Sandia National Laboratories

Bayesian Model Calibration for Functional Data Using Elastic Alignment

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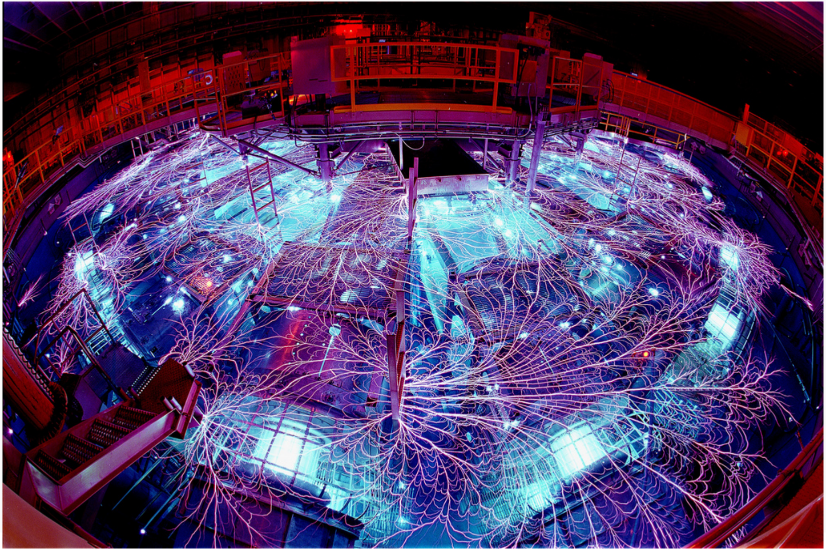
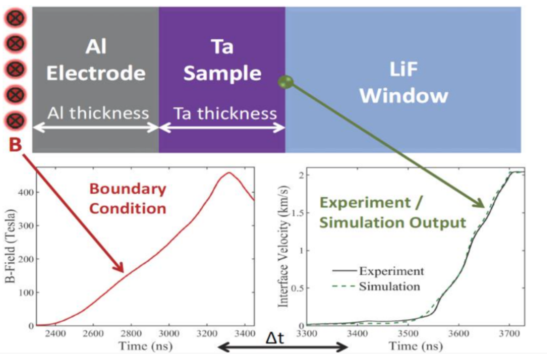
Background

- **Dynamic material properties experiments**: access to the most extreme temperatures and pressures attainable in a laboratory.
- **Sandia National Labs Z-machine**: pulsed power driver that can deliver massive electrical currents over very short timescales (of the order of 25MA over $1\mu s$).
- **Goal:** understanding of material models at extreme conditions by coupling computational simulations with experimental data.
- **Parameters of interest are physical**: material properties with 'true' value that is of interest.
- **Initially**: Calibrate a well-understood model - two parameters of the equation of *state of tantalum*.

Z-Machine



Experimental setup



- By coupling experimental and simulated velocity traces, parameters of the tantalum (Ta) equation of state (EOS) can be estimated
- Massive electric currents treated as boundary conditions.
- Stress wave propagates thru system.

Equation of the state model (Vinet curve)

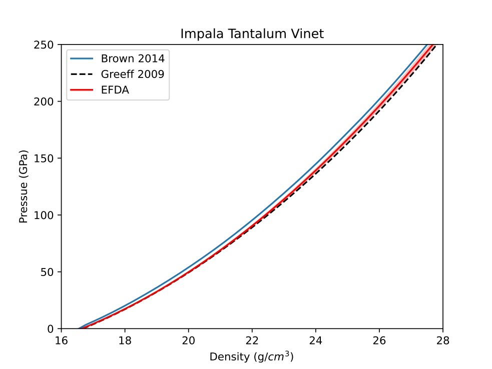


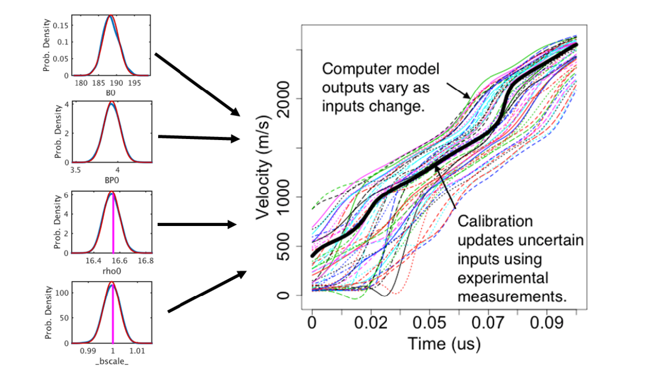
Figure: Elastic BMC compared with the analytic results in Brown et. al 2014 and theoretical calculations in Greef et al. 2009.

- Physically motivated form

$$P(\rho) = 3B_0 \left(\frac{1-\eta}{\eta^2}\right) \exp\left(\frac{3}{2}(B_0' - 1)(1-\eta)\right).$$

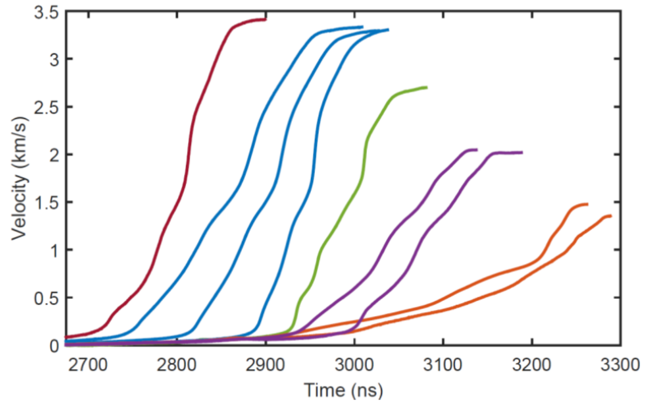
- where $\eta = \sqrt[3]{\rho_0/\rho}$, ρ_0 is the initial density
- B_0 and B_0' are the bulk modulus and its pressure derivative at ambient conditions.

Calibration



- Uncertain inputs generate velocity curves using a computer model.
- Probability distributions look for “agreement” of outputs and measurements.

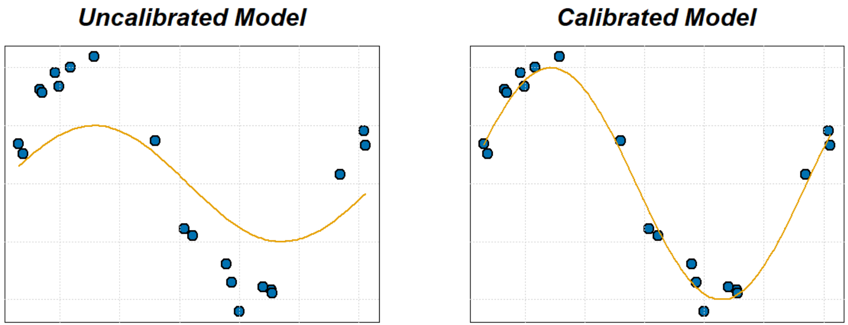
Challenge



- How to accurately estimate uncertainties?
- Calibration parameters have physical interpretation.
- Lots of *nuisance* parameters.
- Bayesian framework is natural in this context

Approach

- Bayesian Model Calibration (BMC) (Kennedy & O'Hagan 2001) often used to "tune" computer model.
- *Calibrated* model for prediction (interpolation).



BMC with Functional Response

- With functional data a common calibration model stems from Kennedy & O'Hagan 2001,

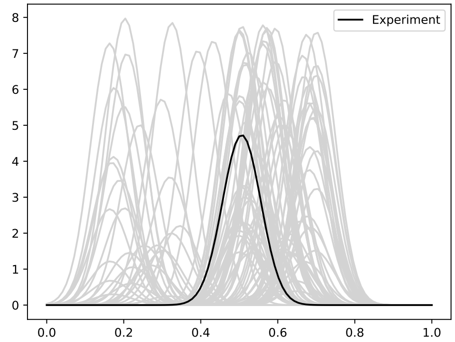
$$y_i^E(t) \quad = f^M(t, \boldsymbol{\theta}, \mathbf{x}_i) + \delta(t, \mathbf{x}_i) + \epsilon_i(t), \quad \epsilon_i(t) \sim N(0, \sigma_i^2(t))$$

- $\boldsymbol{\theta}$ are the calibration (input) parameters.
- $f^M(t, \boldsymbol{\theta}, \mathbf{x}_i)$ denote a simulation on the fixed and known settings.
- $\delta(t, \mathbf{x}_i)$ denotes model discrepancy (typically a G-P).
- $\epsilon_i(t)$ represent all other sources of error.

Goal: infer $\boldsymbol{\theta}$, $\delta(\cdot)$, and $\sigma_i^2(\cdot)$.

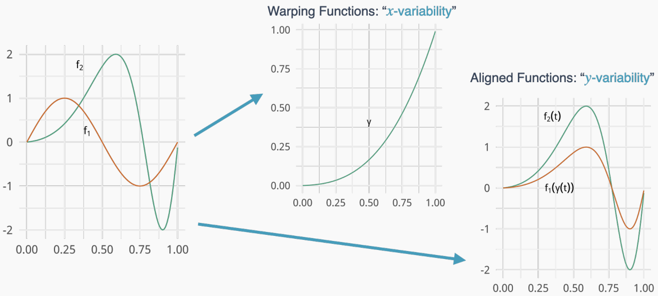
Elastic BMC Example

- Grey curves are computer generated functions with random parameters.
- Black curve is presumed experimental data under certain initial conditions.
- Calibration will be hard!



Elastic BMC Example

Idea: Align the functions using elastic FDA before calibration so phase and amplitude variability can be treated separately



Left: Original functions. Middle: Warping Function ("phase variability"). Right: Aligned functions ("amplitude variability").

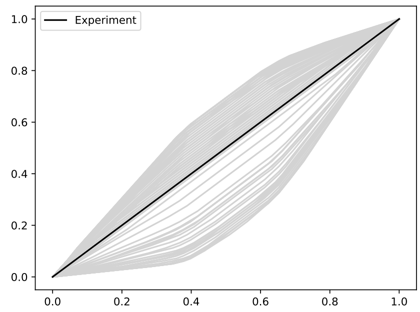
Elastic BMC Example

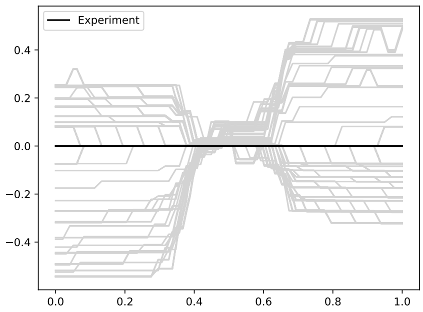
- Each function is a parameterized Gaussian pdf:

$$y(t,\boldsymbol{u}) = \frac{u_1}{0.05\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{t-(\sin(2\pi u_0^2)/4 - u_0/10 + 0.5)}{0.05}\right)^2\right) + 0u_2.$$

- The calibration parameters are $\boldsymbol{u} = [u_0, u_1, u_2]$, though the model only uses the first two of these parameters.
- 100 functions (model runs) using $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_{100}$ where each $\boldsymbol{u}_j$ was sampled uniformly within the unit cube.
- The 'experimental data' was generated using the parameter values $\boldsymbol{u}^* = [0.1028, 0.5930, 0]$

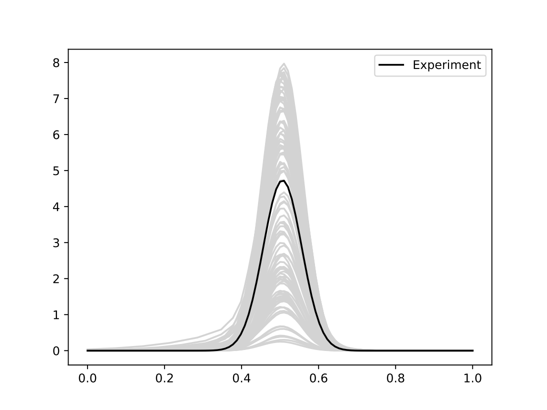
Elastic Functional Data Analysis





- Decompose functions into “warping functions” and “shooting vectors”.
- This accounts for amplitude/phase variability.

Elastic Functional Data Analysis



- Mapping back aligns simulation with the experimental data.

Elastic Bayesian Model Calibration

- We decompose the observations into aligned functions and warping functions with

$$y_i^E(t) = y_i^E(t^*) \circ \gamma_i^E(t) \tag{1}$$

- Similarly we decompose the computer output into aligned functions and warping functions with

$$y^M(t, \mathbf{x}_j) = y^M(t^*, \mathbf{x}_j) \circ \gamma^M(t, \mathbf{x}_j). \tag{2}$$

- The decomposition can occur by aligning the model to the experimental.

Elastic Bayesian Model Calibration

- To facilitate modeling, we transform the warping functions into shooting vector space with

$$\boldsymbol{v}_i^E = \exp_\psi^{-1}\left(\sqrt{\dot{\gamma}_i^E}\right) \tag{3}$$

$$\boldsymbol{v}^M(\boldsymbol{x}) = \exp_\psi^{-1}\left(\sqrt{\dot{\gamma}_i^M(\boldsymbol{x})}\right). \tag{4}$$

- We then calibrate the aligned data and shooting vectors with

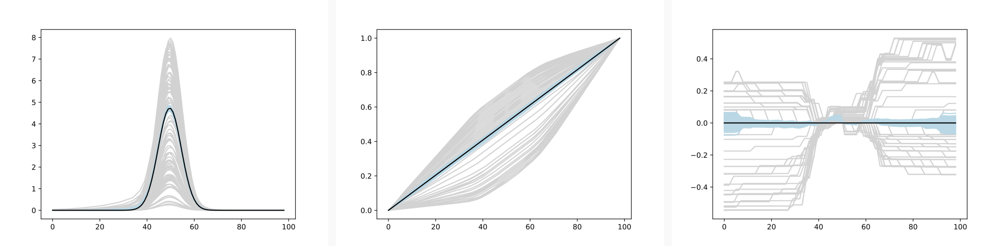
$$y^E(t^*) = y^M(t^*, \theta) + \delta_y(t^*) + \epsilon_y(t^*), \quad \epsilon_y(t^*) \sim N(0, \sigma_y^2) \tag{5}$$

$$\boldsymbol{v}^E = \boldsymbol{v}^M(\theta) + \boldsymbol{\delta}_v + \boldsymbol{\epsilon}_v, \quad \boldsymbol{\epsilon}_v \sim N(0, \sigma_v^2 \boldsymbol{I}). \tag{6}$$

- Implemented in framework named 'Impala' : Python tool for modular BMC.

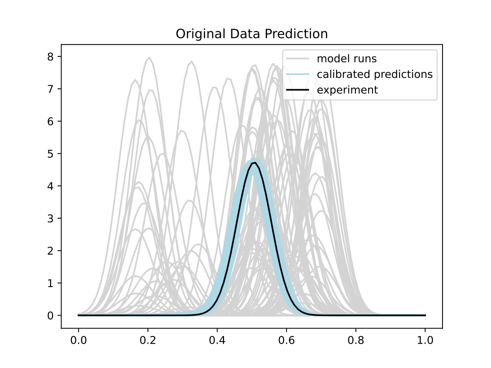
Elastic BMC Example Results

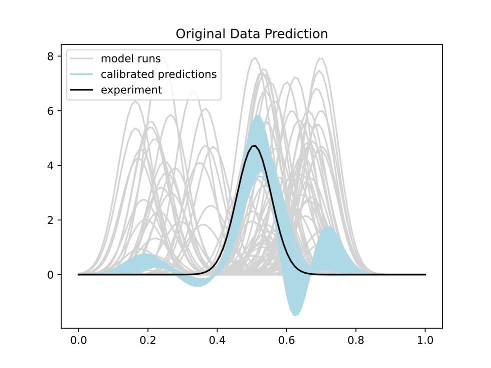
After fitting separate BMARS emulators for the aligned curves and the shooting vectors and performing a (modular) elastic Bayesian model calibration:



- Predictive posterior samples of curves/warping functions/shooting vectors after calibration of the simulated data variability.

Elastic BMC Example Results

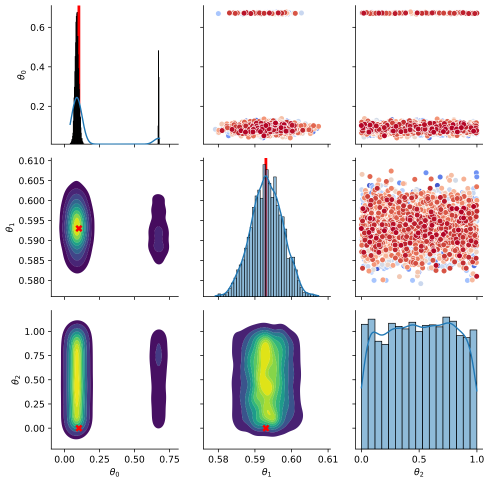




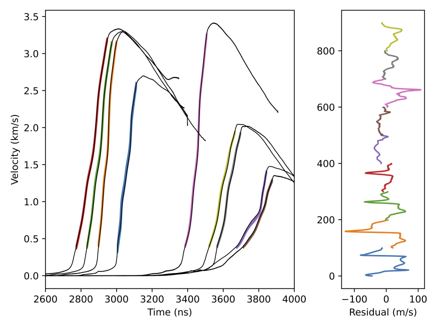
- Left: Predictive posterior samples using elastic BMC
- Right: Predictive posterior samples without alignment

Elastic BMC Example Results

- Posterior distributions. Truth shown by x's and vertical line
- Posterior distributions capture true values with less uncertainty using elastic BMC

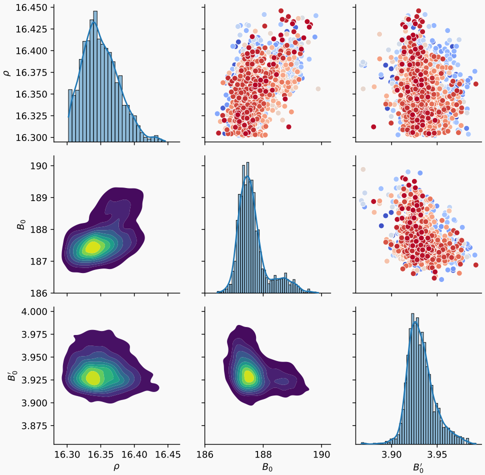


Dynamic material property calibration

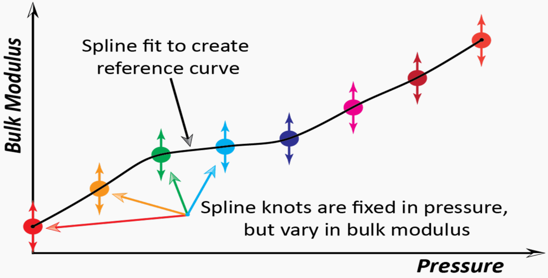


- Left: Experiment velocities of Ta shown in black compared with 95% prediction intervals from the elastic functional Bayesian calibration.
- Right: Corresponding color- coded residuals (difference between experiment and calibration mean) for each experiment

Dynamic material property calibration



Extension



- Extend BMC to cases where key relationships are "semi-parametric" or "non-parametric"
- These results will feed into NNSA's dynamic material program and are used by design labs (LANL, LLNL).
- Inform a variety of models and assessments.

Paper/Software

Paper

- **Francom, D. Tucker, J.D., Huerta, G., Shuler, K.W., Ries, D. (2023). Elastic Bayesian Model Calibration.**
- Pre-print: https://arxiv.org/abs/2305.08834

Software

- Elastic FDA: https://github.com/jdtuck/fdasrsf_python
- Impala: https://github.com/lanl/impala
- BASS: https://github.com/lanl/pyBASS

Publications

- Brown J. and Hund, L.B. (2018). Estimating material properties under extreme conditions by using Bayesian model calibration with functional outputs. In *Journal of the Royal Statistical Society-Series C*
- Rumsey, K., Huerta, G., Brown, J. and Hund, L.B. (2020). Dealing with Measurement Uncertainties as Nuisance Parameters in Bayesian Model Calibration. In *ASA/SIAM Journal of Uncertainty Quantification*
- Rumsey, K. and Huerta, G. (2021). Fast Matrix Algebra for Bayesian Model Calibration. In *Journal of Statistical Computation and Simulation.*
- Rumsey, K., Huerta, G. and Tucker, J.D. (2023). A Localized Ensemble of Approximate Gaussian Processes for Fast Sequential Emulation (in revison).