ACBICI – A Library for the Calibration of Complex and Expensive Models

Christina Schenk (christina.schenk@imdea.org), IMDEA Materials
Ignacio Romero, Universidad Politécnica de Madrid, IMDEA Materials

CMN 2024, Aveiro, Portugal

The AID4GREENEST project has received funding from Horizon Europe under Grant Agreement nº 101091912

Agenda

1. Introduction and Motivation
2. Bayesian Calibration
3. Results
4. Conclusions

Introduction and Motivation

Background: Modeling

Models

...the sciences do not try to explain, they hardly even try to interpret, they mainly make models. By a model is meant a mathematical construct which, with the addition of certain verbal interpretations, describes observed phenomena.

- John von Neumann (1903-1957)

- Many models exist for every single phenomenon
- Predictions are as good as the model
- Models are as good as their calibration
- Calibrations are as good as the data

Background: Calibration

Calibration

The process of finding optimal values for the parameters in a model that make the predictions of the latter as close as possible to physical events.

But optimal in which sense?

- Not too difficult or costly to be estimated -> fast
- Yield a model that accurately reproduces calibration data -> accurate
- That also predicts behavior for left-out experimental data -> uncertainty quantification
- That yield a robust model -> uncertainty quantification
- That they reflect expected behavior/values -> uncertainty quantification

Standard Least-Squares Calibration

Pros and cons

- Simple ✓
- Solution depends on regularization parameter ✗
- Local minima? ✗
- How sure are we and Sensitivity? -> can give confidence intervals but often very wide ✗
- What is the effect of experimental errors? -> Assumed to be Gaussian ✗

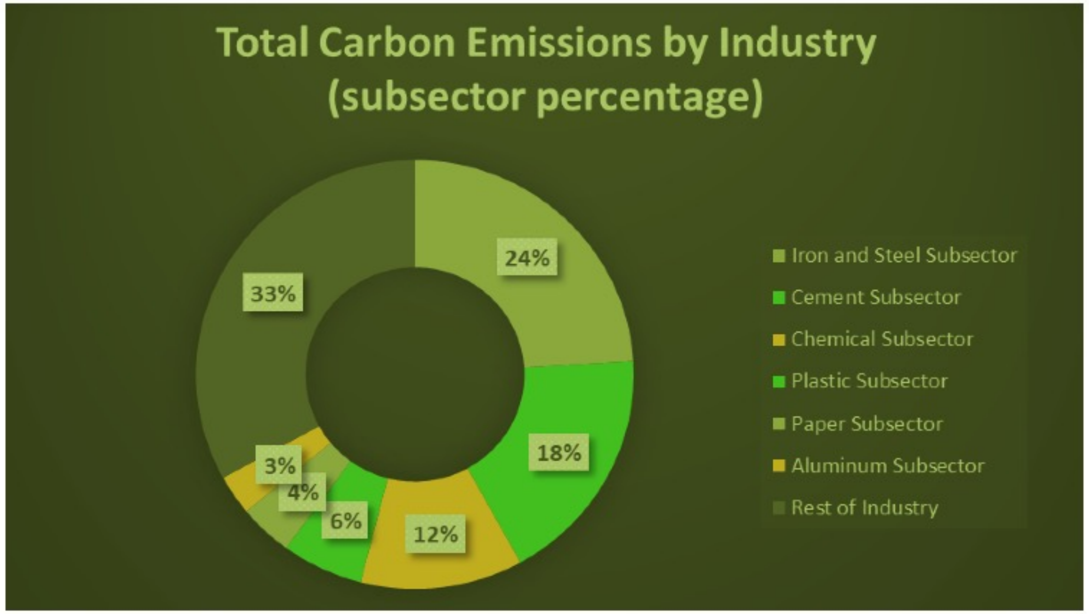
Advanced Bayesian Calibration (ACBICI) as a "better" way of calibrating any model

- Fast predictions via surrogate for expensive models
- Aleatoric (data, statistical) and epistemic (model, systematic) uncertainty quantification
- Estimation of experimental errors

Base approach not new in statistics community but first Python library with additional features

Motivation

- **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:**
  - ✓ Better/faster predictions
  - ✓ uncertainty quantification

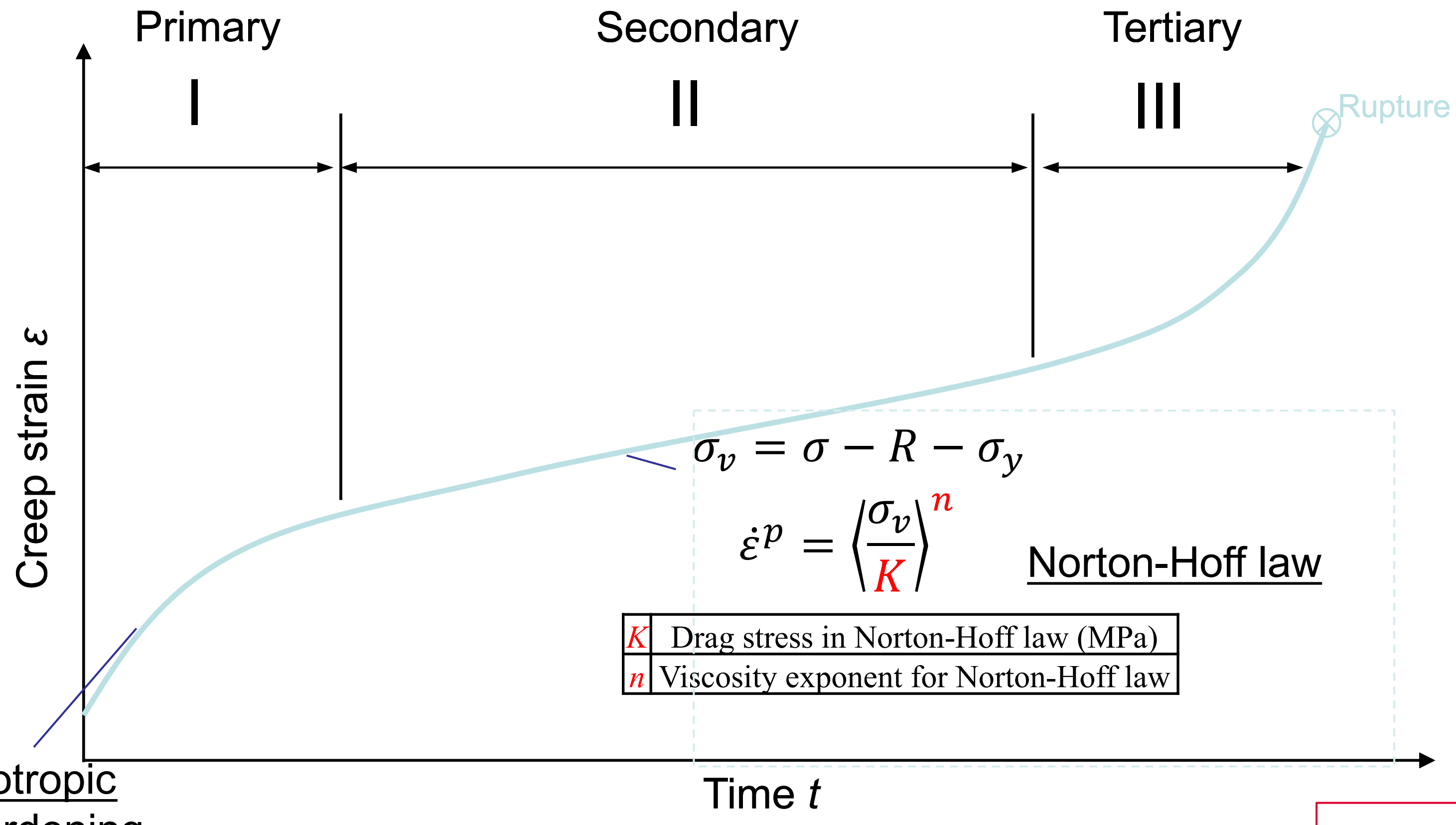


[8billiontrees.com]

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

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

"**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)

Here to-be-estimated parameters

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: 4)

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

→ 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

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

Output = Simulator + discrepancy + exp. error

$$y_i = \eta(x_i, \theta) + \delta(x_i) + \varepsilon(x_i), \quad i = 1, \cdots, N$$

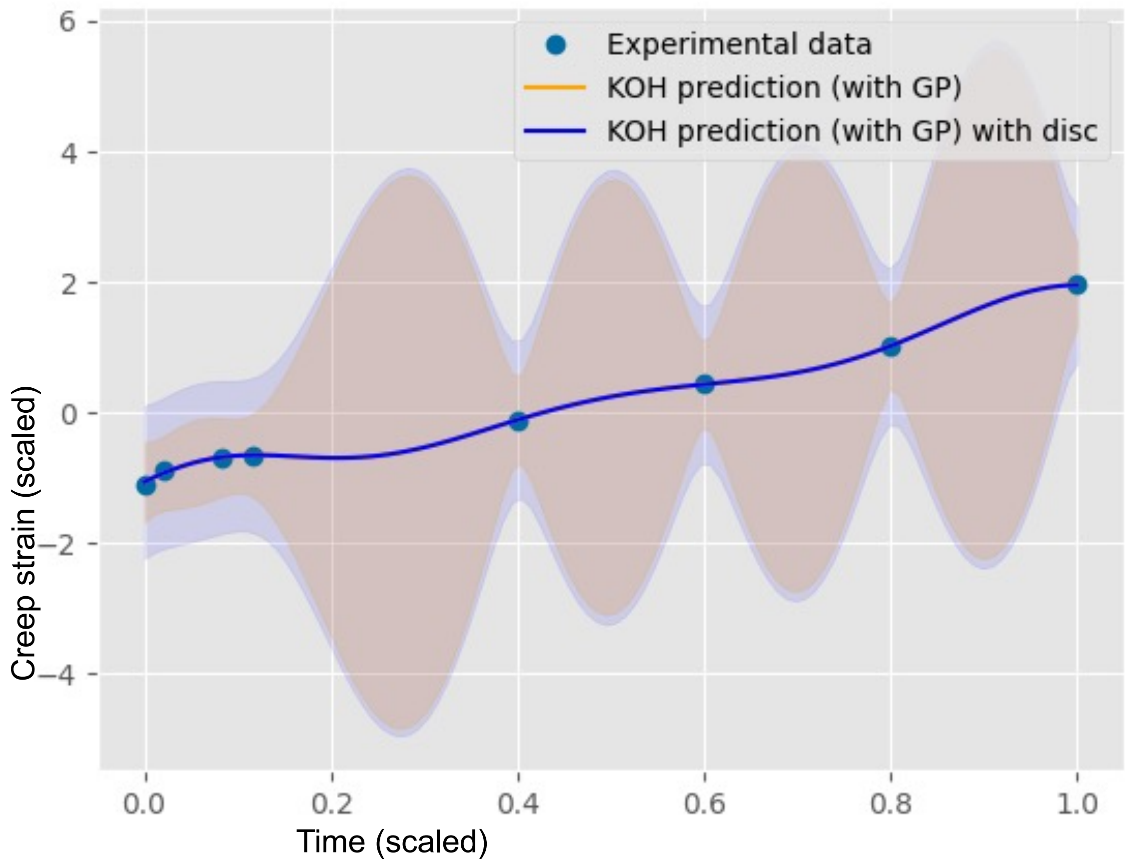
Goals:
- Surrogate for expensive FE model (FEMo)
- Estimate FEMo parameters
- Uncertainty quantification
- Predict creep strain

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.

Results

Bayesian Calibration with Discrepancy Estimation

100,000 emcee[5] samples



Data:

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

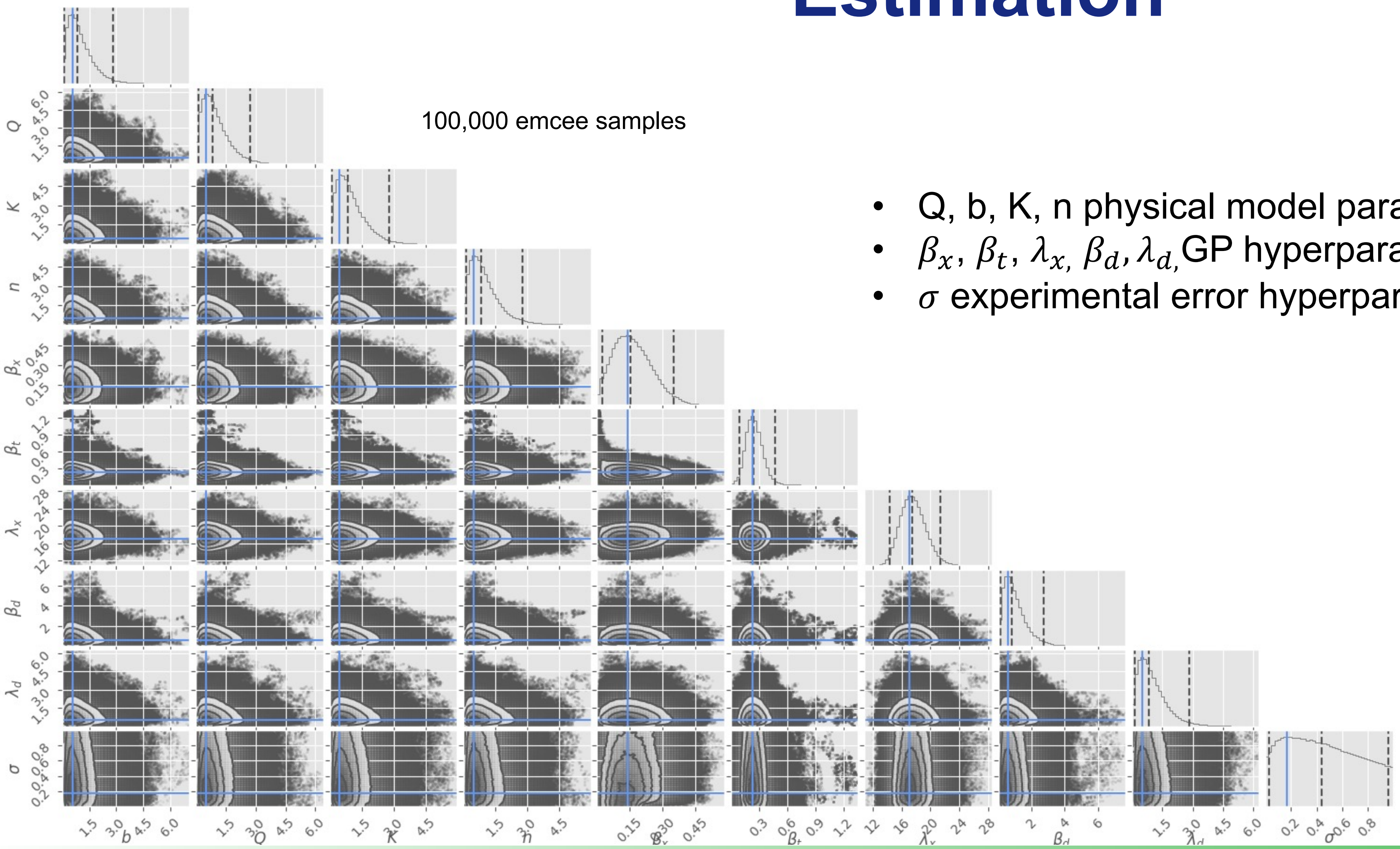
Uncertainty:

- Uncertainty (aleatoric and epistemic)
- Uncertainty (with quantified model discrepancy)

**** 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 with Discrepancy Estimation



100,000 emcee samples

- Q, b, K, n physical model parameters
- β_x, β_t, $\lambda_{x,}$ β_d, $\lambda_{d,}$GP hyperparameters
- σ experimental error hyperparameter

Conclusions

Conclusions

- ✓ Bayesian calibration has many advantages over standard least-squares calibration:
  - ✓ Uncertainty quantification (model and data)
  - ✓ Distributions of the parameters -> sensitivities
  - ✓ Estimation of experimental error
  - ✓ Surrogate models for faster predictions
  - ✓ Option of using priors
- ✓ ACBICI as **first python library with all these features**
- ✓ ACBICI has been successfully applied for different types of models from **creep (here)** to cell calibration

Outlook

Outlook:

- Creep:
  - Estimate parameters of all creep stages (including damage)
  - Include fracture time prediction
  - Estimation for different loads
  - Estimation for microscopic model
- ACBICI: More models/applications and enhancements
- …

Acknowledgements

(l2r) Contributors and Collaborators: Ignacio Romero (UPM, IMDEA Materials), Ilchat Sabirov (IMDEA Materials), Fan Chen, Carlos Rojas, Anne Marie Habraken (University of Liège)

Funded by the European Union

Disclaimer:
This project has received funding from the European Commission under the European Union's Horizon Research and Innovation programme (Grant Agreement No. 101091912).
Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

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!