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Can Machine Learning and Explainable Artificial Intelligence Help to Improve an Expert Model for Predicting Thermomechanical Fatigue?

URAI – 2024

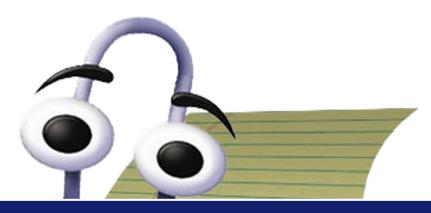
Stefan Glaser, Prof. Dr. Thomas Seifert, Prof. Dr. Daniela Oelke | 14.11.2024

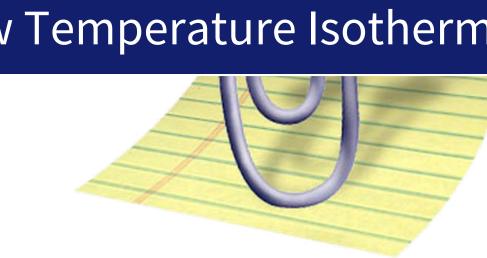
Mechanical Fatigue Domain background

Low Temperature Isothermal Fatigue

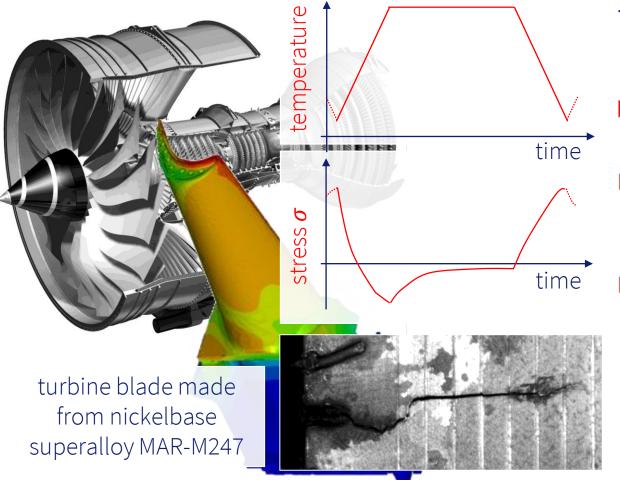


Image: Microsoft Clippy





Motivation Domain background

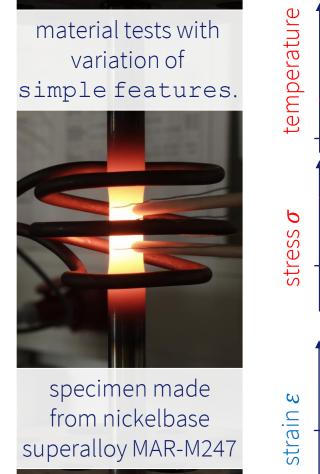


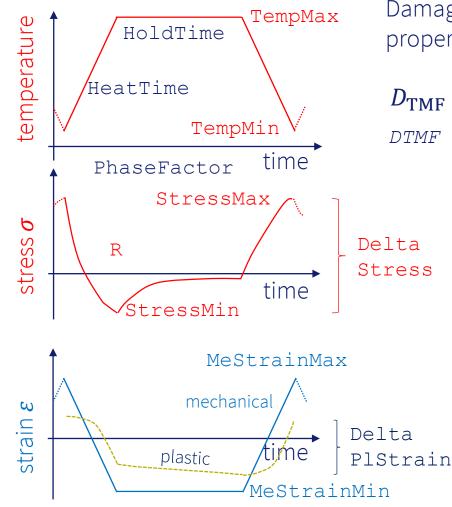
Thermomechanical fatigue (TMF) limits the lifetime of high temperature components:

- Heat-up and cool-down cycles result in stresses in the material.
- Stresses initiate TMF cracks that grow due to fatigue and creep damage mechanisms during service until they reach a technical critical length.
- Models are used for the prediction of the number of cycles to failure N_f of components.

Expert model and features Simple and expert features







Damage parameter calculated from material properties and load characteristics:

$$D_{\text{TMF}} = \left(1.45 \frac{\Delta \sigma_{\text{eff}}^2}{E \sigma_{CY}} + \frac{2.4}{\sqrt{1+3n'}} \frac{\Delta \sigma \Delta \varepsilon^p}{\sigma_{CY}}\right) F_{\text{creep}}$$

Material properties: E, SigmaCY, ROHardCy

Correlation of damage parameter with number of cycles to failure with fitting parameters:

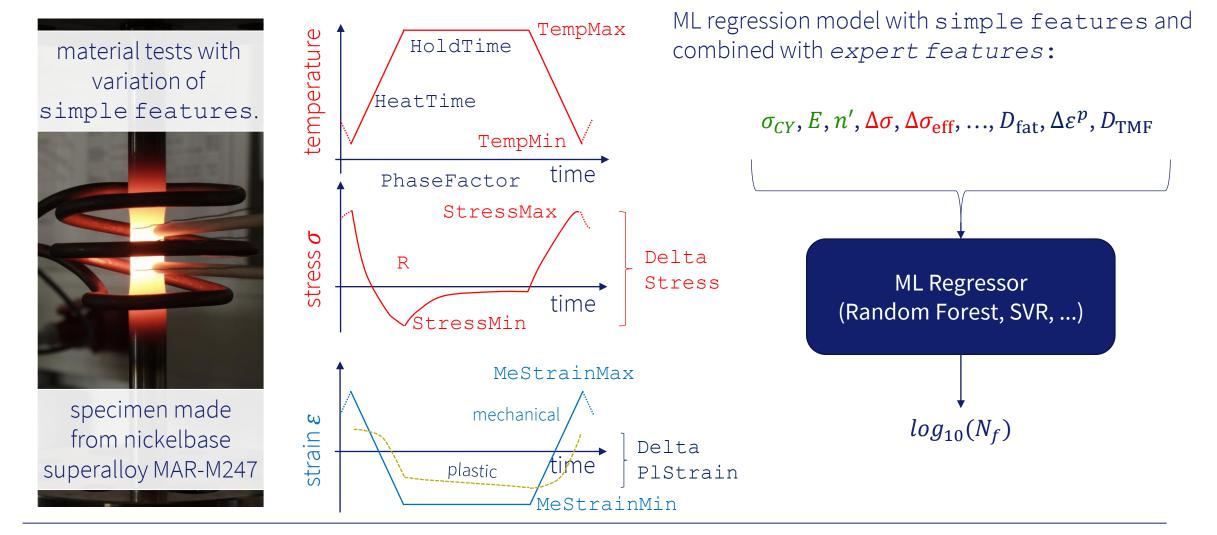
$$N_f = \frac{A}{D_{\rm TMF}^B}$$

Damage portion due to fatigue:

$$D_{\text{fat}} = \frac{1}{\frac{1}{F_{\text{creep}}^B}}$$

ML model and features Simple and expert features





Model Evaluation

Dataset

- ▶ 185 isothermal and
- ▶ 117 thermomechanical experiments

Error Function

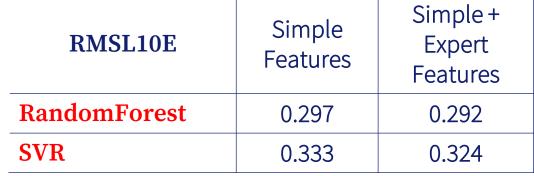
$$\text{RMSL10E} = \sqrt{\sum_{i} \left(\log_{10} \left(N_{\text{f}i} \right) - \log_{10} \left(\widehat{N}_{\text{f}i} \right) \right)^2}$$

Error factor more important than absolute error value!

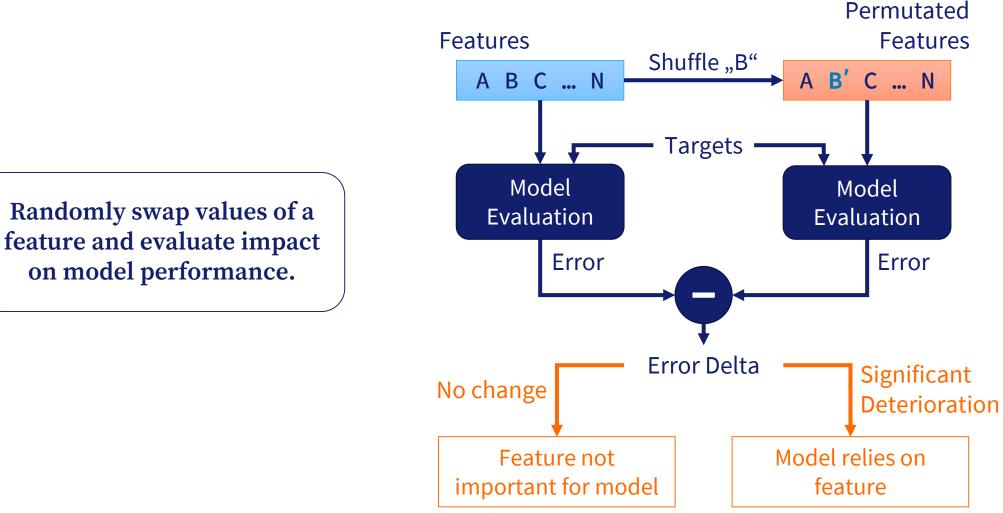
orest	0.297	0.292
	0.333	0.324
		1. 1

5-fold cross-validation results

Expert model based on material properties from a subset of the data reached a RMSL10E of 0.496.

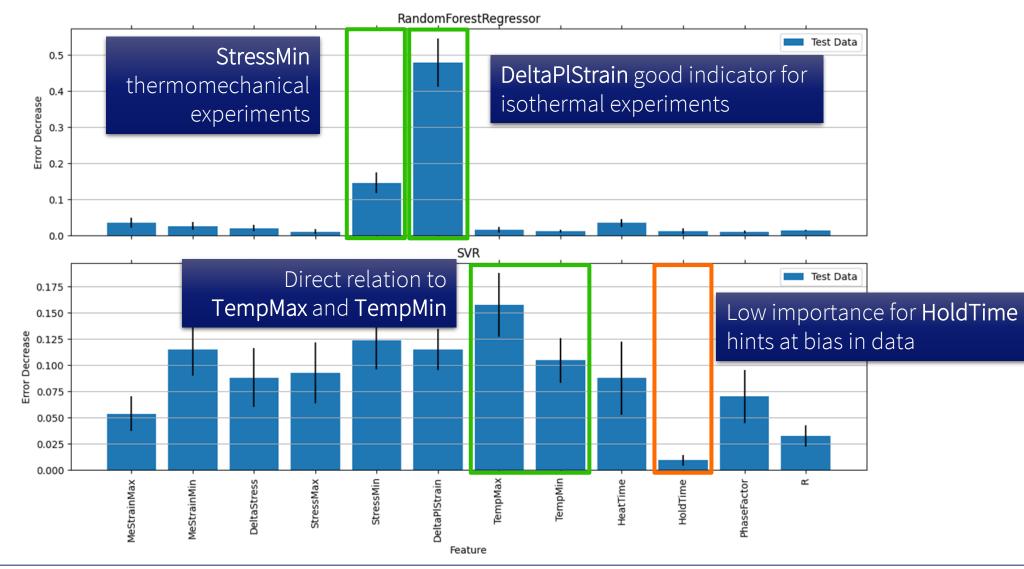


XAI – Permutation Feature Importance (PFI)

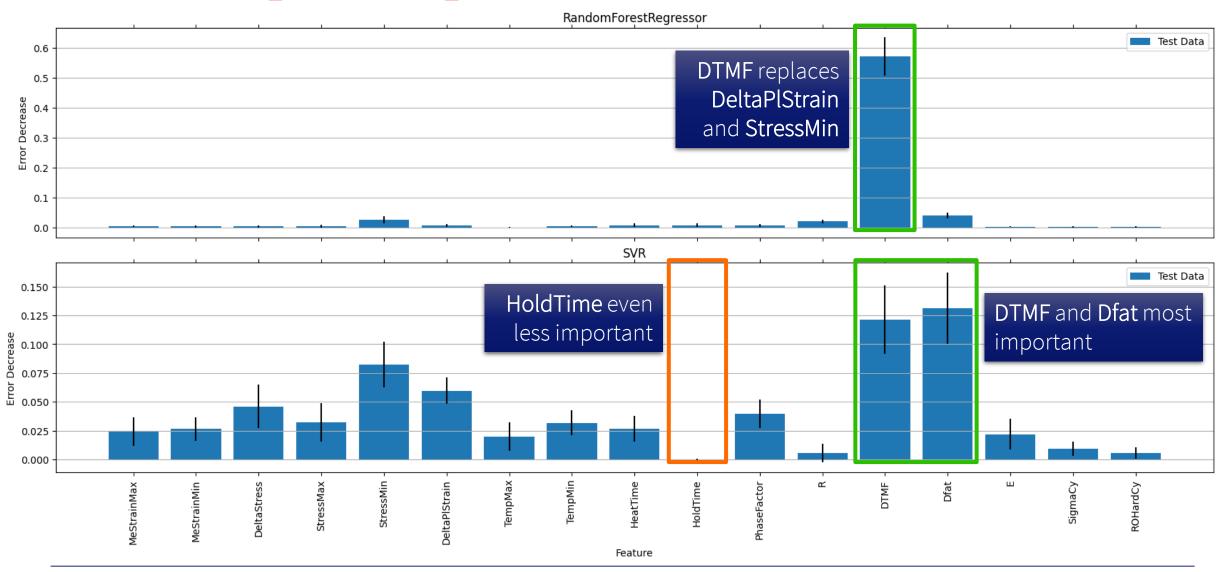


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PFI – Simple Features



PFI – Simple + Expert Features

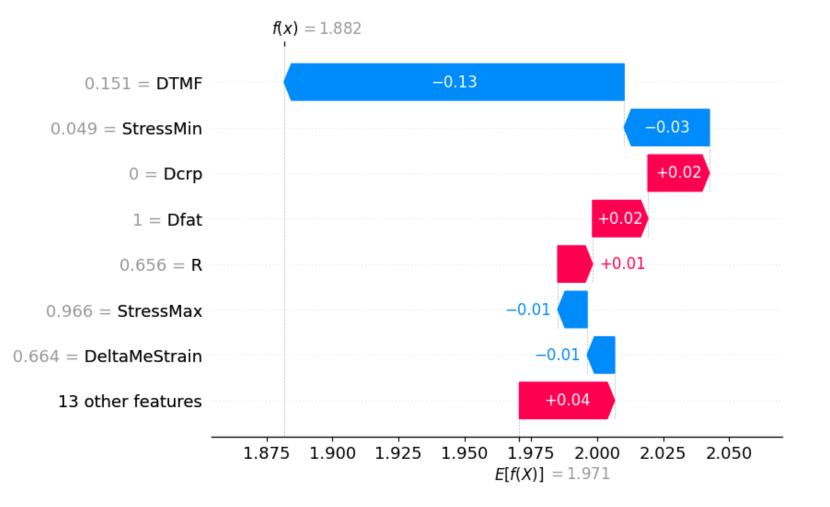


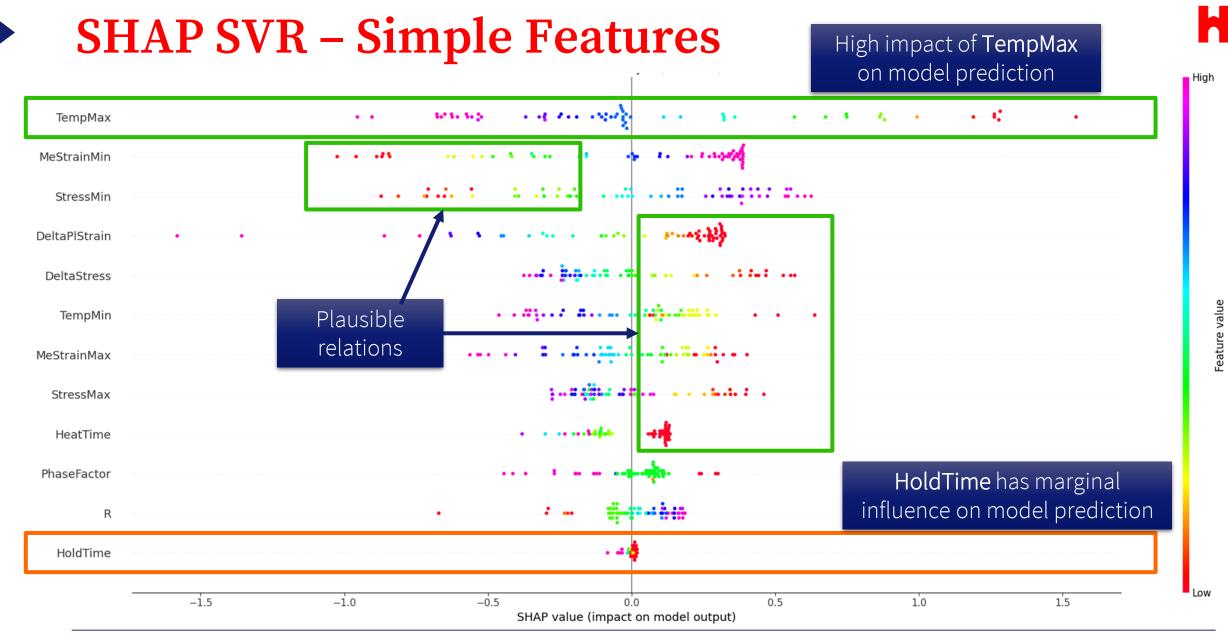
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XAI – Shapley Additive Explanations (SHAP)

- SHAP value (φ) measures contribution of feature to the deviation from the expected value (E[f(x)])
- Model Prediction as sum of expected and SHAP values:

$$f(x) = E[f(x)] + \sum_{i} \phi_{i}$$





Conclusion & Future Work

- > XAI able to discover multiple plausible relations of domain
- Results indicate that certain features could be better represented by the expert model
 - However, not clear yet how
- ML model more susceptible to biases in dataset compared to expert model
 - Different data required for calibrating expert models and for training ML models

Future Work

Boosting approach

Use ML model to correct the expert model ("Where is the expert model wrong?")

ightarrow better suited to discover potential improvements



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