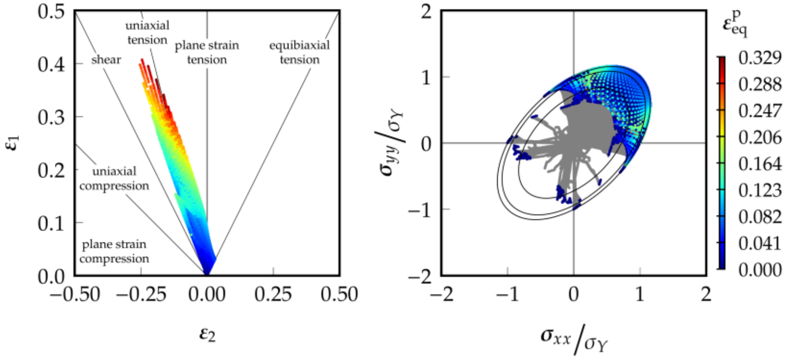
Learning curves

Learning from a single test (with multiple loads)





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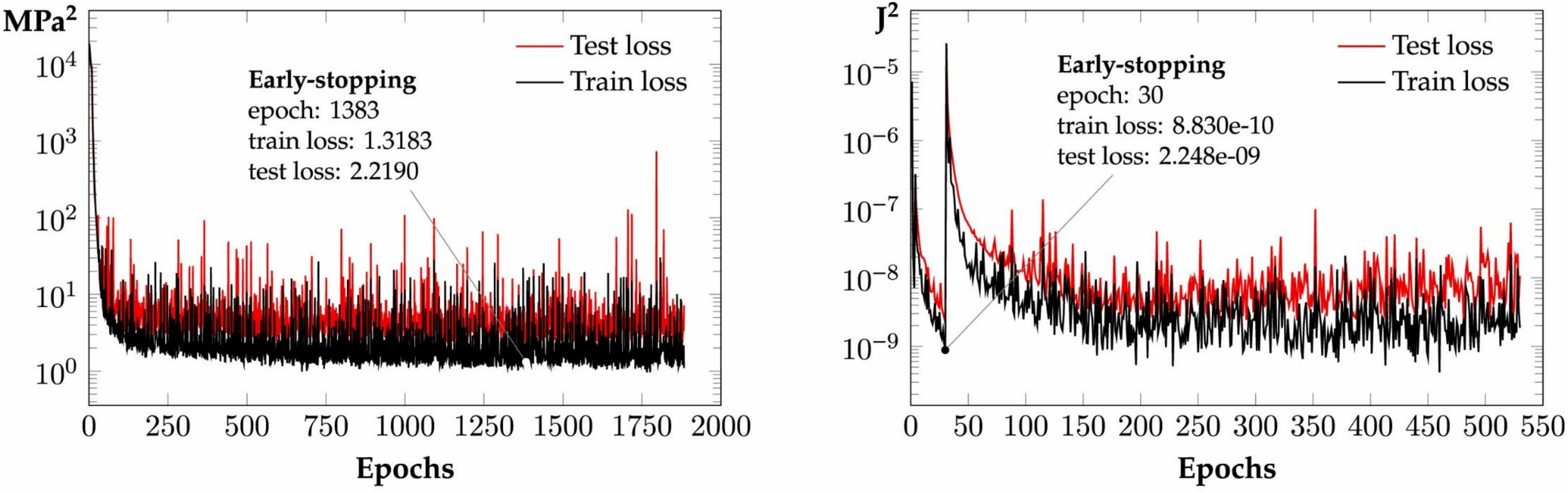
Learning curves

(a) the Dir-RNN model and

(b) the Ind-RNN model based on the VFM



(a) (b)

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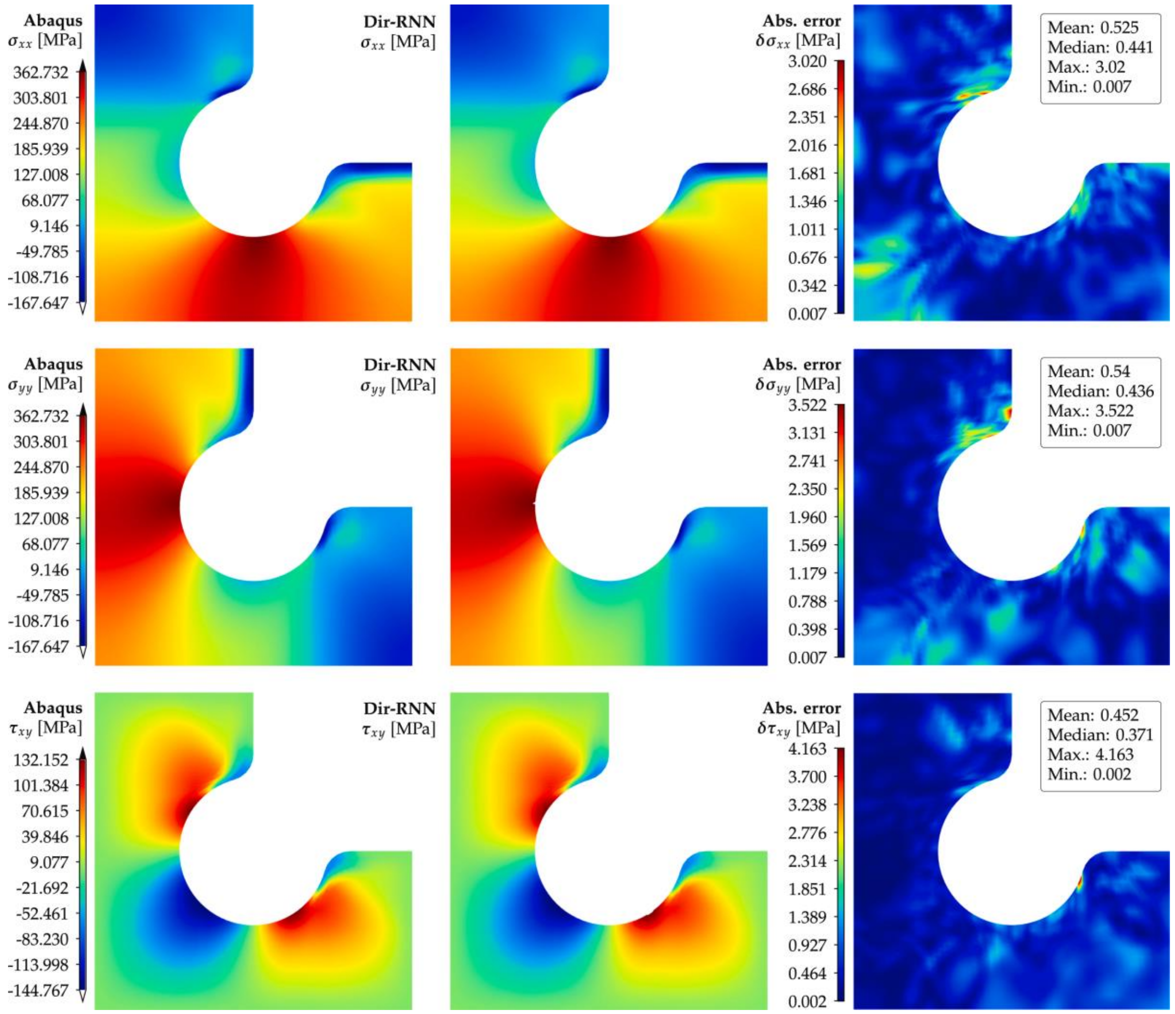
Implicit data-driven constitutive modelling

Results
u_x: 15 mm
u_y: 15 mm
last stage



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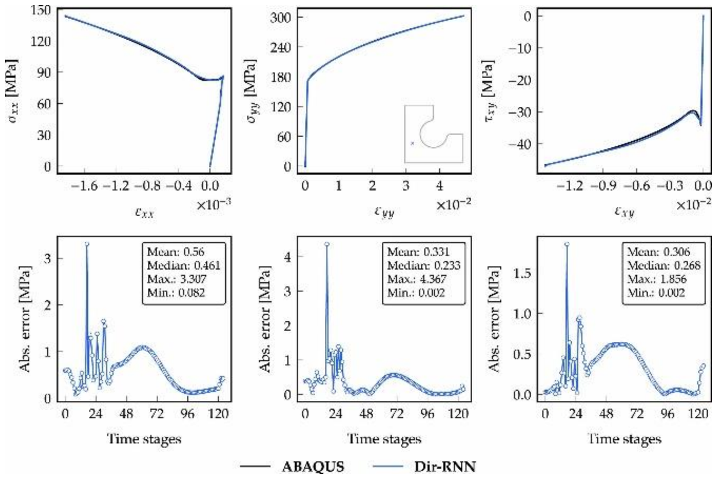
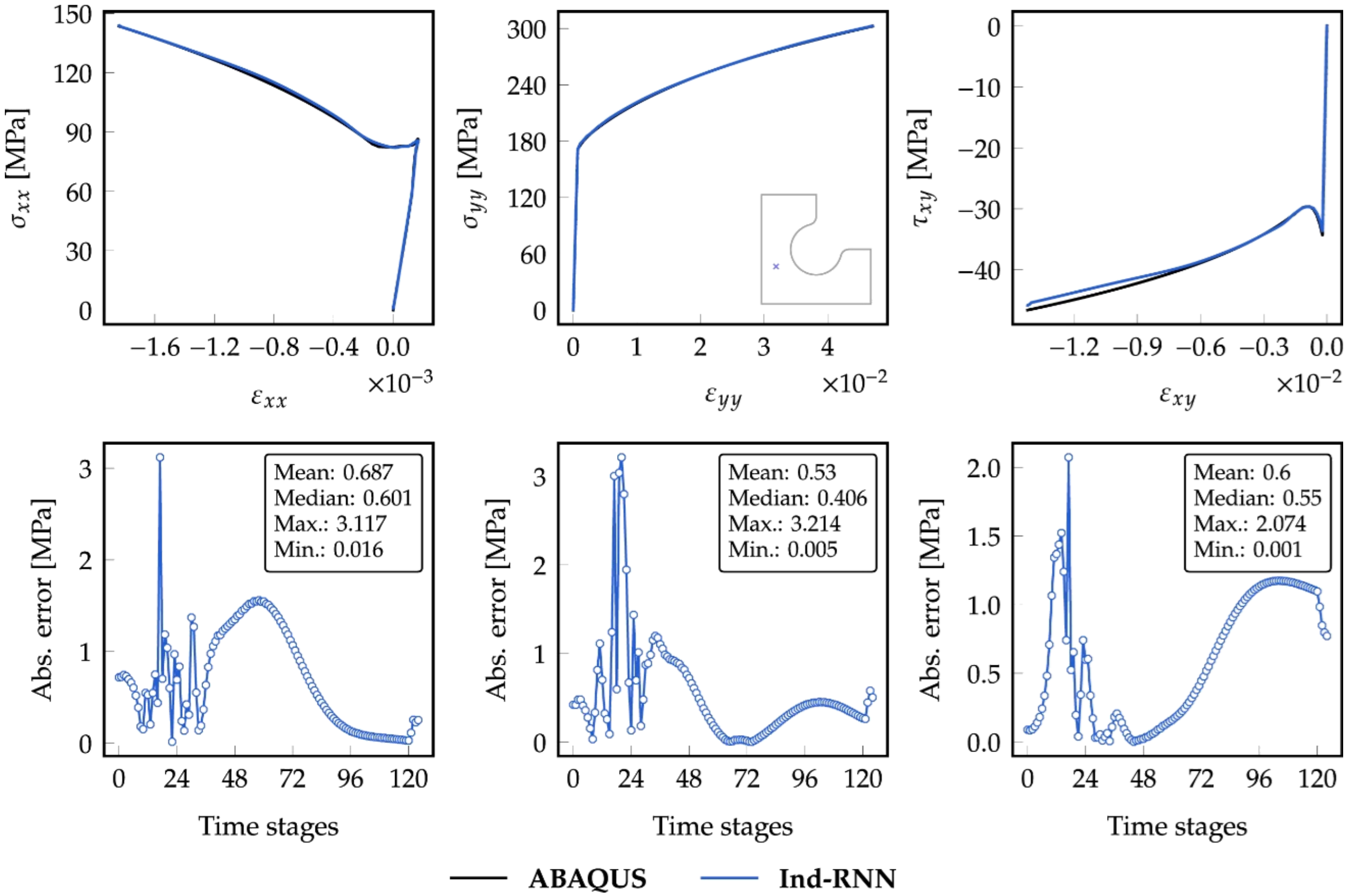
Direct training



Indirect training



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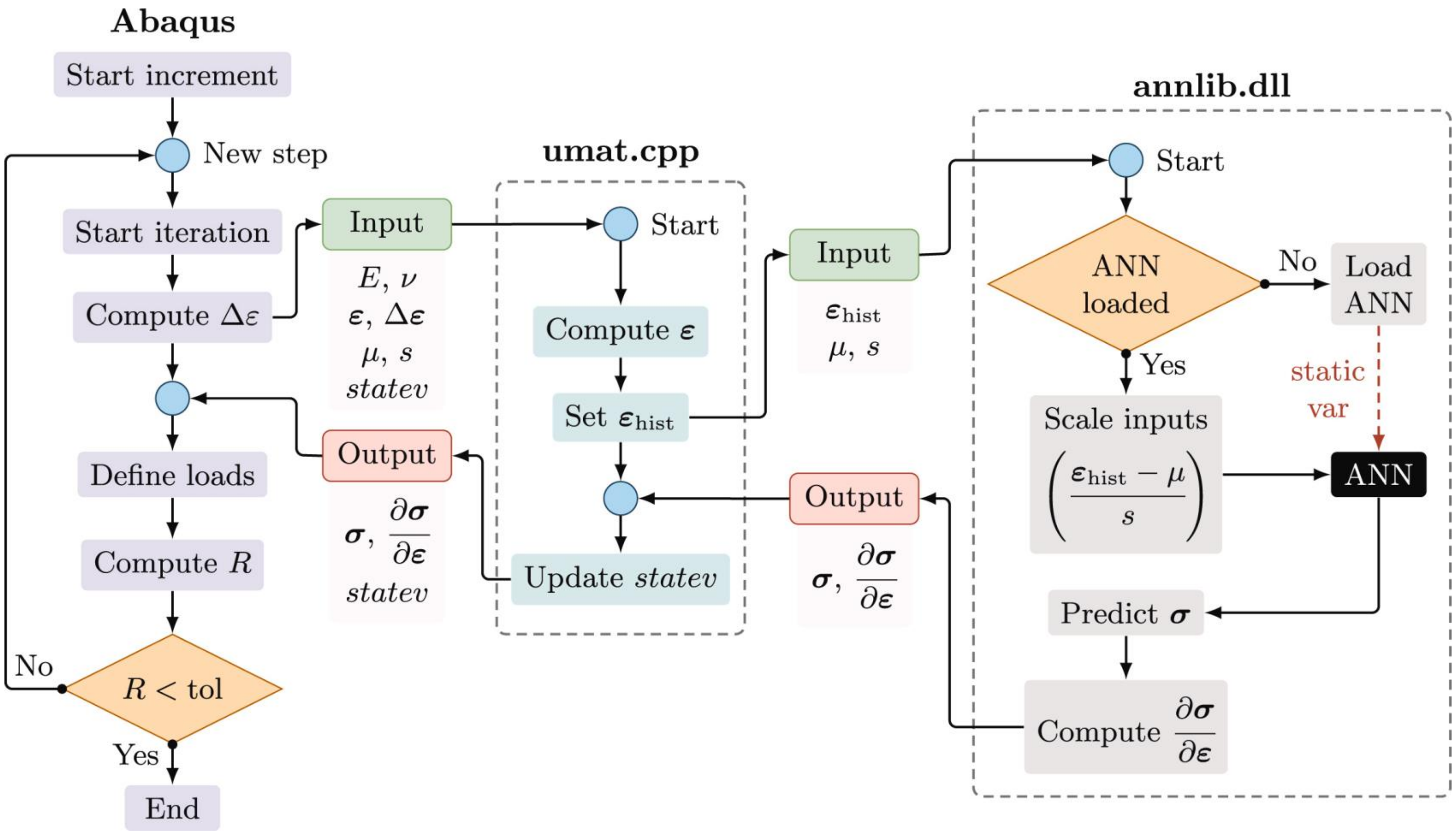
Implicit data-driven constitutive modelling

FEA implementation as UMAT (Abaqus)



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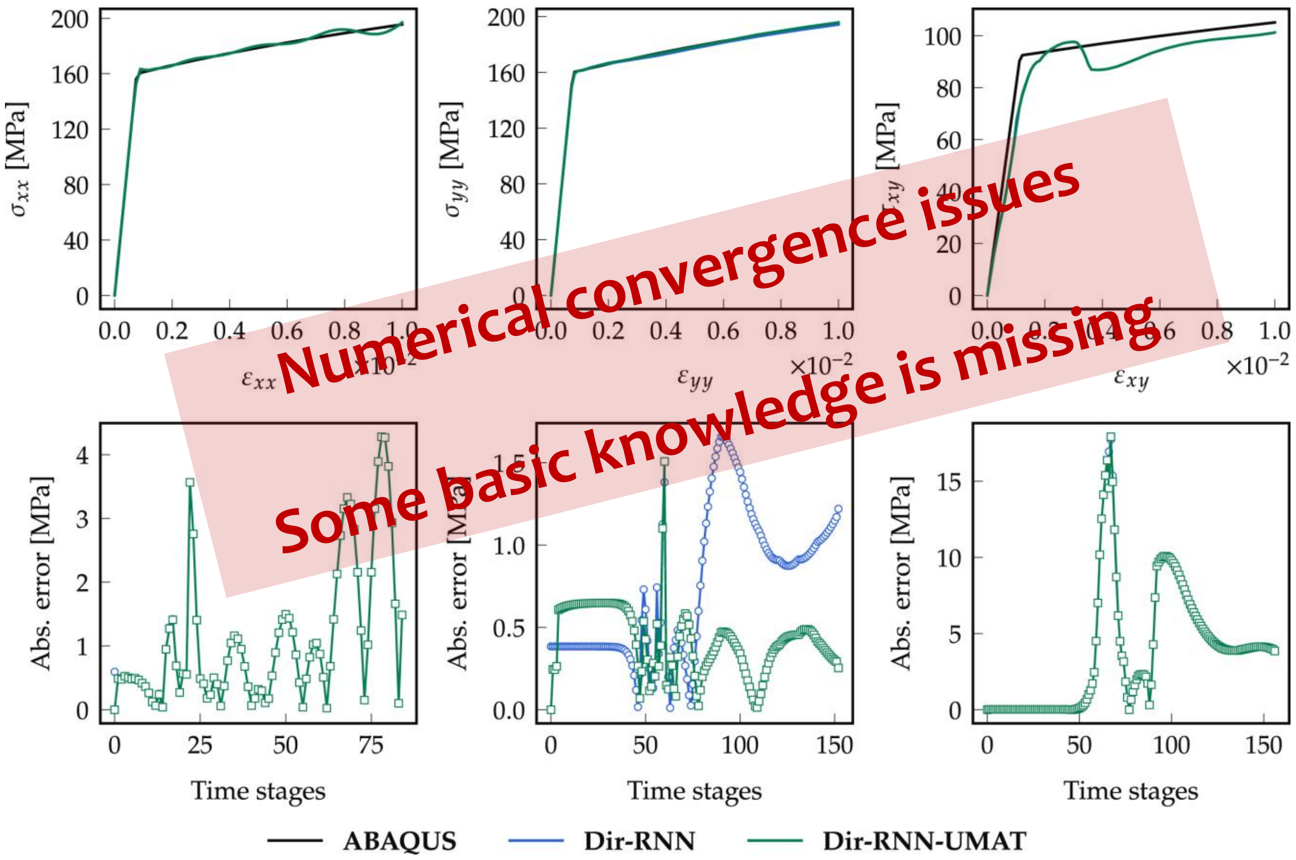
Implicit data-driven constitutive modelling

Uniaxial tensile and shear strain-stress curves. Comparison between the FEA solution based on the Swift's law and the UMAT implementation of the RNN model



Numerical convergence issues

Some basic knowledge is missing

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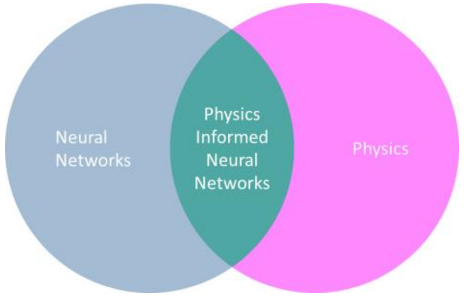
Implicit data-driven constitutive modelling



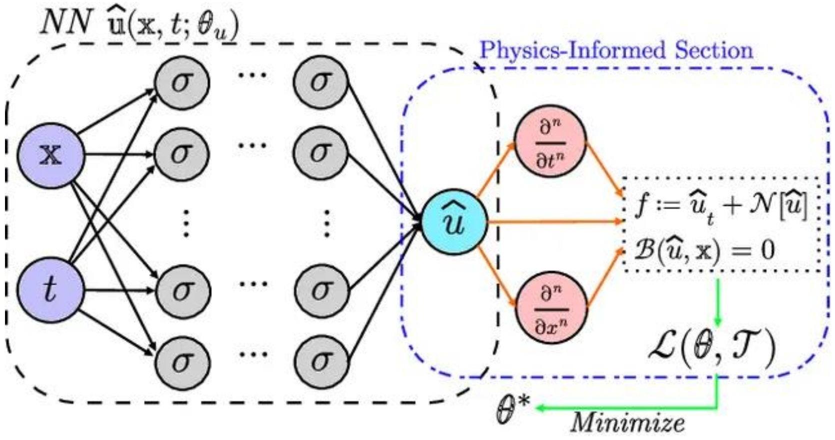
Training NN-based constitutive models using data is not sufficient.

Extra information related to the physics behind the problem need to be enforced.

Model can learn new information that is usually not possible to learn with training data by using some laws of physics as constraints
(Physics informed neural networks)

Advantages of physics-based constraints

- Improved accuracy and stability
- Reduction in data requirements
- Increases trustworthiness
- Prevention of non-physical predictions



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Implicit data-driven constitutive modelling

	Formulation	Loss term	Description
1st law of thermodynamics	$\gamma_{\text{loc}} = \boldsymbol{\sigma} : \dot{\varepsilon} + \theta\dot{\eta} + \dot{\mathrm{E}}$		The work done by stress must either be stored as recoverable internal energy in the solid or dissipated as heat [2]
2nd law of thermodynamics (Clausius-Duhem)	$\gamma_{\text{loc}} \geq 0$ $\frac{1}{2}(\boldsymbol{\sigma} - \boldsymbol{\sigma}^*) : \Delta\varepsilon \geq 0$	$\mathcal{L}_{\text{CD}} = \frac{\lambda}{2N}\sum_{k=1}^{N}\text{ReLU}\left(-\frac{1}{2}\left(\boldsymbol{\sigma}_{(k)} - \boldsymbol{\sigma}^*_{(k)}\right) : \Delta\varepsilon_{(k)}\right)^2$	For a sample of material subjected to a cycle of deformation, starting and ending with identical strain and internal energy, the total work must be positive or zero [2, 4, 6]
Plastic power	$\dot{w}^{\text{P}} = \boldsymbol{\sigma} : \dot{\varepsilon}^{\text{P}} \geq 0$	$\mathcal{L}_{\text{W}_\text{P}} = \frac{\lambda}{2N}\sum_{k=1}^{N}\text{ReLU}\left(-\boldsymbol{\sigma}_{(k)} : \dot{\varepsilon}^{\text{P}}_{(k)}\right)^2$	Plastic power must be non-negative to obey the 2nd law of thermodynamics Negative plastic dissipation implies a decrease in temperature as a result of inelastic deformation and therefore is nonphysical [1]
Accumulated plastic work	$w^{\text{P}} = \int_0^t \dot{w}^{\text{P}} \mathrm{d}t$		Since the plastic power should be non-negative, the accumulated plastic work should be non-decreasing [1]
Drucker's postulate (Material stability)	$\Delta\boldsymbol{\sigma} : \Delta\varepsilon \geq 0$	$\mathcal{L}_{\text{Drucker}} = \frac{\lambda}{2}\sum_{k=1}^{N}\text{ReLU}\left(\Delta\boldsymbol{\sigma}_{(k)} : \Delta\varepsilon_{(k)}\right)^2$	The work done by the tractions through the displacements is positive or zero [2, 6]

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Implicit data-driven constitutive modelling

	Formulation	Loss term
Tangent symmetry	$\mathbf{C} = \dfrac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}} \succ 0$	$\mathcal{L}_{\mathrm{TS}} = \sum_{k=1}^{N}\sum_{i=1}^{2}\sum_{j=1}^{2}\left(C_{ij(k)} - C_{ji(k)}\right)^2$
Time-consistency	$\lim_{\Delta\boldsymbol{\varepsilon}\to 0} \boldsymbol{\sigma} = 0$	$\mathcal{L}_{\mathrm{Cons}} = \dfrac{\lambda}{2N}\sum_{k=1}^{N}\sum_{i=1}^{N_s}\left(\boldsymbol{\sigma}(\boldsymbol{\varepsilon} = \mathbf{0})_{i(k)}\right)^2$
Momentum balance	$\nabla_x \cdot \boldsymbol{\sigma} = 0 \text{ in } x \in \Omega$	$\mathcal{L}_{\mathrm{MB}} = \dfrac{\lambda}{2N}\sum_{k=1}^{N}\sum_{i=1}^{N_g}\left(\nabla_x \cdot \boldsymbol{\sigma}_{i(k)}\right)^2$
Boundary conditions	$\mathbf{n} \cdot \boldsymbol{\sigma} = \mathbf{T} \text{ on } x \in \Gamma_{\mathrm{T}}$	$\mathcal{L}_{\mathrm{BC}} = \dfrac{\lambda}{2N}\sum_{k=1}^{N}\sum_{i=1}^{N_{\mathrm{BC}}}(\boldsymbol{\sigma} \cdot \mathbf{n} - \bar{\mathbf{T}})^2$
Stress triaxiality	$\mathcal{T} = \dfrac{\sigma_{\mathrm{h}}}{\sigma_{\mathrm{vM}}}$ Plane stress: $\mathcal{T} \in \left[-\dfrac{2}{3}, \dfrac{2}{3}\right]$	$\mathcal{L}_{\mathrm{Triax}} = \dfrac{\lambda}{2}\sum_{k=1}^{N}\mathrm{ReLU}\left(-\lvert\mathcal{T}_{(k)}\rvert + \dfrac{2}{3}\right)^2$

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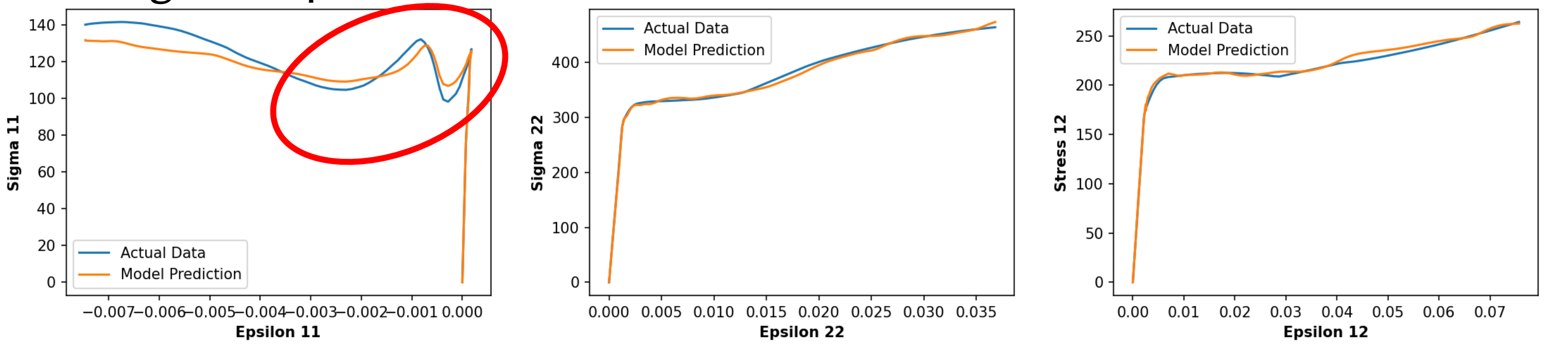
Implicit data-driven constitutive modelling

Example: Comparison of Constraints

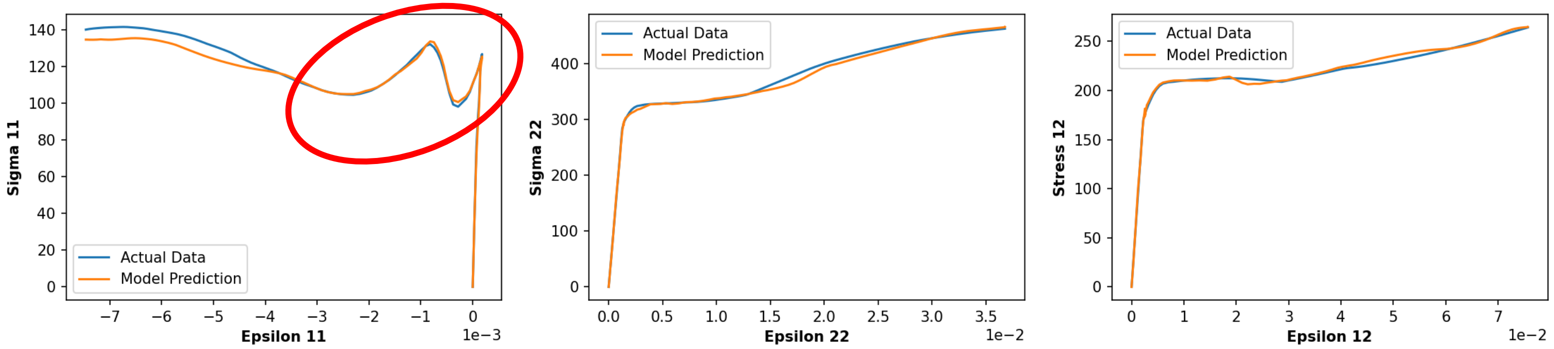
Metric	Data loss	Clausius-Duhem	Stress triaxiality	Lode angle	Plastic power
R^2	0.999	0.999	0.999	0.999	0.999
MSE	7.22	9.76	10.5	11.7	5.80
RMSE	2.68	3.12	3.24	3.43	2.40
MAE	1.26	1.41	1.51	1.71	1.13

Example for one integration point

Data loss →



Data loss + Plastic power →



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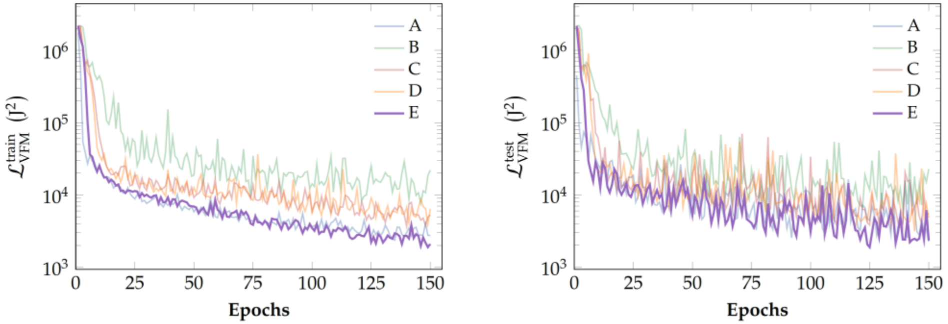
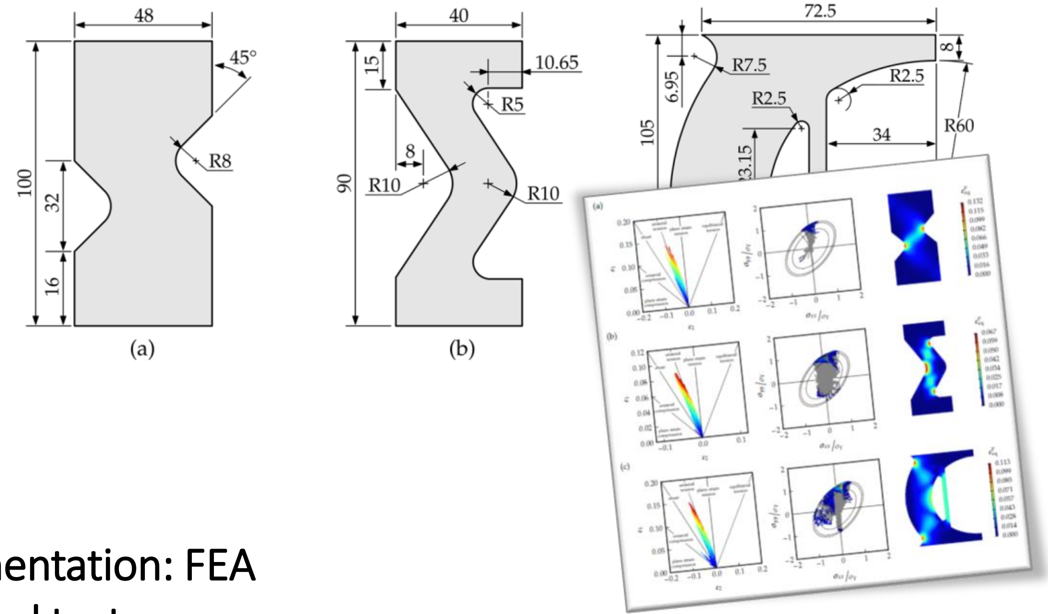
data-driven modelling: validation procedure

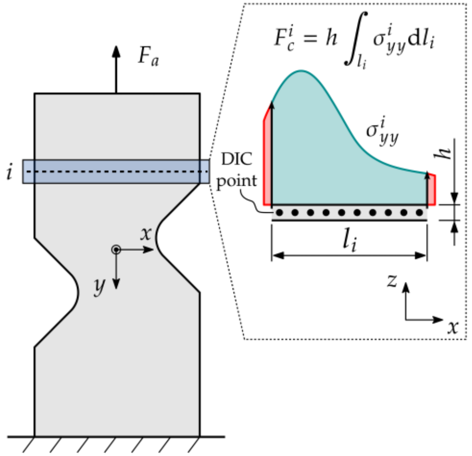
1. Error statistics



2. Validation database



3. Validation KPI

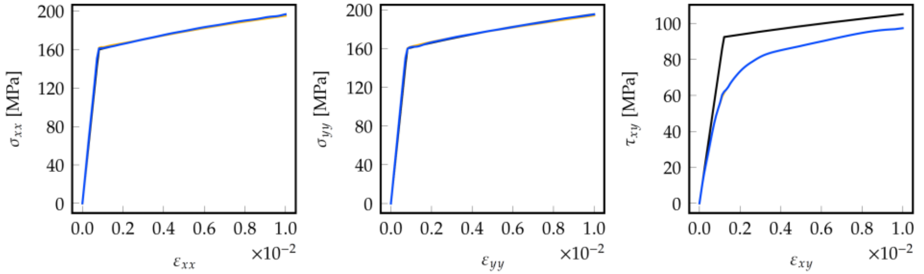


The 'RAF'

(Resconstructured axial force)

A. Peshave, F. Pierron, P. Lava, D. Moens, D. Vandepitte, Strain 2024, e12473. https://doi.org/10.1111/str.12473

4. UMAT implementation: FEA results for classical tests



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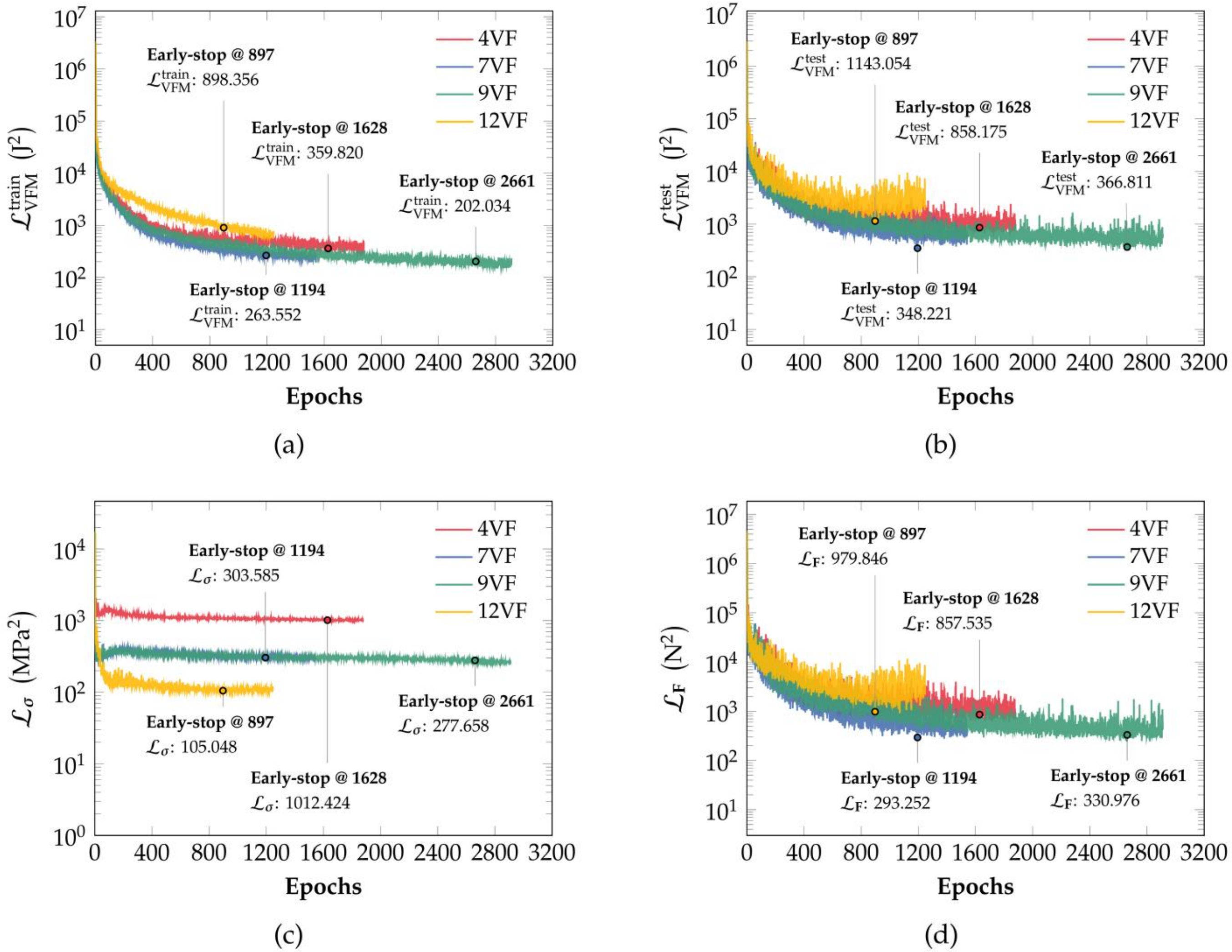
data-driven modelling: validation procedure

1. Error statistics



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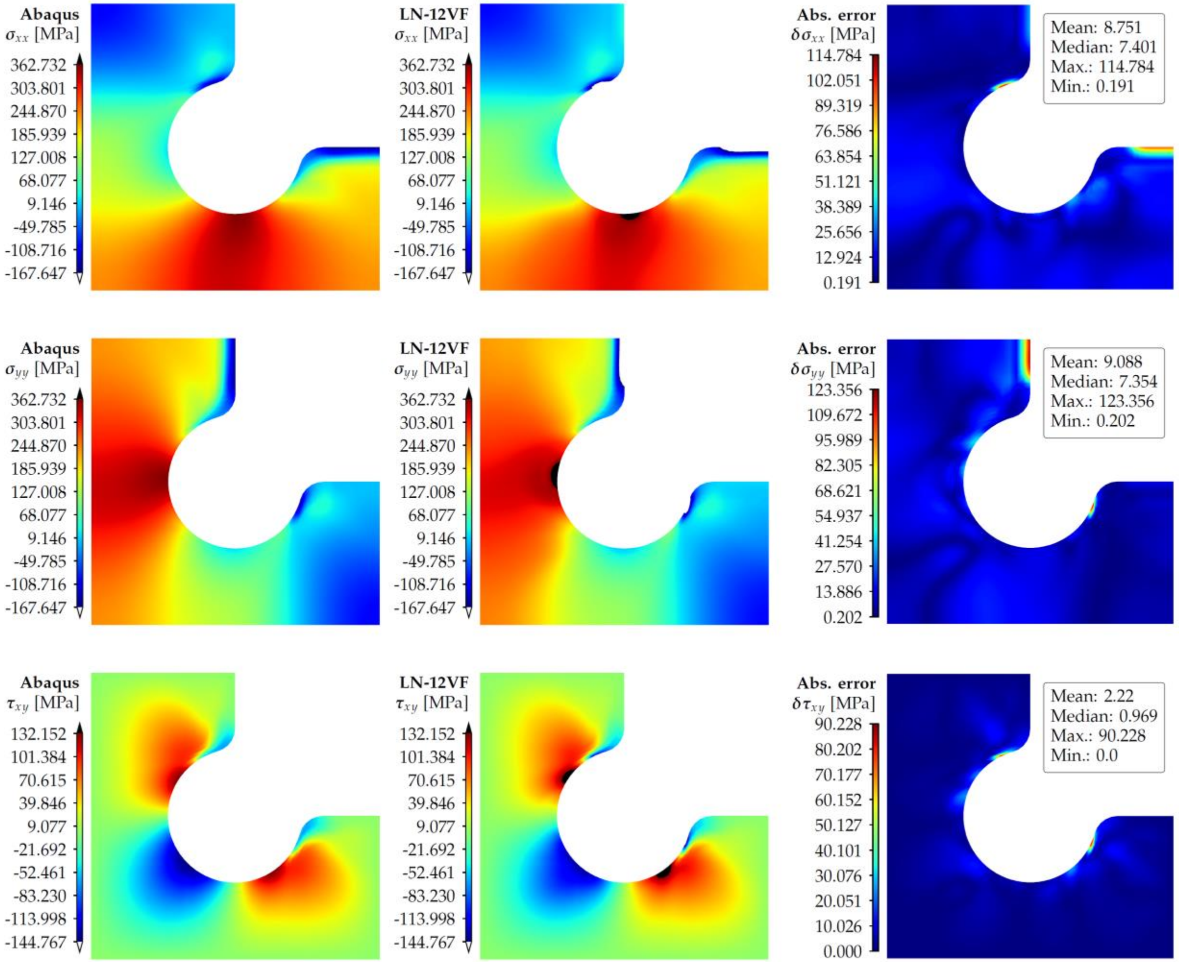
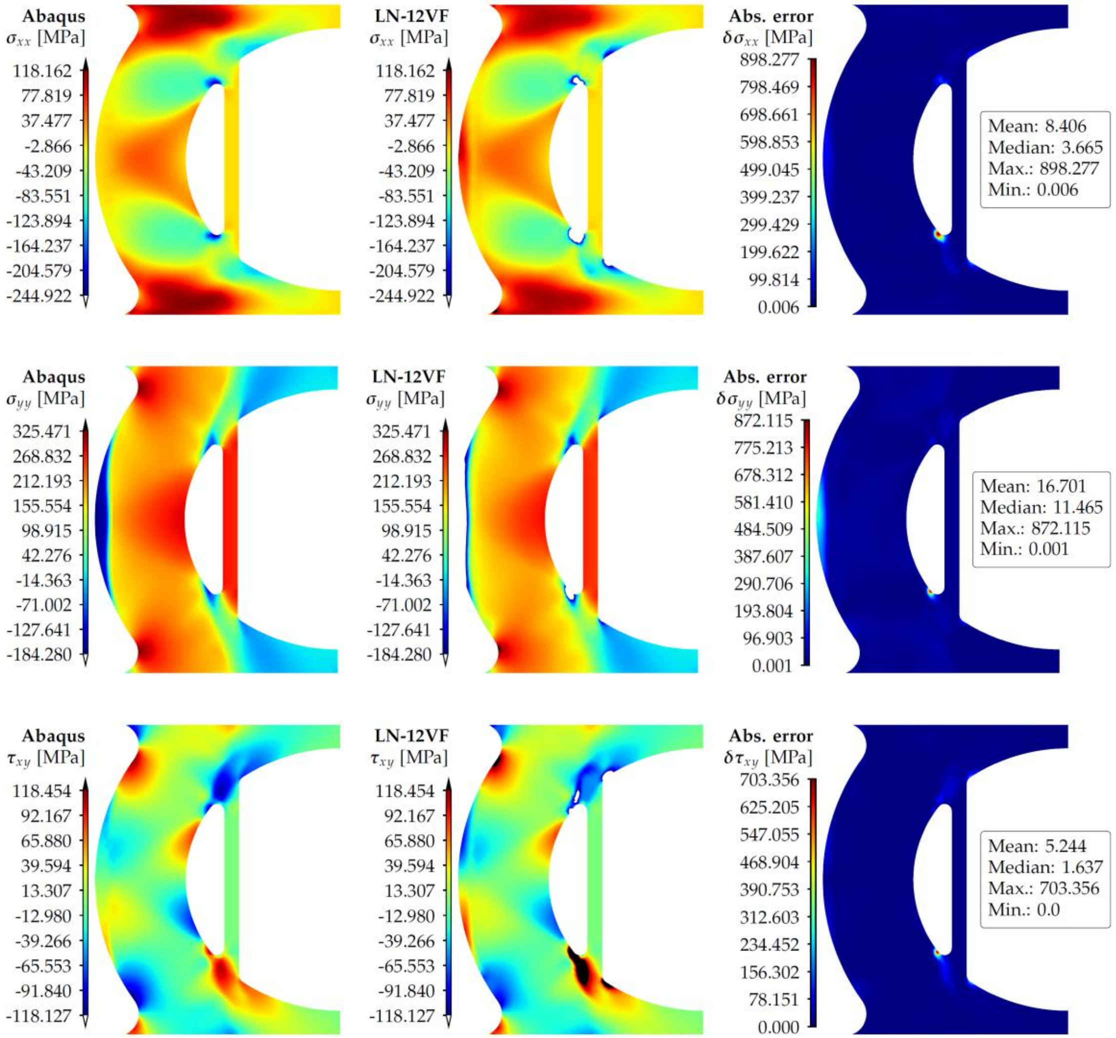
data-driven modelling: validation procedure

2. Validation database





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data-driven modelling: validation procedure

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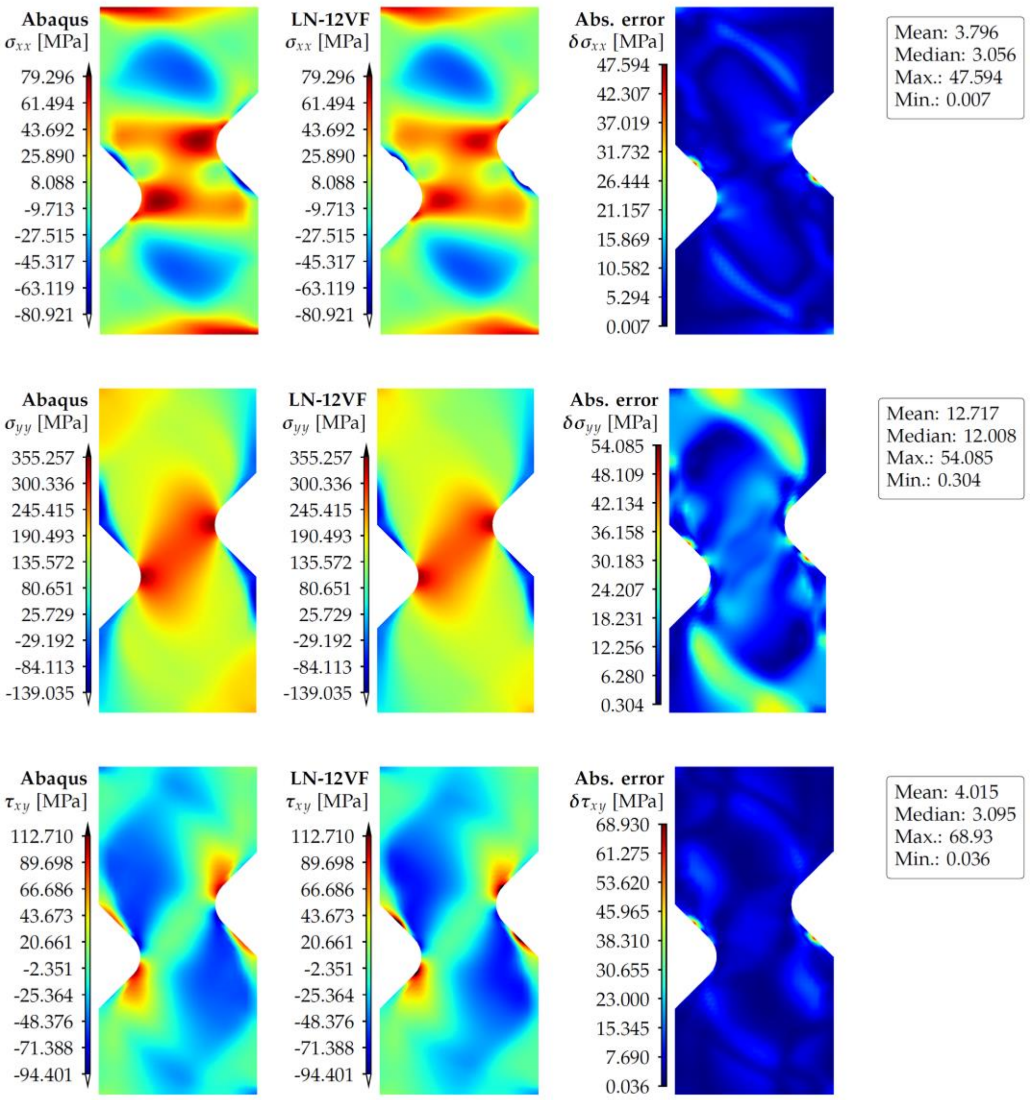

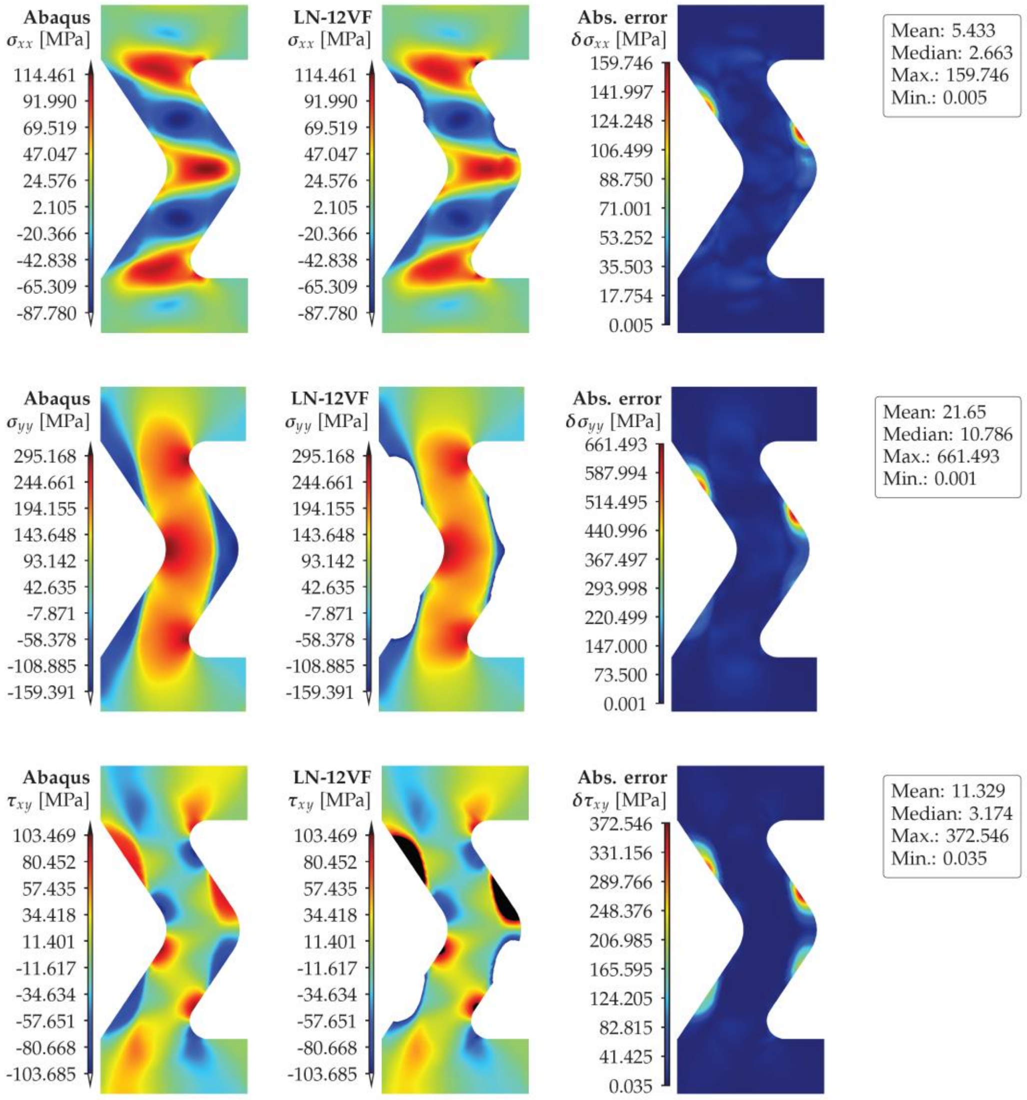

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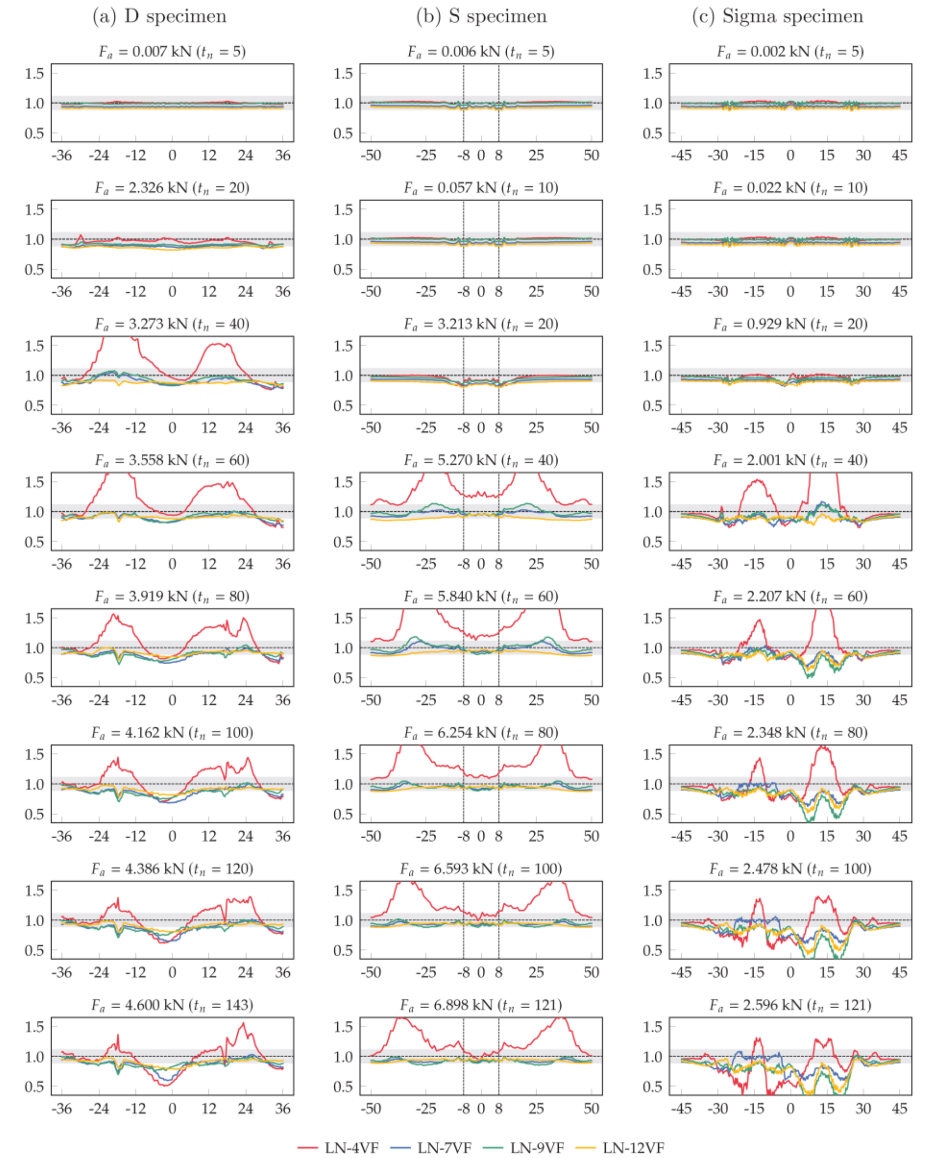
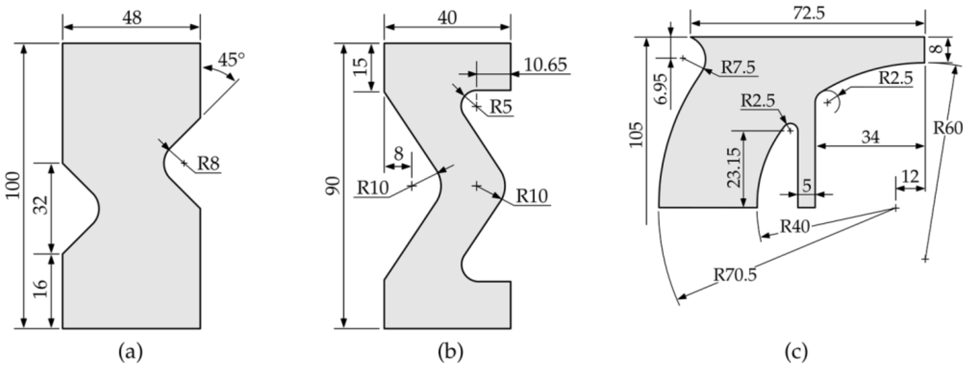
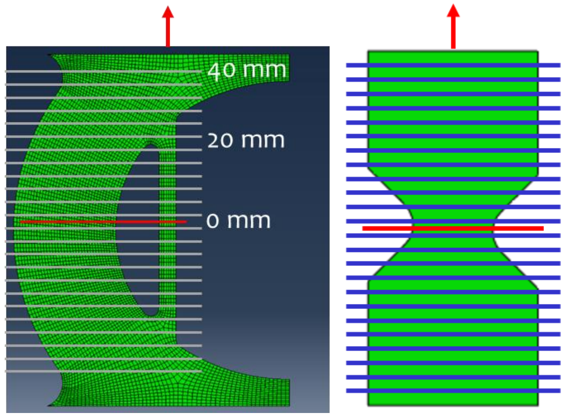
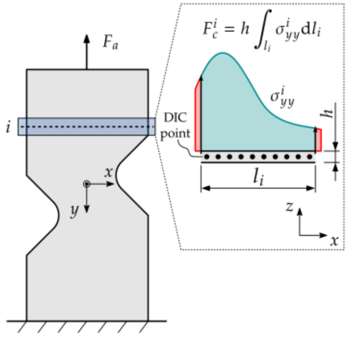
data-driven modelling: validation procedure

3. Validation KPI









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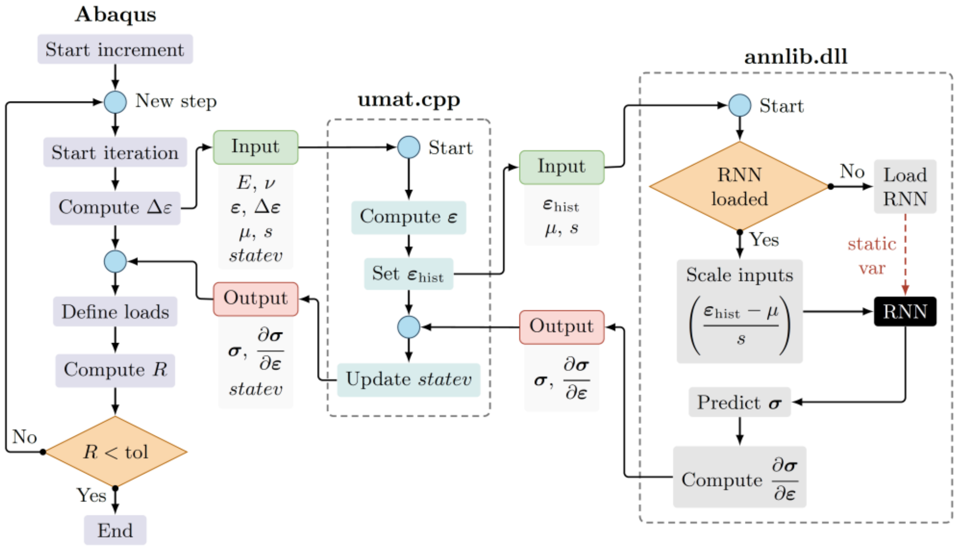
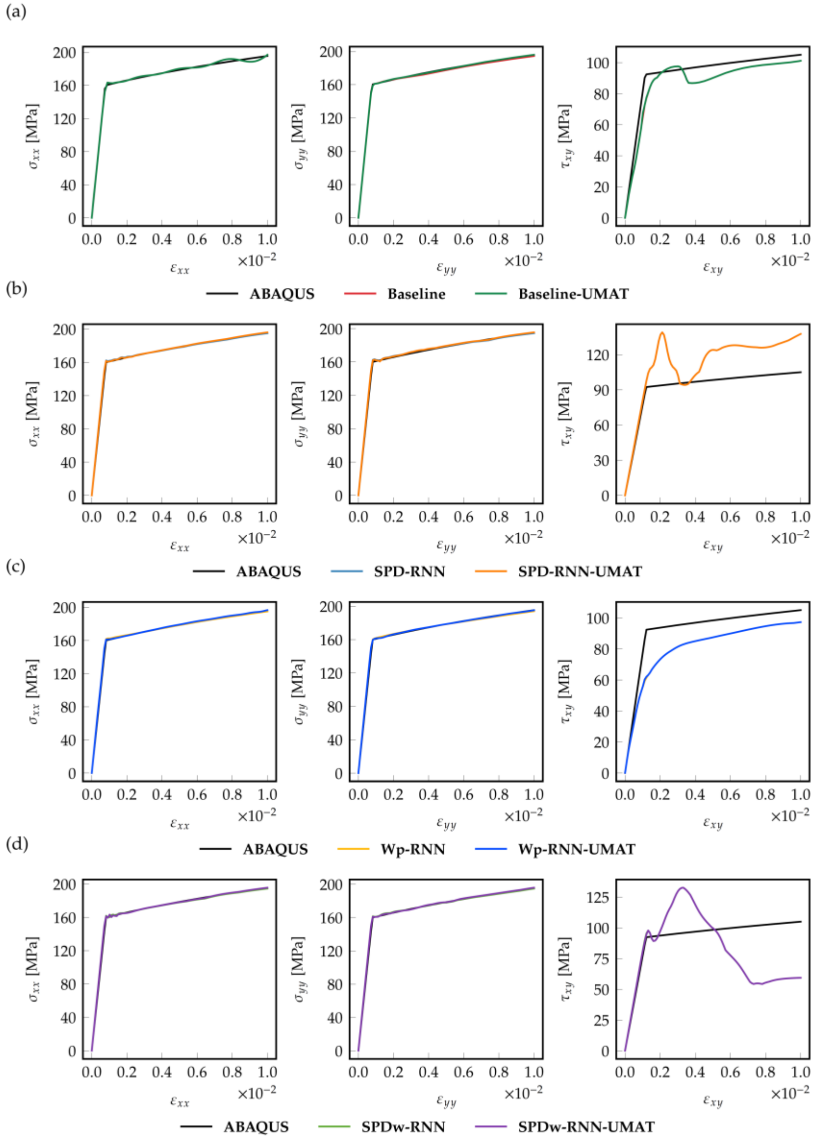
data-driven modelling: validation procedure

VForm-xSteels

4. UMAT implementation: FEA results for classical tests





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Conclusion

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Conclusion

VForm-xSteels

Major evolutions have been made for data-driven constitutive modelling

However, the is still a long way to go

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Closing remarks

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VForm-xSteels

VForm-xSteels

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