Hybrid twins for production processes

Benjamin Klusemann

Acknowledgement:
Frederic E. Bock, Norbert Huber,
Zina Kallien, Sören Keller, Nikolai Kashaev,

Helmholtz-Zentrum hereon GmbH
Institute of Materials Mechanics
Solid State Materials Processing

Leuphana University Lüneburg

MSE Day 2023
14.11.2023

European Research Council
Established by the European Commission

LEUPHANA
UNIVERSITÄT LÜNEBURG

Helmholtz-Zentrum
hereon

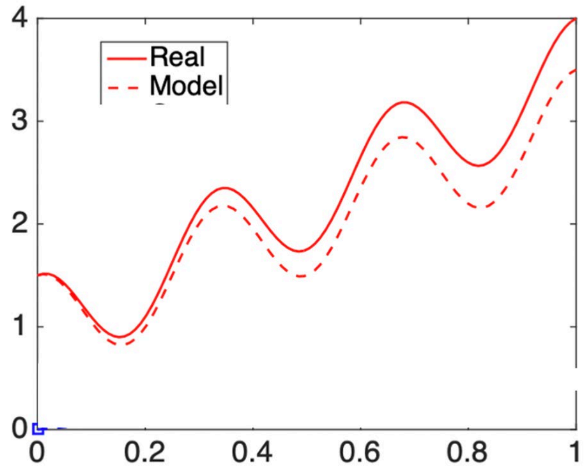
Introduction

Motivation – Physics vs. Data Science

Process parameters > **(Micro-)structure** > **Mechanical properties** > **Performance**

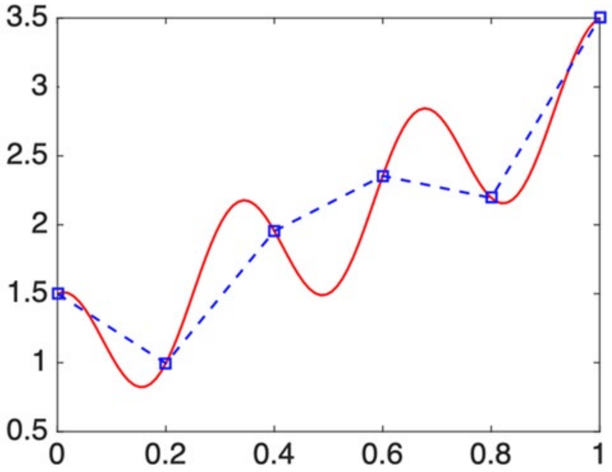
Two perspectives on: **Materials mechanics and processing**

Physics:
- Experiments
- Analytical modelling
- Numerical modelling



Variability
Uncertainty
Computing cost
Explanation
Extrapolation
….

Data science:
- Data management and analysis
- Machine learning



Amount of data
Explanation
Accuracy
Generality
…

Source: Chinesta, F; Cueto, E.; Abisset-Chavanne, E.; Duval, J.L.; Khaldi, F.E.B. Virtual, Digital and Hybrid Twins: A New Paradigm in Data-Based Engineering and Engineered Data. Arch. Comput. Methods Eng. 2018, 27, 105–134.

Introduction

Motivation – Physics and Data Science

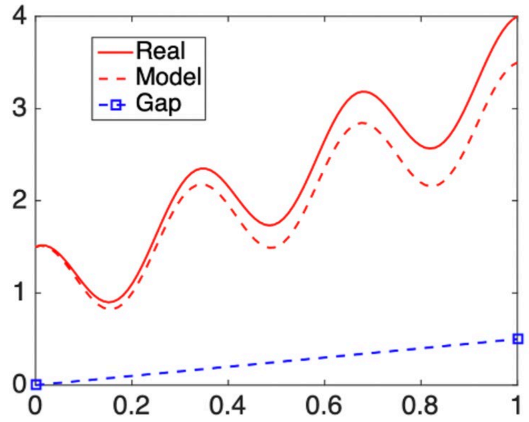
Process parameters → **(Micro-)structure** → **Mechanical properties** → **Performance**

Two perspectives on: **Materials mechanics and processing**

Physics:
- Experiments
- Analytical modelling
- Numerical modelling

Data science:
- Data management and analysis
- Machine learning

Reality
=
Physics-based model "The Art of Modelling"
+
The part of the reality that the model ignores "The Ignorance"



Chinesta, F; Material forming digital twins: the alliance between physics-based and data-driven models. ESAFORM plenary lecture 2022.

Introduction
Motivation – Physics and Data Science

Process parameters → (Micro-)structure → Mechanical properties → Performance

Challenges for data in material mechanics and engineering:

→ Low availability and high in cost for acquisition

→ Are often sparse with respect to time, space, variables and targets

To increase efficiency

Use:
- Minimum amount of data
- Established knowledge

⇒

Achieve:
- Low prediction error
- Good generalization
- Parameter space expansion

Introduction
Physics-integration into machine learning

Level of integration

Surrogate modelling of physical process simulations

Upadhyay, V., Jain, P. K., and Mehta, N. K. Conf. Proc. of SocProS 2011, 761–768 (2012).

Xiong, J., Zhang, G., Hu, J., and Wu, L.; J. Intell. Manuf. 25, 157–163 (2014).

Sahu, N. K., Andhare, A. B., Andhale, S., and Abraham, R. R. IOP Conf. Ser. Mater. Sci. Eng. 346:12037 (2018).

Physics-based feature engineering

- Physical relationships between features
- Physical normalization of inputs and outputs via dimensionality analysis

Verleysen, M.; François, D.; Simon, G.; Wertz, V. *IWANN 2003*, LNCS 2687, pp. 105-112, (2003).

Huber, N.; Tsakmakis, C. *J. Mater. Res.* 19, 101–113 (2004).

Hybrid / discrepancy modelling

- Using underlying physics that show discrepancies to target
- Compensating discrepancies with machine learning

González, D; Chinesta, F; Cueto, E. *Front. Mater.* 6, 752 (2019).

Moya, B.; Badías, A.; Alfaro, I.; Chinesta, F.; Cueto, E.; *Int. J. Numer. Methods Eng.* 25, 87 (2020).

Havinga, J.; Mandal, P.K.; van den Boogaard, T. *Int. J. Mater. Form.* 13, 663–673 (2020).

Physics-informed artificial neural networks

- Loss function formulated with respect to governing equations
- Required knowledge of governing equations (i.e. nonlinear PDEs)
- Via data-driven solution of nonlinear PDEs: they are fulfilled at sample points

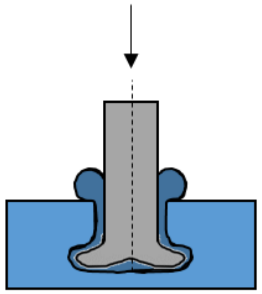
Raissi, M.; Perdikaris, P.; Karniadakis, G.E. *arXiv:*1711.10561 (2017).

Linka, K.; Hillgärtner, M.; Abdolazizi, K.P.; Aydin, R.C.; Itskov, M.; Cyron, C.J.; *J. Comput. Phys.* 429, 110010 (2021).

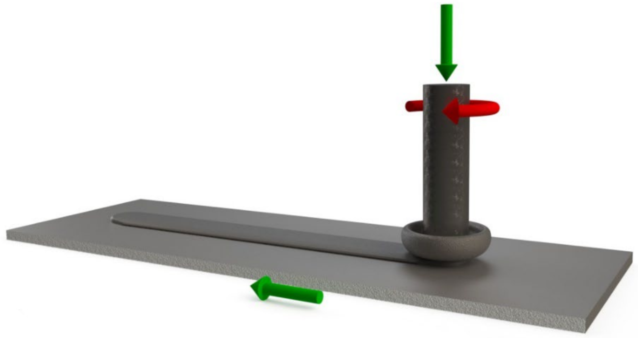
Haghighat, E.; Raissi, M.; Moure, A.; Gomez, H.; Juanes, R. *Comput. Methods Appl. Mech. Engrg.* 379, 11374 (2021).

Examples overview
Hybrid twins for production processes

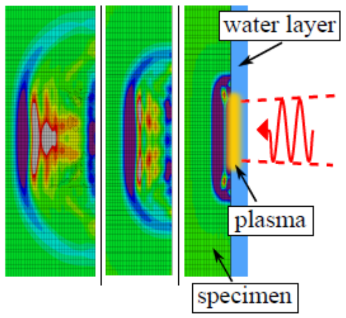
Case study 1
Physical feature engineering to improve mechanical performance prediction (Friction Riveting)



Case study 2
Simulation-assisted machine learning predictions of process behaviour and deposit geometry (Friction Surfacing)

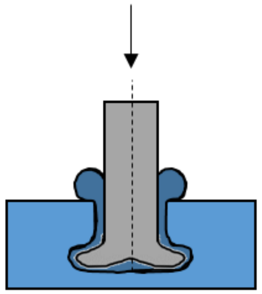


Case study 3
Hybrid modelling via machine learning correction of physical model output (Laser Shock Peening)

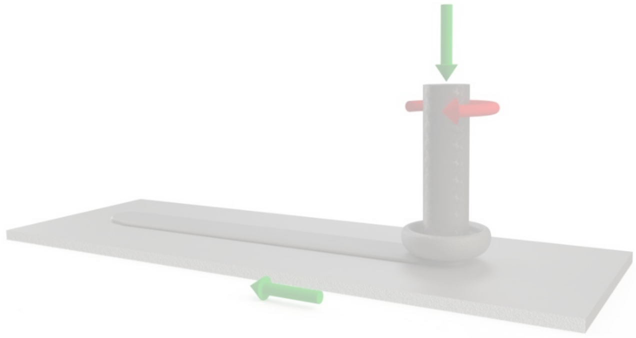


Examples overview
Hybrid twins for production processes

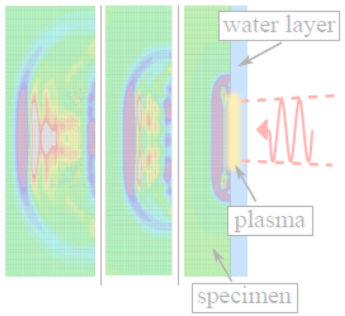
Case study 1
Physical feature engineering to improve mechanical performance prediction (Friction Riveting)



Case study 2
Simulation-assisted machine learning predictions of process behaviour and deposit geometry (Friction Surfacing)



Case study 3
Hybrid modelling via machine learning correction of physical model output (Laser Shock Peening)



F.E. Bock, L.A. Blaga, and B. Klusemann. Mechanical performance prediction for friction riveting joints of dissimilar materials via machine learning. *Procedia Manufacturing*, 47:615–622, 2020.

Case study 1: Introduction & Methodology
Friction Riveting – a solid state joining process

Advantages:

- Metal is processed below melting temperature
- No defects such as pores or hot cracking (in contrast to fusion-based joining processes)
- Bonding is achieved via mechanical anchoring and adhesion forces
- No surface pre-treatment or post-processing required

Process parameter variables

- Rotational speed
- Friction time and force
- Forging time and force

Physics-based feature engineering

- Mechanical energies E_M
  - Friction E_f
  - Plastic deformation E_d

$$\boxed{\begin{aligned} E_M &= E_f + E_d \\ &= \int M \cdot \omega \cdot dt + \int F \cdot \vartheta \cdot dt \end{aligned}}$$

torque

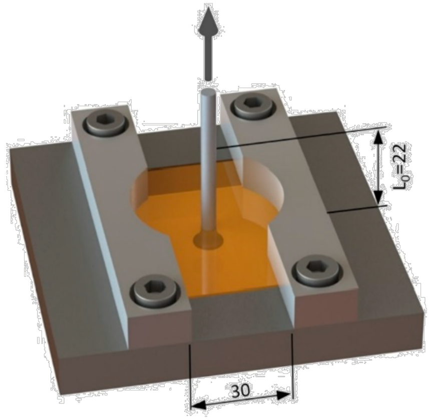
rotational speed

axial force

deformation rate

Aim: predict ultimate tensile force

T-pull test setup

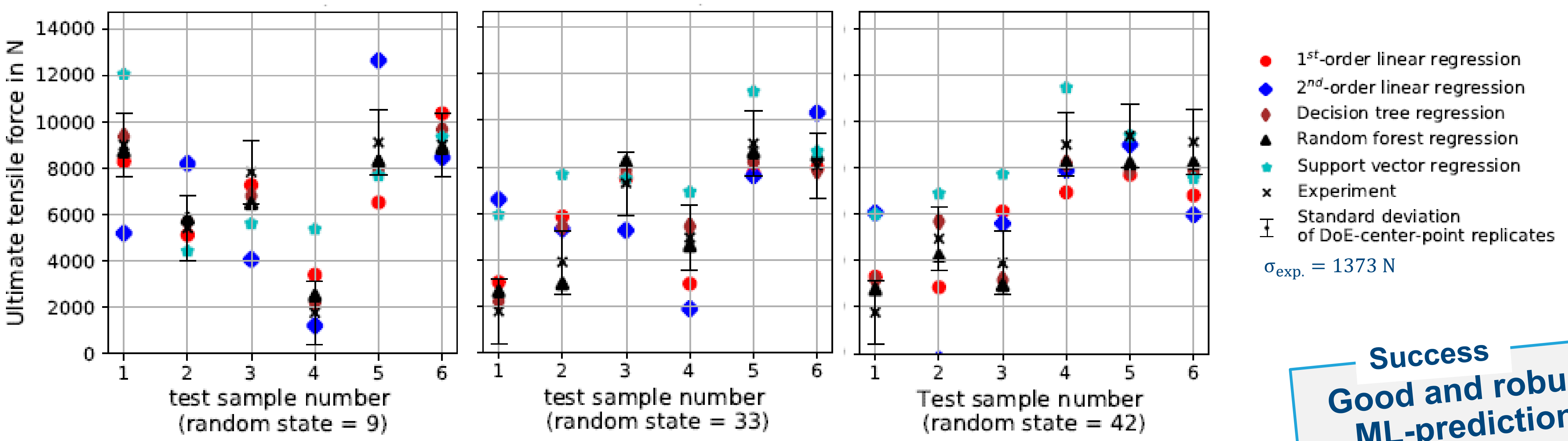


Rivet: AA2024-T351
Plate: Polyetherimide

Image: Pina Cipriano et al. 2018

Case study 1: Results

Input features: process parameters and mechanical energies



Success

Good and robust ML-prediction

Performance measure	Random state	1st-LR	2nd-LR	SVR	DTR	RFR
R^2	9	0.72	-0.15	0.48	**0.92**	**0.92**
	33	0.71	-0.2	0.11	0.90	**0.92**
	42	0.55	-0.13	0.21	0.86	**0.90**
Standard deviation in N	9	1404	2839	1917	748	**702**
	33	1356	2741	1384	719	**691**
	42	1860	3082	1358	1056	**719**

Main observations:

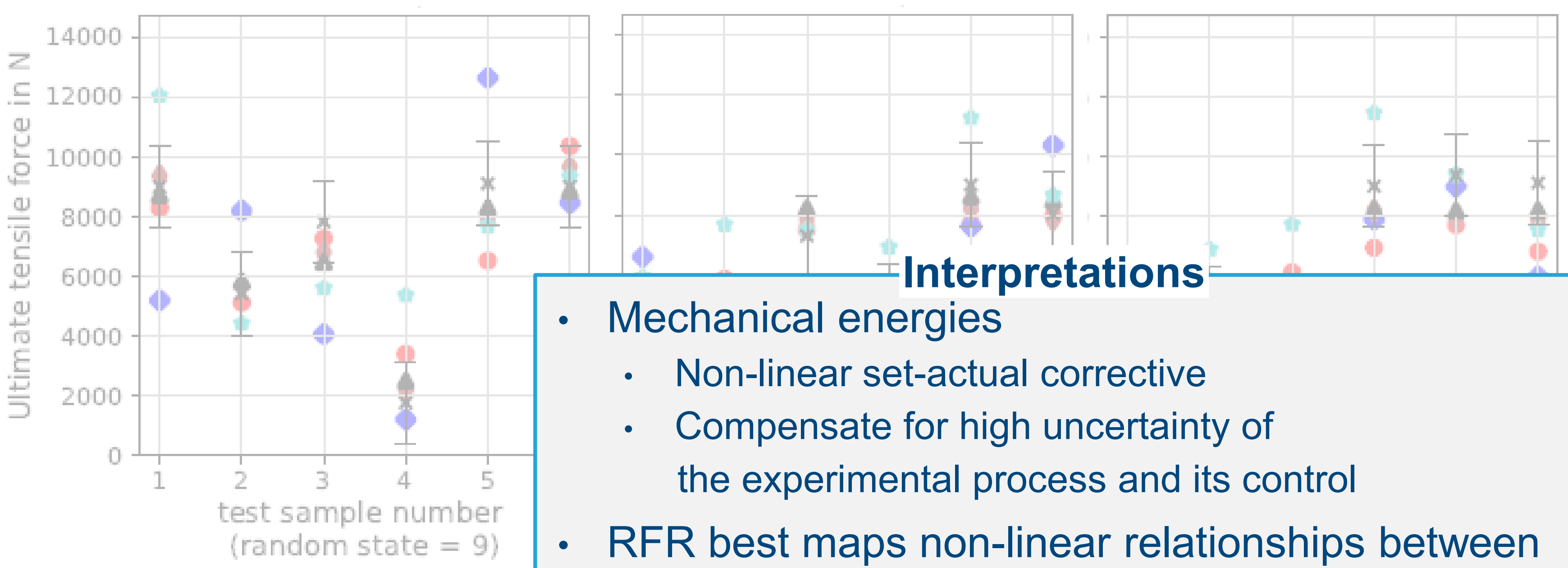
- LR and SVR predictions did not improve
- DTR and RFR predictions improve (best)

Result: Benchmark (R^2 = 77.9%) is exceeded (previously established linear model)

Helmholtz-Zentrum hereon

Case study 1: Results

Input features: process parameters and mechanical energies



1st-order linear regression
2nd-order linear regression
Decision tree regression
Random forest regression
Support vector regression
Experiment
Standard deviation
of DoE-center-point replicates
xp. = 1373 N

Interpretations

- Mechanical energies
  - Non-linear set-actual corrective
  - Compensate for high uncertainty of the experimental process and its control
- RFR best maps non-linear relationships between
  - Process parameter
  - Mechanical energies
  - Ultimate tensile force

Success
Good and robust ML-prediction

Performance measure	Random sta…					
R^2	9					
	33					
	42	0.55	-0.13	0.21	0.86	**0.90**
Standard deviation in N	9	1404	2839	1917	748	**702**
	33	1356	2741	1384	719	**691**
	42	1860	3082	1358	1056	**719**

…ns did not improve

- DTR and RFR predictions improve (best)

Result: Benchmark (R^2 = 77.9%) is exceeded (previously established linear model)

Helmholtz-Zentrum hereon

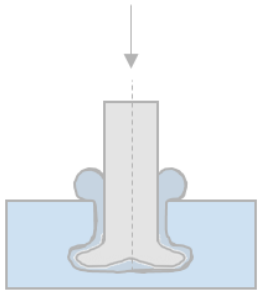
Examples overview
Hybrid twins for production processes

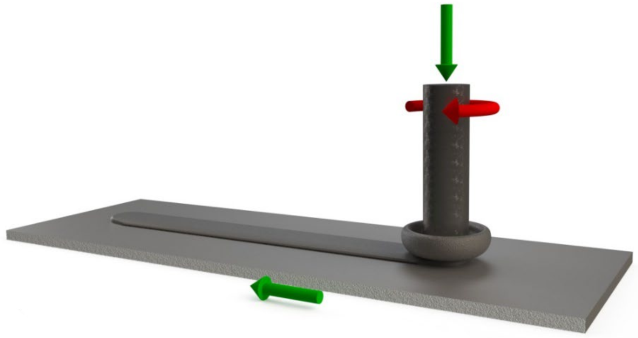
European Research Council
Established by the European Commission

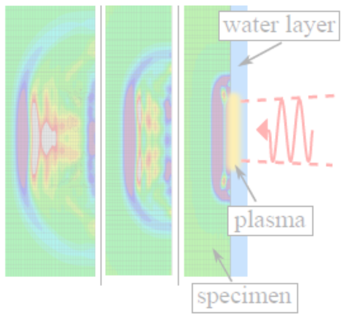
Case study 1
Physical feature engineering to improve mechanical performance prediction (Friction Riveting)

Case study 2
Simulation-assisted machine learning predictions of process behaviour and deposit geometry (Friction Surfacing)

Case study 3
Hybrid modelling via machine learning correction of physical model output (Laser Shock Peening)







Bock, F.E.; Kallien, S.; Huber, N.; Klusemann, B. (**2024**). Data-driven and physics-based modelling of process behaviour and deposit geometry for friction surfacing, *Computer Methods in Applied Mechanics and Engineering* 418, 116453.

Helmholtz-Zentrum hereon

Case study 2
Friction surfacing

Advantages

+ Deposition of dissimilar and non-fusion weldable materials
+ Fine-grained recrystallized microstructure
+ Low requirements for the process environment
+ Environmentally friendly (‘green’ process)
+ Low heat input

Disadvantages

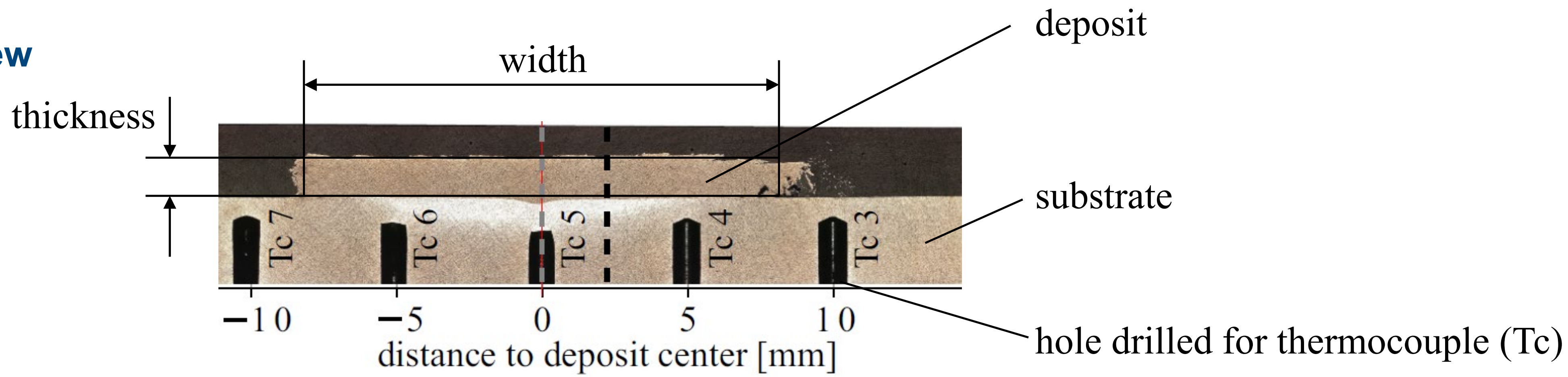
– Discontinuous process
– Remaining stud needs to be recycled

Process parameters: Axial force (F) F, Rotation speed (RS) ω , Travel speed (TS) v

Helmholtz-Zentrum hereon

Case study 2: Introduction
Problem statement

Cross section view



Main modelling challenges for geometry & process behaviour

- Required a priori
- Depend on process temperatures
- Process temperatures, in turn, depend on process parameters and substrate & backing materials

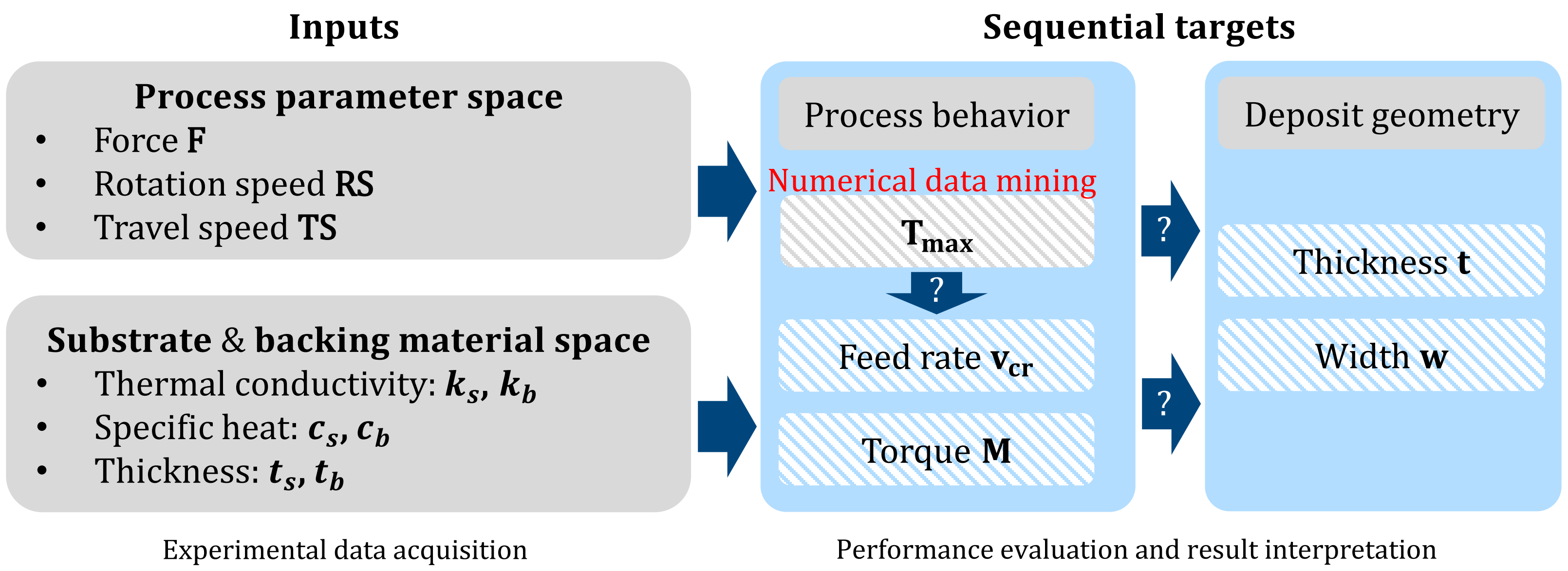
Question: How can the **number of experiments** be reduced to a **minimum**?

Solution proposal: Use **machine learning** and exploit physics contained in **heat-transfer model**

Image: Kallien, Z.; Klusemann, B. Combined experimental-numerical analysis of the temperature evolution and distribution during friction surfacing. *Surf. Coat. Technol.* 437, 128350 (2022).

Case study 2: Methodology

Proposed solution – simulation assisted machine learning



Milestones

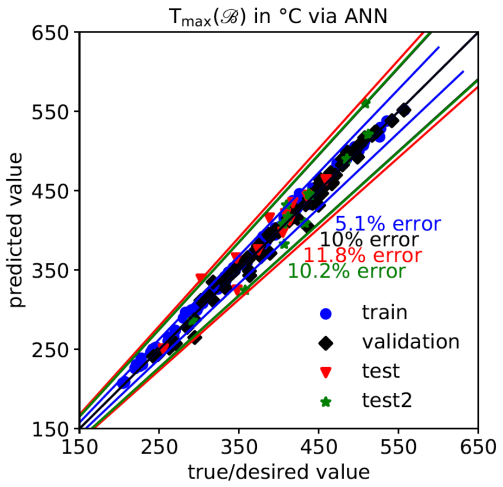
- Experimental variation of process parameters and material properties (to obtain v_{cr}, M, t, w)
- Data-mine numerical heat transfer model to obtain T_{max}
- Build predictive models for targets T_{max}, feed rate v_{cr} and torque M
- Build predictive models for targets: thickness t and width w
- Evaluate the use of process behaviour targets as features to predict deposit geometry

Helmholtz-Zentrum hereon

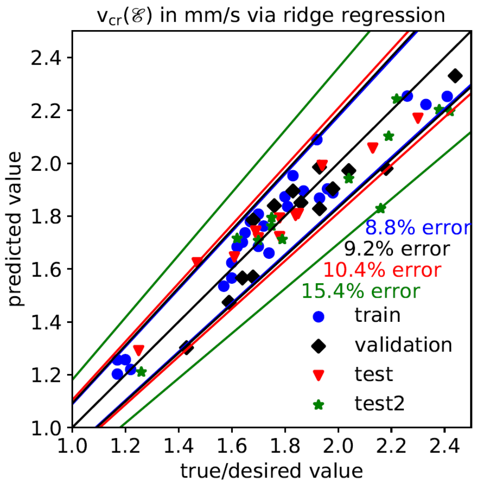
Case study 2: Result overview

Predicted versus true values for all targets

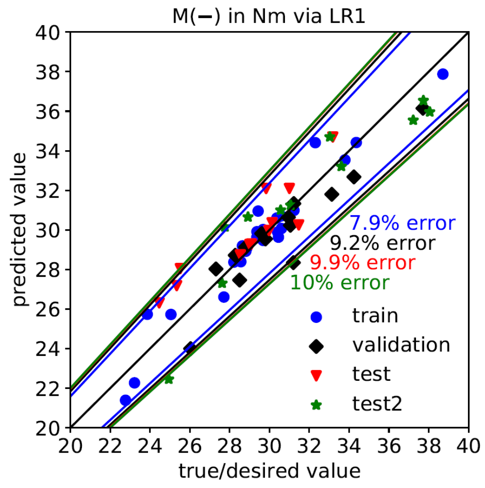
Maximum temperature



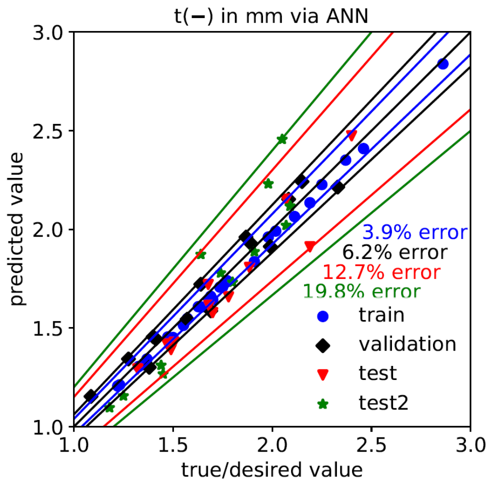
Feed rate



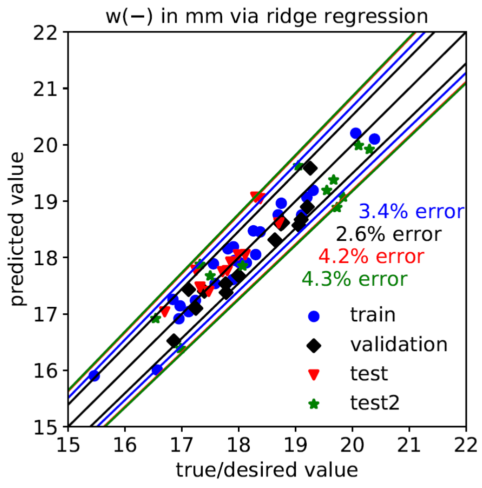
Torque



Thickness



Width

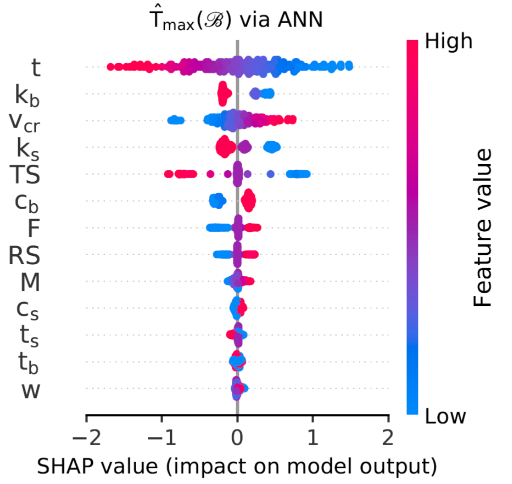


Achievements:

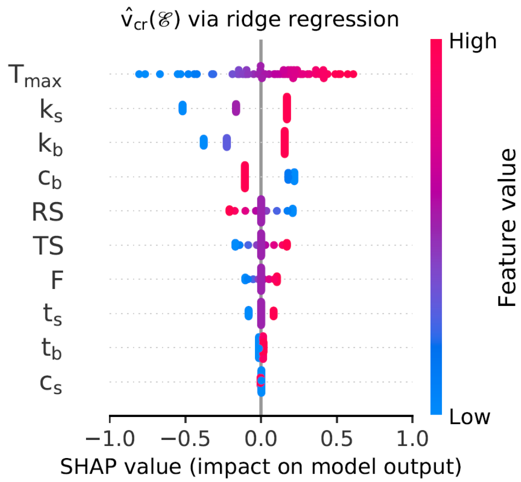
- Successful prediction of all targets
- Very good, good and acceptable agreements between predicted and true values
- Generalization is also good and acceptable based on low error on cross-space (test2 set)

Case study 2: Result overview
Feature dependence of all targets

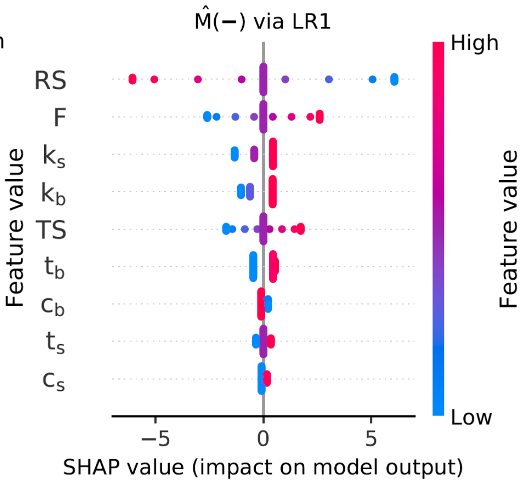
Maximum temperature



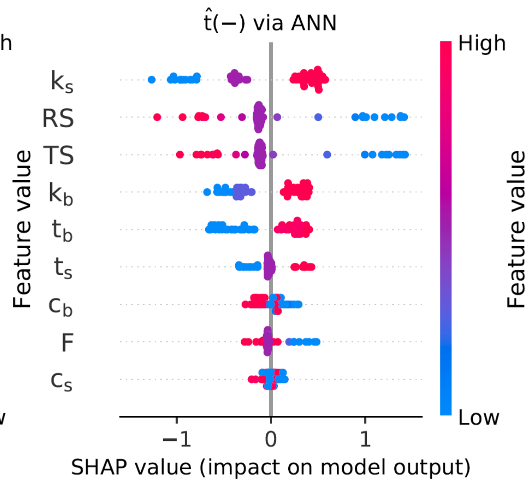
Feed rate



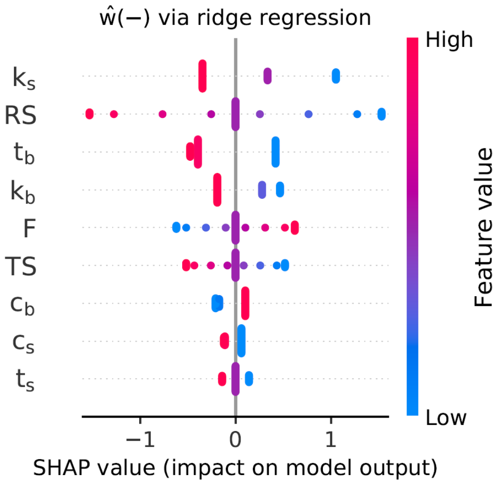
Torque



Thickness



Width



Evaluation of machine learning models

- **Validation**: Relations between targets and process parameters F, RS, TS agree with literature
- **Identification**: Significant impacts by thermal material properties besides process parameters
- **Finding**: k_s and k_b among top 4 features for all targets

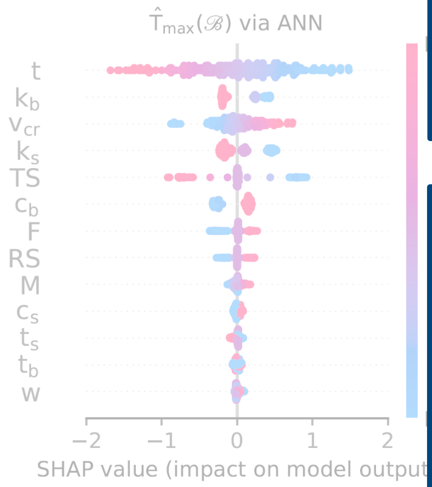
  → Indirect confirmation: high impact of temperature on all targets

SHAP

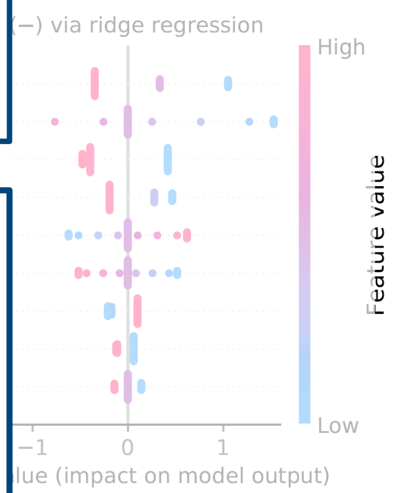
Image: https://github.com/slundberg/shap

Case study 2: Conclusion

Maximum temperatu



Width



Main achievements

- Physics-based data augmentation improved prediction performance
- Built ML models show acceptable prediction performance for all targets

Lessons learned

- Prediction of feed rate v_{cr} was improved by T_{max} as feature
- Depending on the target → Different ML techniques served as best models
- Explainable AI: SHAP values enabled determination of feature dependence
  - Influence of process parameters
  - T_{max} influences t, w and v_{cr} (in agreement with literature)
  - Thermal conductivity shows high impact (always among top 4 features)

Impact

- Thickness and width can be tailored separately by adjusting process parameters and material properties according to the presented findings

Evaluation of ma

- **Validation**: Relations between targets and process parameters F, RS, TS agree with literature
- **Identification**:
- **Finding**: k_s an

→ Ind

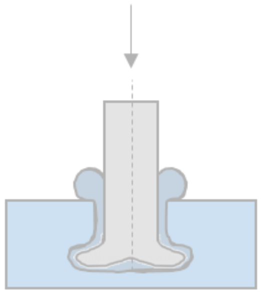
Helmholtz-Zentrum hereon

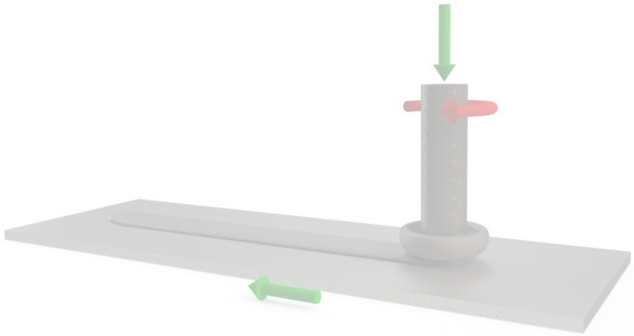
Examples overview
Hybrid twins for production processes

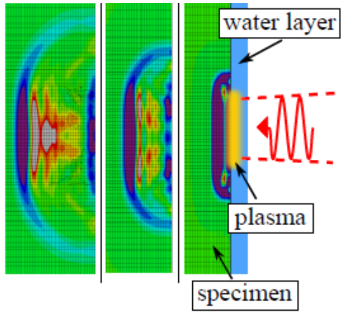
Case study 1
Physical feature engineering to improve mechanical performance prediction (Friction Riveting)

Case study 2
Simulation-assisted machine learning predictions of process behaviour and deposit geometry (Friction Surfacing)

Case study 3
Hybrid modelling via machine learning correction of physical model output (Laser Shock Peening)



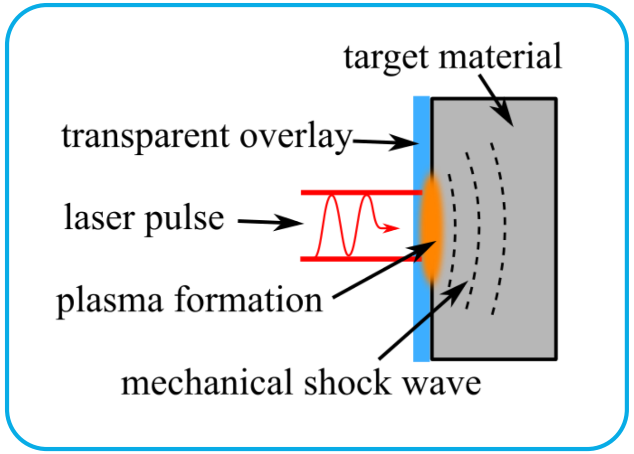




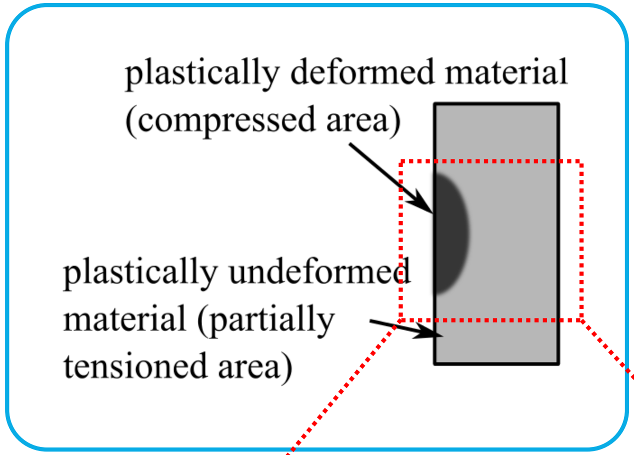
F. E. Bock, S. Keller, N. Huber, and B. Klusemann. Hybrid modelling by machine learning corrections of analytical model predictions towards high-fidelity simulation solutions. *Materials*, 14(8):1883 (19p.), 2021.

Case study 3: Introduction
Laser shock peening

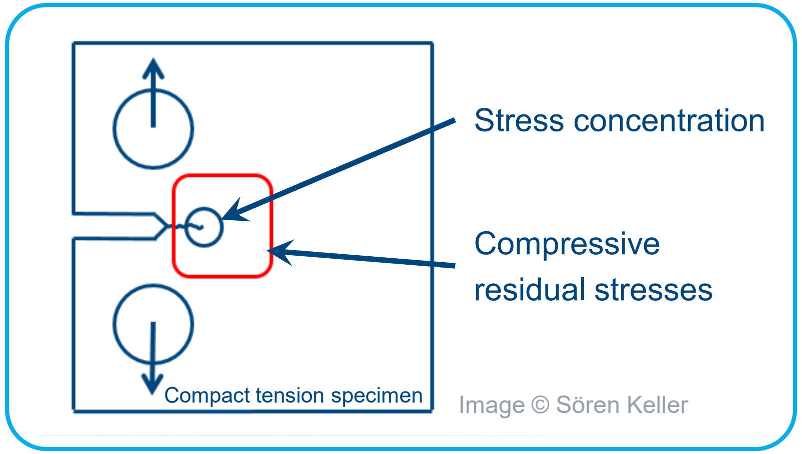
Process



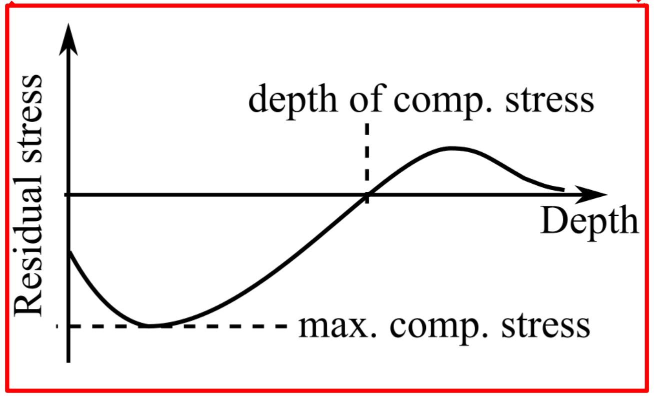
Result



Improving damage tolerance



Induced stress distribution



Process advantages

- Locally induced residual stresses
- Flexible controllability
- Minimal material changes

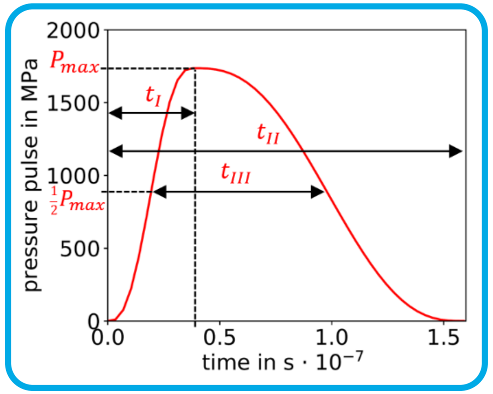
Residual stress fields can

- Slow down crack growth
- Increase fatigue resistance

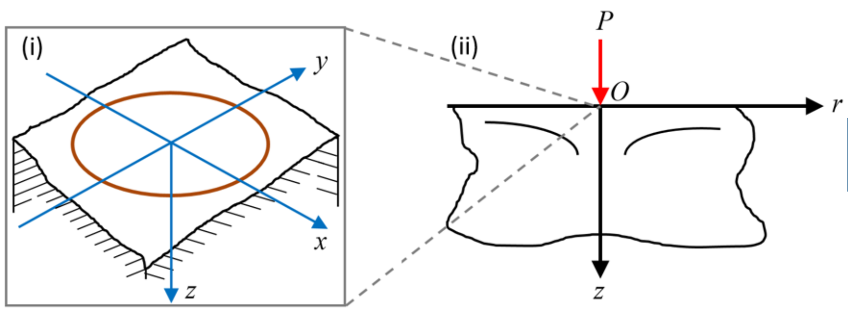
Helmholtz-Zentrum hereon

Case study 3: Problem statement
Enhance analytical model via ML to reach FE solution

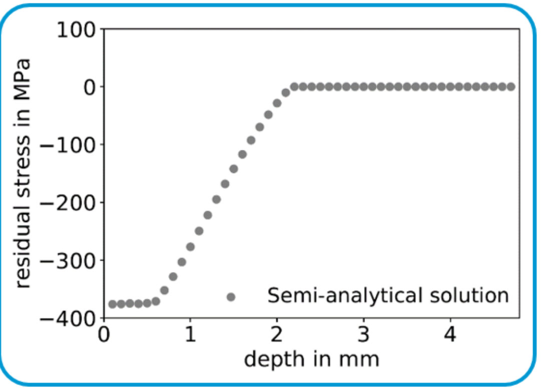
Input: Pressure pulse



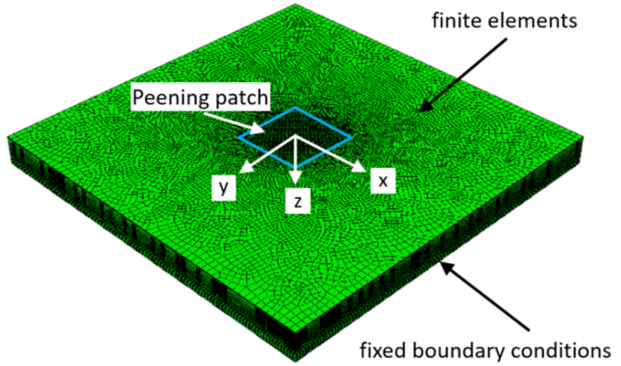
Low fidelity semi-analytical model



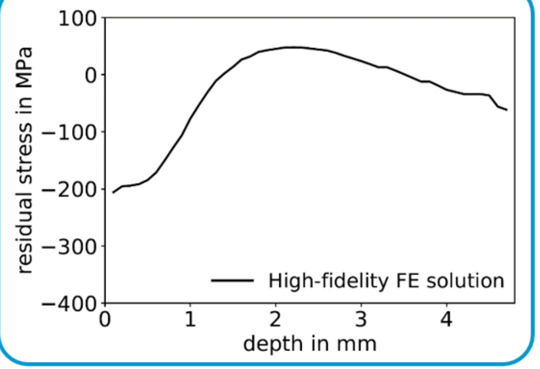
Output: Residual stress



High-fidelity finite element model

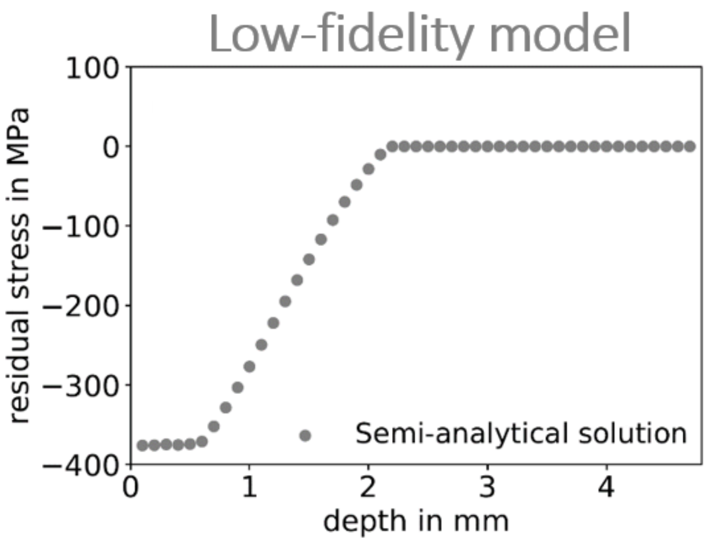


Output: Residual stress



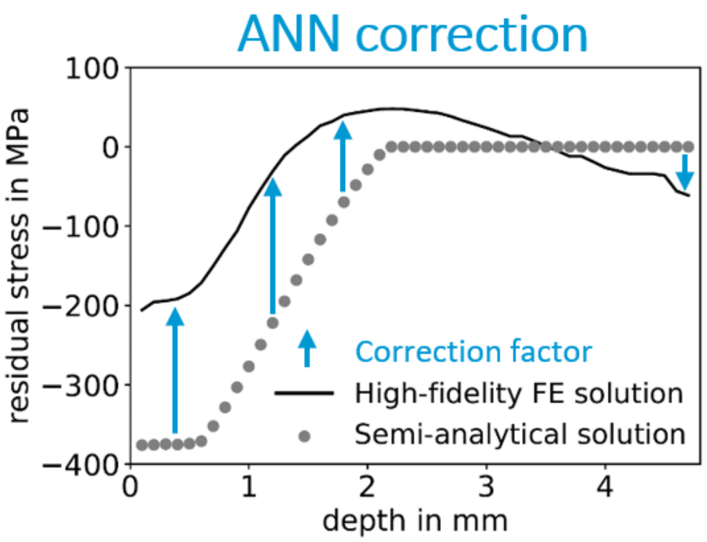
Helmholtz-Zentrum hereon

Case study 3: Methodology
Hybrid modelling implementation



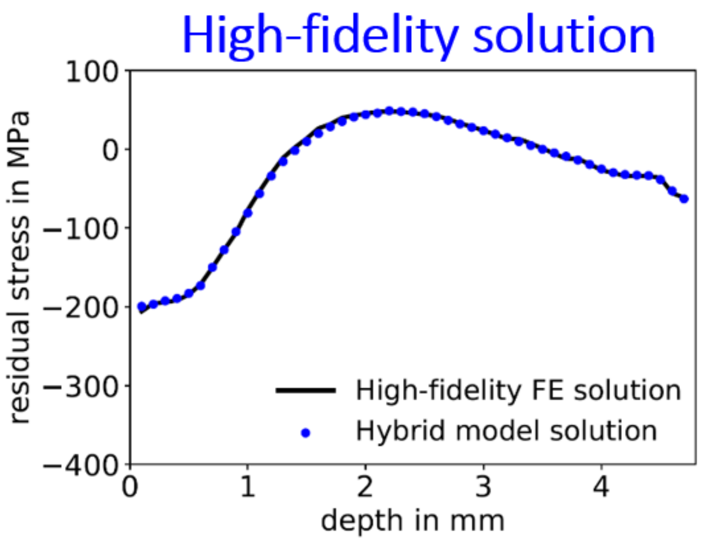
✓ physics-based
× high error

+



✓ data-driven
✓ reducing error

=



✓ data-driven
✓ physics-based
✓ low prediction error

Pulse parameter ranges:

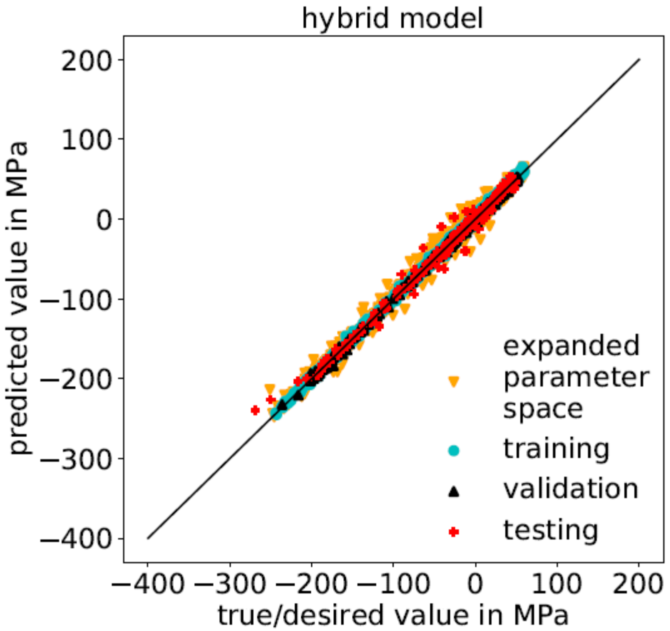
	P_{max} [MPa]	t_I [ns]	t_{II} [ns]
Min.	800	12	43
Max.	2200	66	300

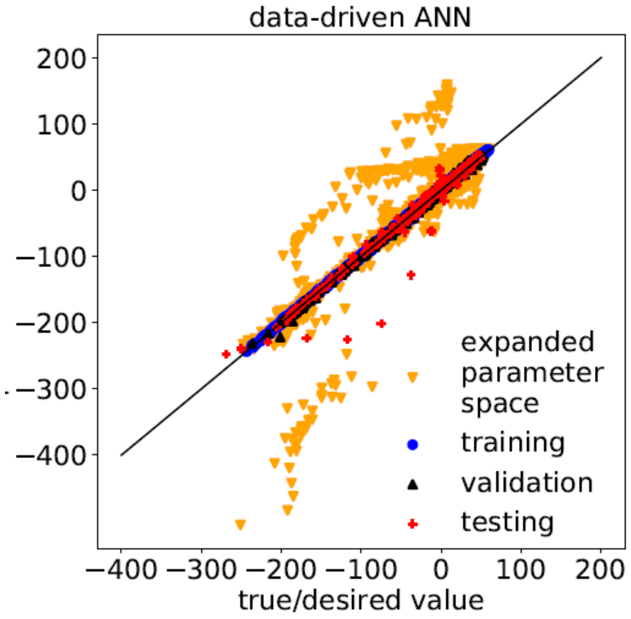
Material: AA2024-T3

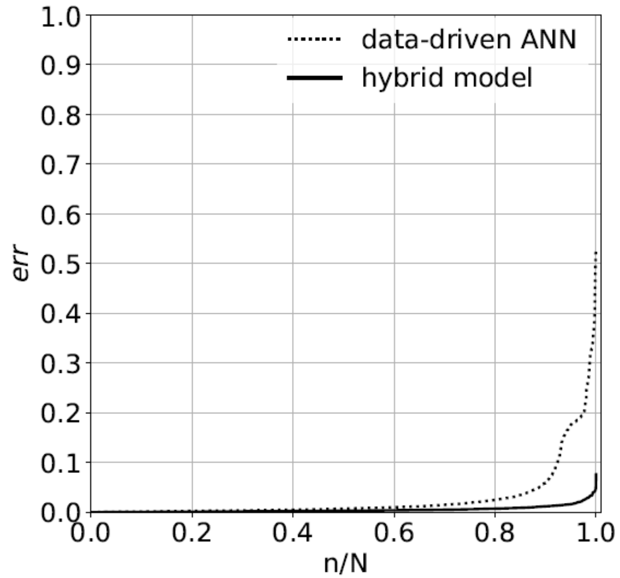
→ frequently used in aircrafts

Case study 3: Results

Benchmark: Extrapolation via hybrid and data-driven model







$$err := \left| \frac{d - y^N}{d} \right|$$

	Hybrid Model		Data-Driven ANN	
Data Set	**R^2 in %**	***MSE***	**R^2 in %**	***MSE* in MPa^2**
Training	99.90	4.33	99.86	6.32
Validation	99.86	7.38	99.76	12.39
Test	99.15	28.63	95.89	137.58
Expanded space	99.39	30.17	65.00	1717.18

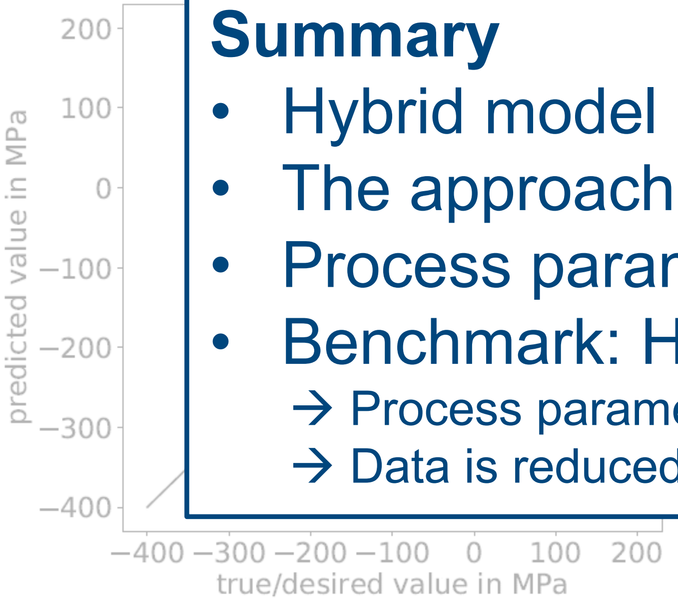
Main observations

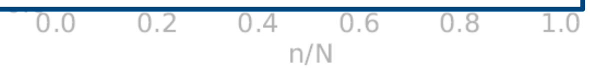
- Hybrid model: Very good performance
- Data-driven: inferior generalization

Helmholtz-Zentrum hereon

Case study 3: Results

Benchmark: Extrapolation via hybrid and data-driven model





Summary

- Hybrid model is efficient & accurate
- The approach exhibits good generalization
- Process parameter space is expandable within trained corrections
- Benchmark: Hybrid model outperformed data-driven model when
  → Process parameter-space is expanded
  → Data is reduced

$$err := \left| \frac{d - y^N}{d} \right|$$

	Hybrid Model		Data-Driven ANN	
Data Set	R^2 in %	MSE	R^2 in %	MSE in MPa^2
Training	99.90	4.33	99.86	6.32
Validation	99.86	7.38	99.76	12.39
Test	99.15	28.63	95.89	137.58
Expanded space	99.39	30.17	65.00	1717.18

Main observations

- Hybrid model: Very good performance
- Data-driven: inferior generalization

Conclusions

Case study 1 (Friction Riveting)

- Physics-based feature engineering improves prediction performance

Case study 2 (Friction Surfacing)

- Physics-based data-augmentation and data-mining enhances predictions
- Simulation assisted machine learning allows to keep experiments to a minimum

Case study 3 (Laser Shock Peening)

- Hybrid model is efficient & accurate with good generalization
- Process parameter space is expandable within trained corrections
- Hybrid model outperformed data-driven model (generalization on scarce data)

The authors gratefully acknowledge funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 101001567) within the ERC consolidator grant MA.D.AM.

erc
European Research Council
Established by the European Commission

Helmholtz-Zentrum
hereon

Thank You.

Publications:

Bock, F; Aydin, R.; Cyron, C.; Huber, N.; Kalidindi, S.R., Klusemann, B. A Review of the Application of Machine Learning and Data Mining Approaches in Continuum Materials Mechanics. Front. Mater. 2019, 6, 443.

Bock, F.; Keller, S.; Huber, N.; Klusemann, B. Hybrid Modelling by Machine Learning Corrections of Analytical Model Predictions towards High-Fidelity Simulation Solutions, *Materials* 2021, 14 (8), 1883.

Bock, F.E.; Kallien, S.; Huber, N.; Klusemann, B. (2024). Data-driven and physics-based modelling of process behaviour and deposit geometry for friction surfacing, Computer Methods in Applied Mechanics and Engineering 418, 116453.

Benjamin Klusemann
Helmholtz-Zentrum hereon GmbH
Institute of Materials Mechanics

Max-Planck-Straße | 21502
Geesthacht T +49 4152 87-2552
benjamin.klusemann@hereon.de

Helmholtz-Zentrum
hereon