Calibrating Complex Material Models: A Comparative Analysis of Hybrid Approaches

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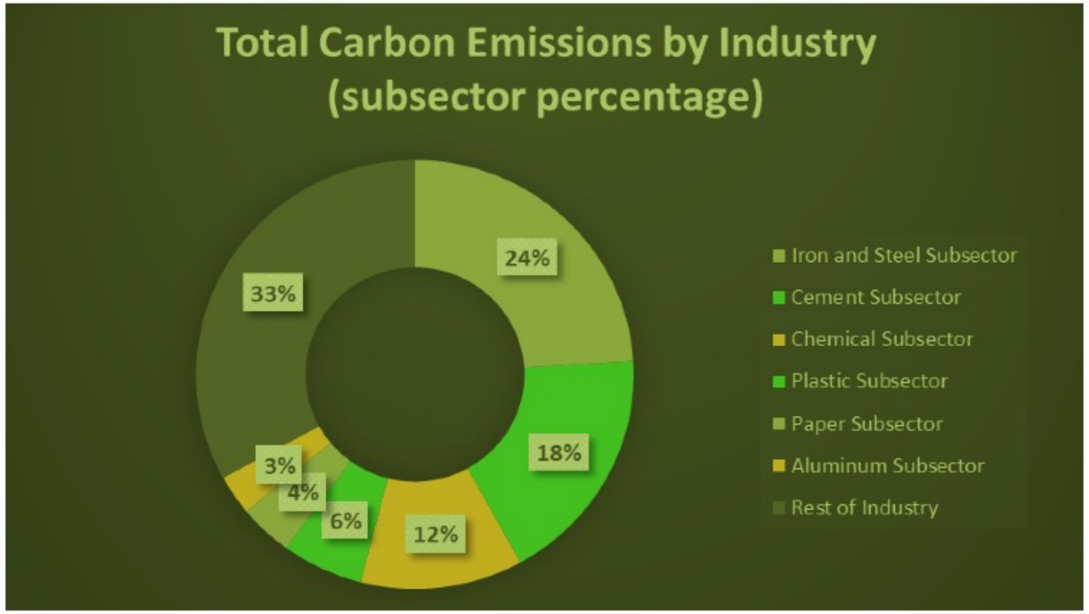
Agenda

1. Introduction
2. Bayesian Calibration
3. Point estimation with neural network model
4. Results
5. Conclusions

Introduction

Introduction

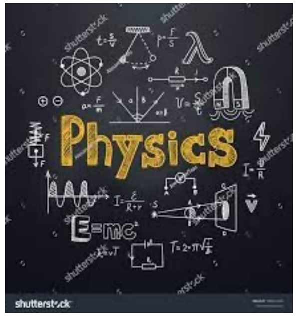
- **Motivation:** Carbon footprint of some materials, e.g. steel production with 20-25% of industrial CO2 emissions[1]
- **Need:** Accurate and fast predictions
- **Challenges:** Costly experiments, small data sets, computationally expensive models, lots of uncertainty
- **Objectives:** Development of hybrid approaches:
  - ✓ Better/faster predictions
  - ✓ uncertainty quantification



[8billiontrees.com]

1. *Clean Steel Partnership, Strategic Research and Innovation Agenda (SRIA) 2021*

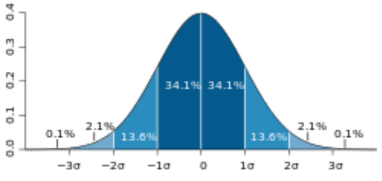
Physical Model-based, Probabilistic and Data-driven Methods


[shuttershock.com]

- Physical model-based methods: Use physical system knowledge and typically not much data e.g. CFD-simulation, Model-based control
- Probabilistic methods: Methods based on probability.

  Key to uncertainty quantification.

  e.g. Monte Carlo methods, Bayesian methods



[wikipedia.org]

- Data-driven methods: Typically use a lot of data and without any knowledge (no physical or probabilistic knowledge)

  e.g. Artificial neural networks


[computerhope.com]

- Recent advances in algorithm developments combine 2 of the 3 or even all 3 in some way
- But why and how?

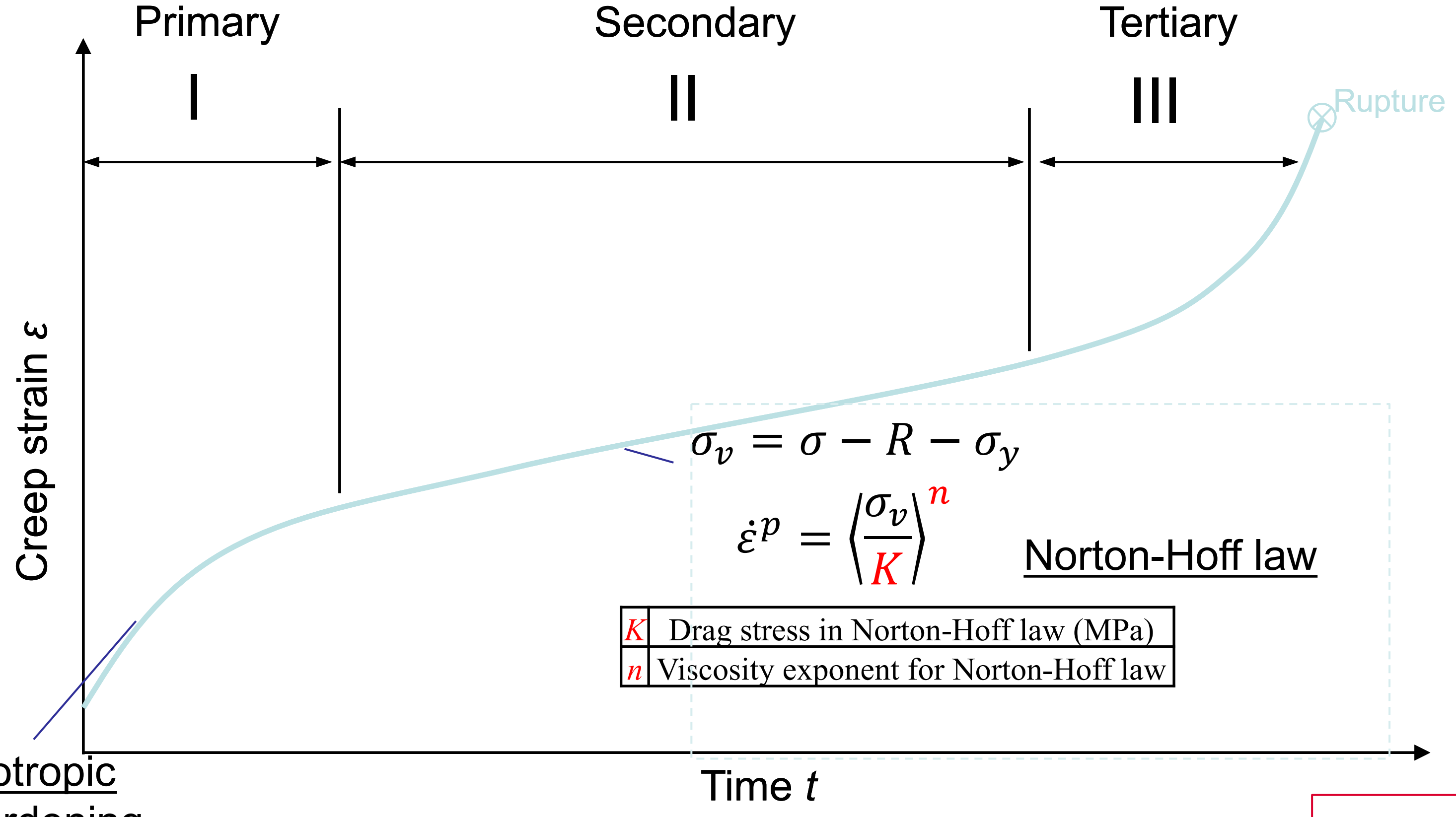
Advantages and Limitations

	Physical-model-based	Data-driven	Probabilistic
Advantages	Incorporate the physics: Provide understanding and visualization of the system	Do not require very much specialized knowledge	Ability to take into account uncertainty and variability in data -> Higher accuracy
	Designing, testing etc. can be quicker and less resource-intensive than building a prototype	Applicable to problems that cannot be analyzed physically	Can help identify patterns and relationships within data
	Allow for early detection of issues…	…	…
Limitations	Rely on assumptions	Ignore the physics	Potential for overfitting
	May involve many parameters to be identified	Accuracy of predictions depends on data quality	Not all data fits well into a probabilistic framework
	Development may be complex and time-consuming	Often require a large amount of data	May be computationally intensive
	Model discrepancies	Correlations are only valid within the range of the underlying dataset	Implementation may require significant resources
	Not easily adaptable to changes	…	…
	Implementation may be complex…		

KEY: combine to use advantages and control limitations

Modeling steel creep behavior

Elasto-visco-plastic model (Norton type + damage)[2]



$$\sigma_v = \sigma - R - \sigma_y$$

$$\dot{\varepsilon}^p = \left\langle \frac{\sigma_v}{K} \right\rangle^n$$

Norton-Hoff law

K	Drag stress in Norton-Hoff law (MPa)
n	Viscosity exponent for Norton-Hoff law

Isotropic hardening

$$R = Q\left(1 - e^{-bp}\right)$$

b	Rate of isotropic hardening
Q	Total isotropic saturation size of the yield surface

Elasticity

T	Temperature (C°)
E	Young's modulus (MPa)
v	Poisson's Ratio

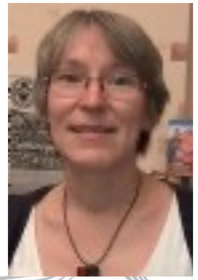
Load: 180MPa

Here to-be-estimated parameters

"**Creep** is a phenomenon of slow plastic deformation (elongation) of a metal at high temperature under a constant load."
- Dr. Dmitri Kopeliovich

Here: neglect III stage/damage

Modified slide from original provided by Fan Chen and Anne Marie Habraken (Uliège)



2. H. Morch (Uliège, 2022): Thermomechanical modelling of the creep-fatigue behaviour and damage of Nickel-alloy receiver tubes used in Concentrated Solar Power plants.

European Commission

Bayesian Calibration

Bayesian Calibration[3]

- 4 cases: 1) no discrepancy error and inexpensive model, 2) no discrepancy error and expensive model, 3) discrepancy error and inexpensive model, 4) discrepancy error and expensive model → Here: 2)

Data:
- Experimental: $\{\bar{x}_i, \bar{y}_i\}_{i=1}^{N}$
- Synthetic: $\{\tilde{x}_j, \tilde{t}_j, \tilde{y}_j\} = \eta(\tilde{x}_j, \tilde{t}_j)\}_{j=1}^{M}$

$\xrightarrow{x,\ t}$ Gaussian Process (GP) Surrogates (for discrepancy error and model) → Bayesian formulation: likelihood, priors, Bayes' theorem & MCMC →

θ physical model parameters
χ GP hyperparameters
σ experimental error hyperparameter

ACBICI tool

Output = Simulator + exp. error

$$y_i = \eta(x_i, \theta) + \epsilon_i$$

Posterior:

$$p(\theta, \chi, \sigma | y) = \frac{p(y|\theta, \chi, \sigma)p(\theta, \chi, \sigma)}{p(y)}$$

Via MCMC with

Likelihood: $p(y|\theta, \chi, \sigma) \propto \det(\Sigma)^{-\frac{1}{2}} \exp(-\frac{1}{2} y\, \Sigma^{-1} y)$

And Priors for θ, χ, σ

Goals:
- Surrogate for expensive FE model (FEMo)
- Estimate FEMo parameters
- Uncertainty quantification
- Predict creep strain

3. Kennedy, M.; O'Hagan, A. Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 2001, 63, 425–464.

Point estimation with NN model

Point estimation with NN model

Challenges:

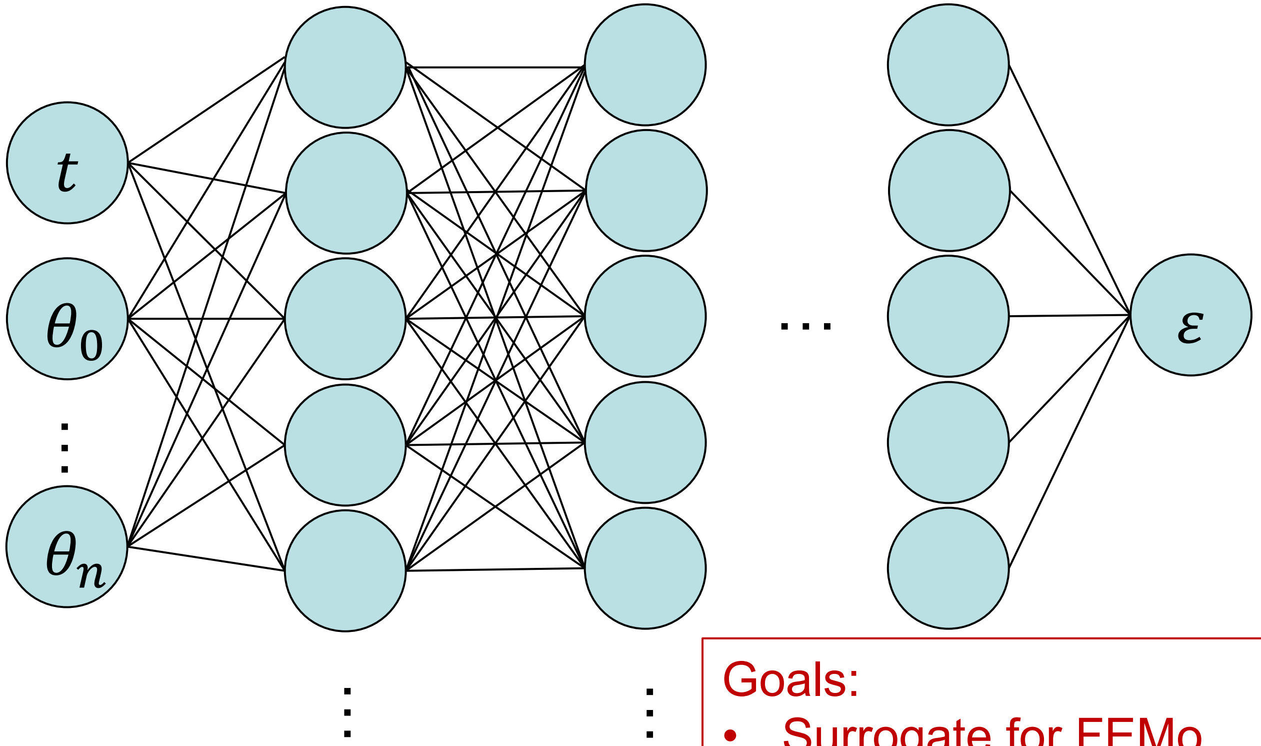
- NN require data set that model has not seen before
- physical model parameters θ for experimental data set unknown

Method:

- Training of m NNs with synthetic data coming from physical simulations (Hyperparameter optimization with Optuna, and varying kernel initializers)
- Point estimation with experimental data and NN models (Nelder-Mead method)

$$min_\theta \parallel \varepsilon_i^{exp} - NN^k\left(t_i^{exp}, \theta\right) \parallel for\ k = 1, \ldots m$$

✓ Optimal model parameters $\theta_0, \ldots, \theta_n$ with uncertainty



Goals:

- Surrogate for FEMo
- Estimate FEMo parameters
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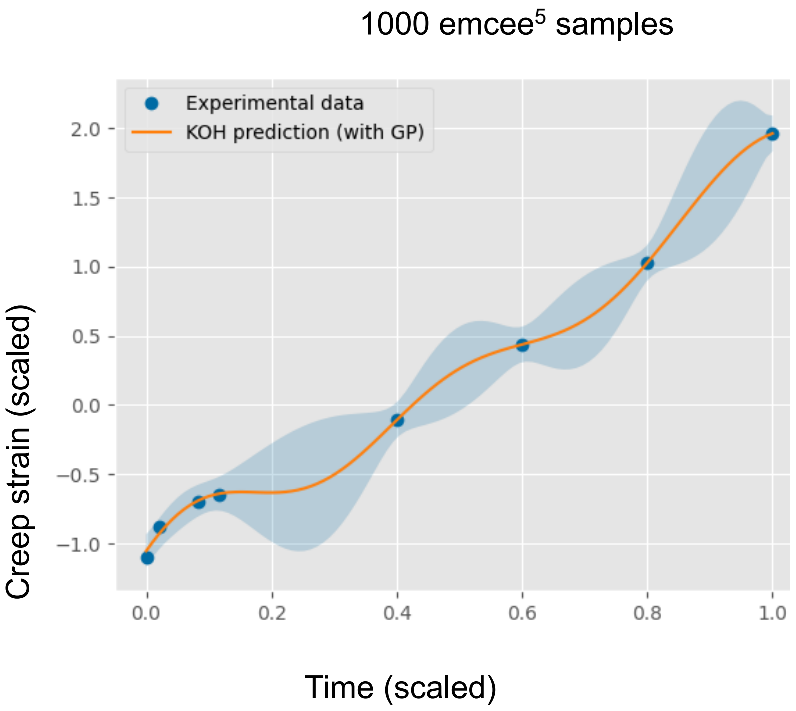
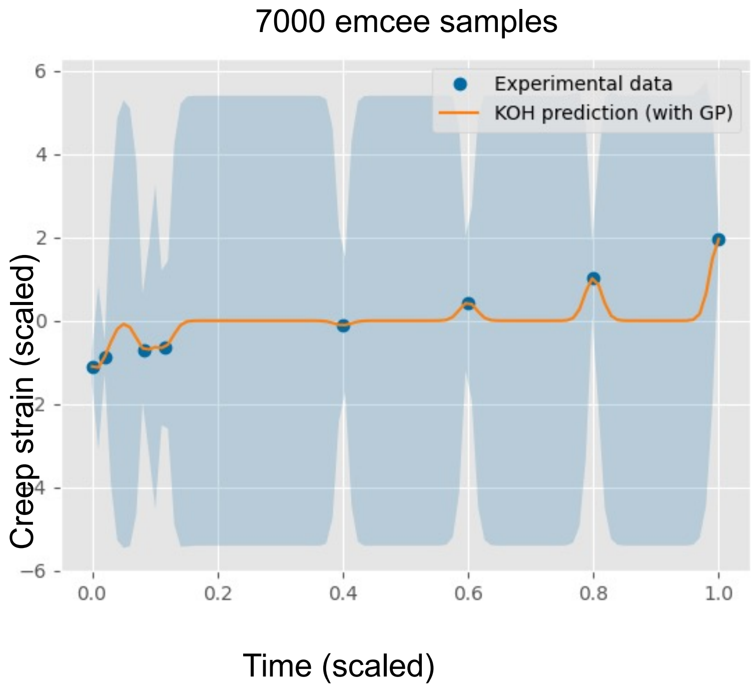
Results

Bayesian Calibration





Data:
- 8 experimental data points[4]
- 200 random synthetic data points from FE simulations (Lagamine from Uliege*)

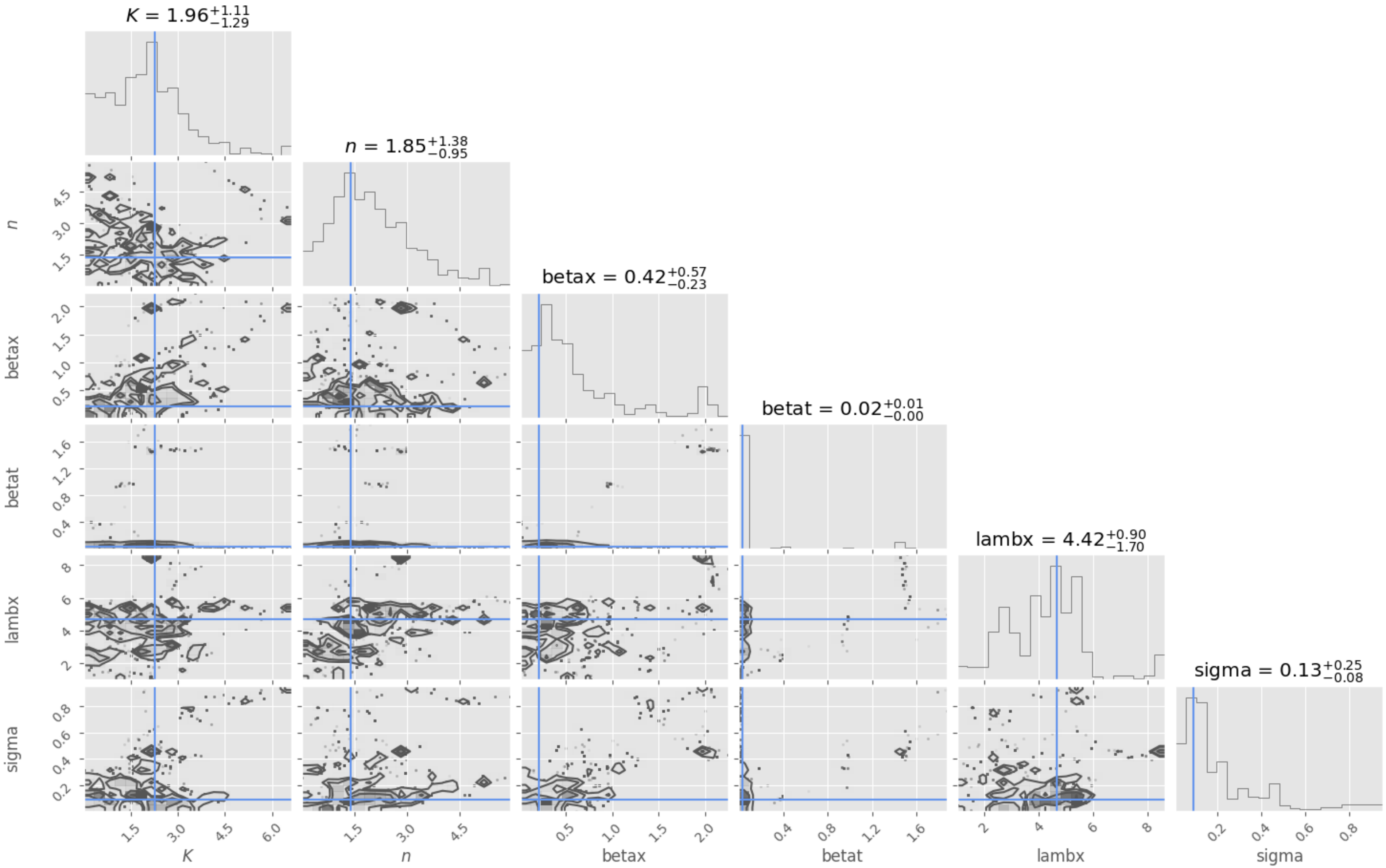
Uncertainty:
- Aleatoric and epistemic uncertainty

**** Fan Chen, Carlos Rojas, Anne Marie Habraken (Uliège)***

4. Schemmel (2003): Beschreibung des Verformungs-, Festigkeits- und Versagensverhaltens von Komponenten im Kriechbereich unter instationärer Beanspruchung mit einem elastisch-viskoplastischen Werkstoffmodell, PhD thesis
5. Foreman-Mackey, Goodman, Weare (2010): emcee: The MCMC Hammer, arXiv:1202.3665

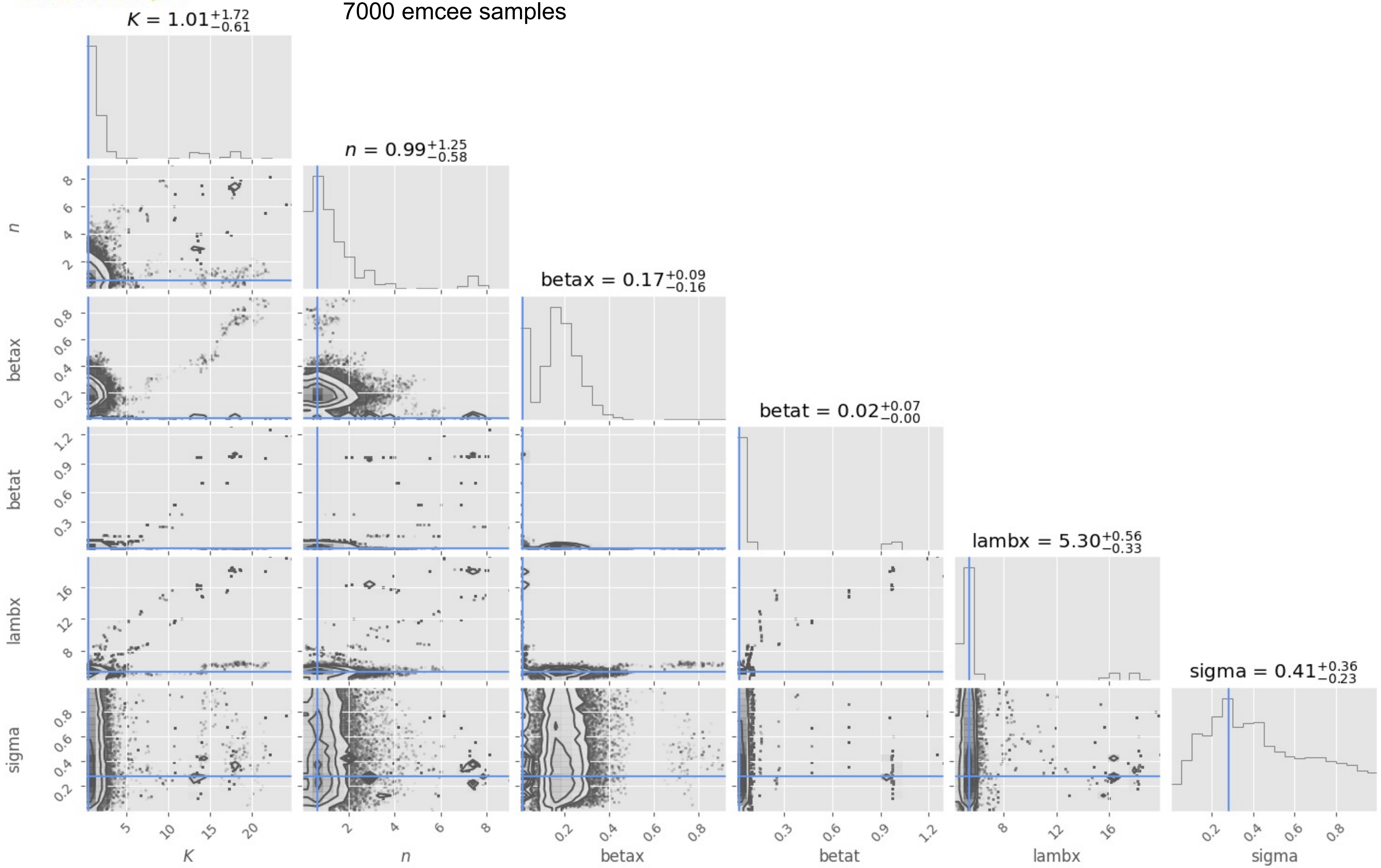
Distributions 1/2

1000 emcee samples

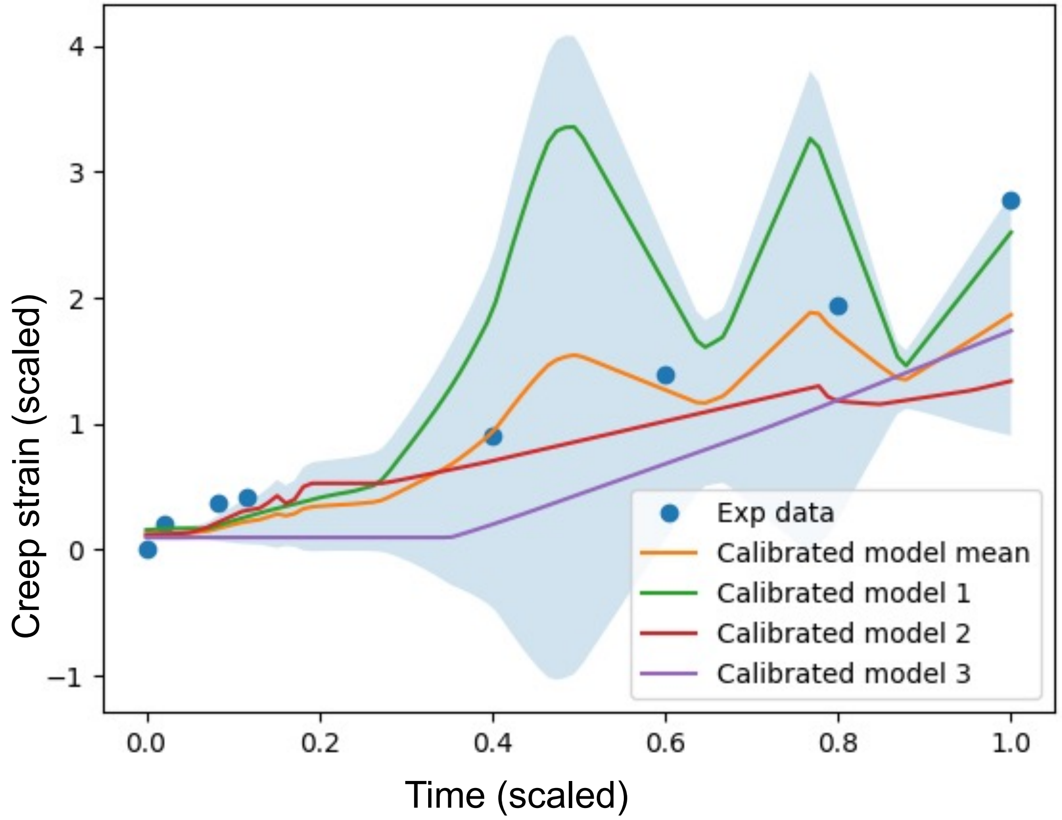


Distributions 2/2

7000 emcee samples



Point estimation with NN model



Data:

- 200 random synthetic data points from FE simulations (Lagamine from Uliege*), 80% for training, 20% for testing
- 8 experimental data points[4] (for point estimation)

Uncertainty:

- Epistemic Uncertainty

Conclusions

Conclusions and Outlook

- ✓ Need for hybrid approaches that are smart and reliable and address common issues such as overfitting, bias, and debugging assistance
- ✓ Bayesian calibration promising candidate less biased and less data-dependent than NN-approach, but still depends on the choice of priors, Gaussian process surrogate and available data
- ✓ NN and point estimation approach much easier to set up but introduces strong bias and is very data-dependent

Outlook:

- ➢ Smart creation of an informative synthetic data set
- ➢ Sampling and convergence studies for Bayesian calibration
- ➢ Include discrepancy error estimation for Bayesian calibration
- ➢ Estimate main parameters of all stages
- ➢ Speed up methodology

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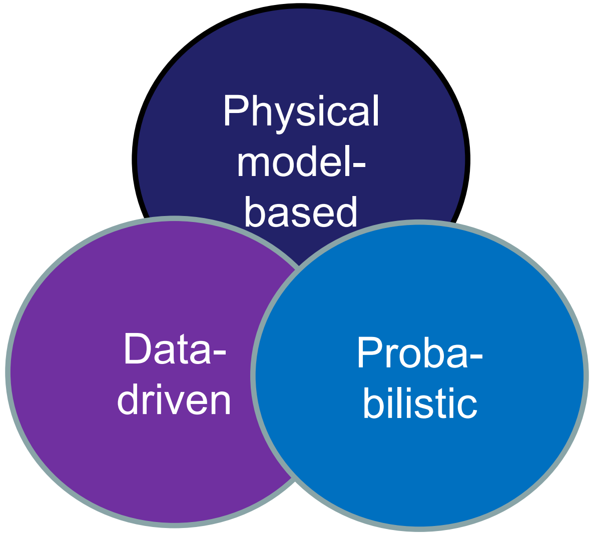
More information

- https://aid4greenest.eu
- https://www.linkedin.com/company/aid4greenest-project/
- http://www.youtube.com/@AID4GREENESTOfficialAccount
- AI guided microstructure exploration. Building database and looking for contributors: https://microstructuredb.com
- About my work:



THANK YOU!