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Calibrating dynamic material properties with functional output using Bayesian model calibration

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Abstract

In experiments conducted on the Z-machine, dynamic material properties cannot be analyzed using traditional analytic methods, necessitating solving an inverse problem with a functional output, velocity over time. Bayesian model calibration (BMC) can be applied to solve the inverse problem, but disentangling input parameter uncertainty and model misspecification is often poorly identified problem. We modify the BMC framework to simplify and improve the estimation of physical parameters with functional outputs. We propose scaling the likelihood function by an effective sample size rather than modeling the discrepancy function; and modularizing input nuisance parameters with weakly identified parameters. We evaluate the performance of these methods using a simulation study and apply these methods to estimate parameters of the tantalum equation of state. We conclude that the approach provides simple, fast, and statistically valid calibration of parameters of the equation of state for tantalum.

Dynamic material property calibration

Objective: Two parameters of the tantalum equation of state (EOS) are estimated by coupling measured and simulated velocity traces. The EOS characterizes the pressure-volume-temperature relationship.

Experimental setup (Figure 1)**:** The time-dependent magnetic field boundary condition results in a time-dependent stress wave propagating through the system. Simulated velocity at the interface of the Ta sample and LiF window can be compared to the experimental measurement.

Uncertainties: Model inputs include Ta material properties (density, bulk modulus B_0, pressure derivative B_0'), magnetic field scaling, and material thicknesses. B_0 and B_0' are physical parameters of interest (Brynstaddor & O'Hagan 2014). Time and velocity are measured with error.

Data (Figure 2)**:** The data consist of 9 different experimental velocity traces, and, for each experiment, 5,000 simulated velocity traces per experiment, using LHS over 7 inputs. Simulated velocity traces were used to build Gaussian process emulators for the outputs.

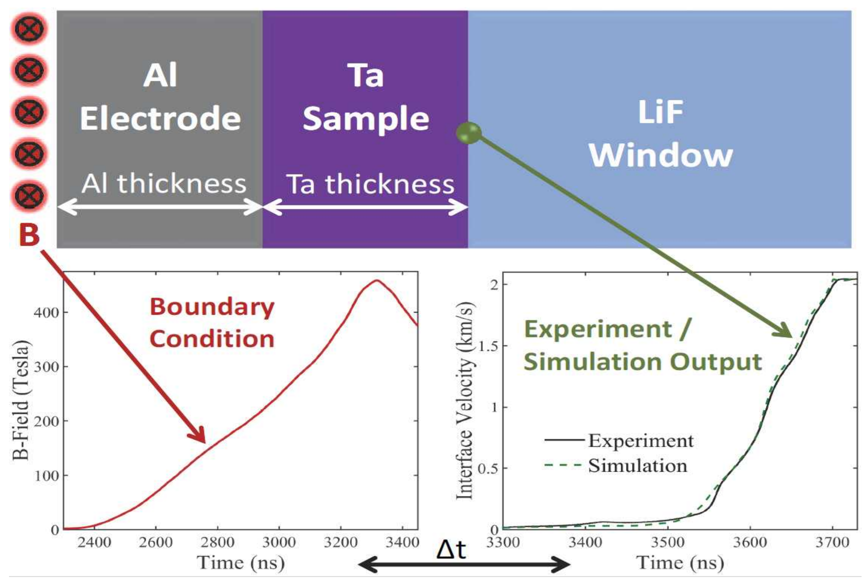

Figure 1: Experimental setup

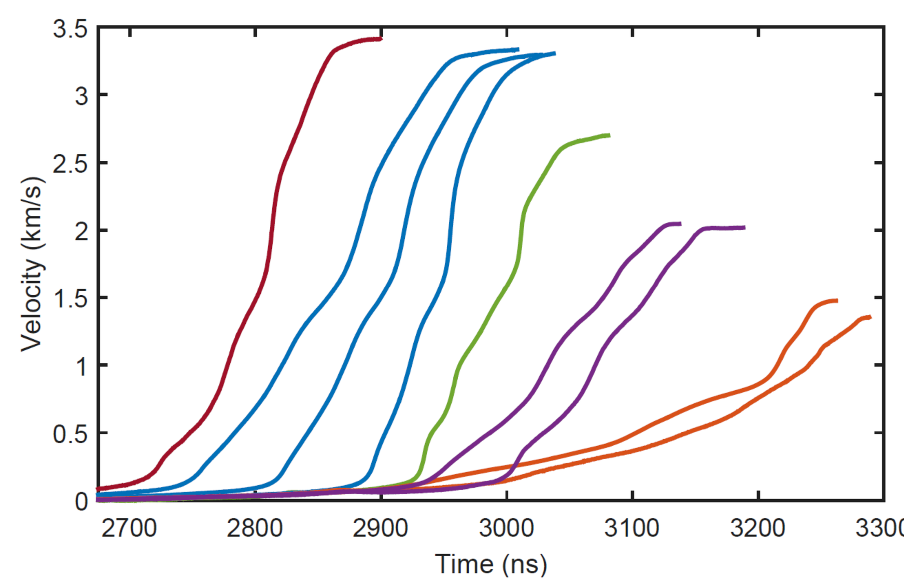

Figure 2: Measured velocity traces

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Modifications to BMC

BMC model (Kennedy and O'Hagan 2001): For each experiment, the measured velocity y is modeled as a function of uncertain inputs α, design parameters x (in this application, x is time), measurement uncertainties ϵ, and model discrepancy δ.

$$y_i = \eta(\alpha, x_i) + \delta(x_i) + \epsilon_i$$
$$\delta \sim GP(\mu, \Sigma), \epsilon_i \sim N(0, \sigma(x_i))$$

Likelihood scaling: Rather than modeling the discrepancy function, we scale the likelihood by an equivalent effective sample size, n_e.

$$y_i = \eta(\alpha, x_i) + \epsilon_i$$
$$\log l\,(y|\alpha,\sigma) = \frac{n_e}{n} \log l^*\,(y|\alpha,\sigma),$$

where l^* is an independent Gaussian likelihood for y based on the model above. The model is fit without updating a discrepancy function. The scaling factor n_e is estimated from the discrepancy function at the posterior mean.

Modularization: When calibrating the tantalum material properties, the number of nuisance parameters is large relative to the number of physical parameters of interest and overfitting in BMC can induce bias in physical parameter estimates. To mimic this forward propagation of uncertainty, we explored modularization of the nuisance parameter uncertainty (Liu et al., 2009; Plummer, 2015) by sampling nuisance parameters from their prior distributions and comparing inferences to full Bayesian inference.

Results

- Scaling the likelihood results in more conservative inferences than modeling the discrepancy function and has reasonable frequentist properties.

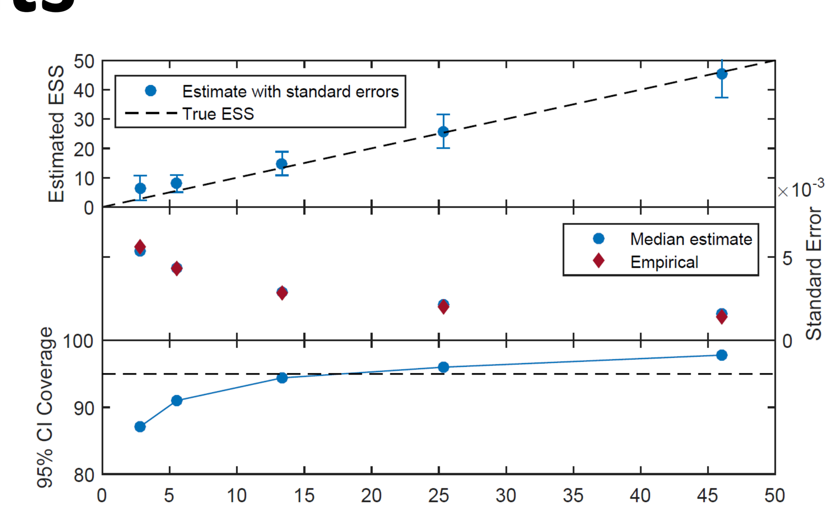

Figure 3: Likelihood scaling simulation study.

- Modularization of nuisance parameters inflates uncertainty in physical parameters to help avoid overfitting; developing a more rigorous approach to modularization is an area for future research.

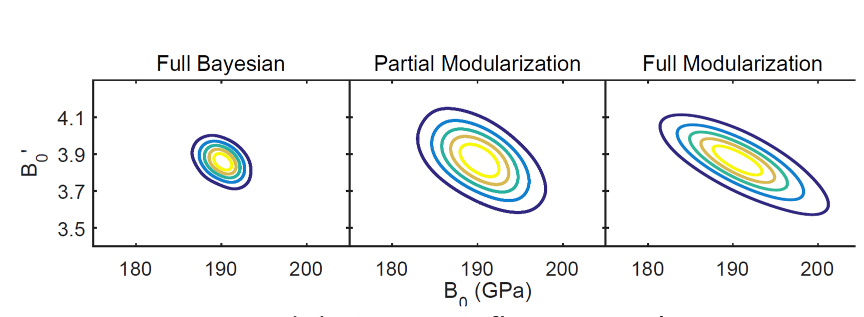

Figure 4: Modularization inflates B_0, B_0' uncertainty.

- Bayesian model calibration appears to be a promising framework for calibration of dynamic material models. Estimated Ta EOS parameters match other results in the literature closely; further, BMC facilitates incorporating more sources of uncertainty than traditional analytic approaches.

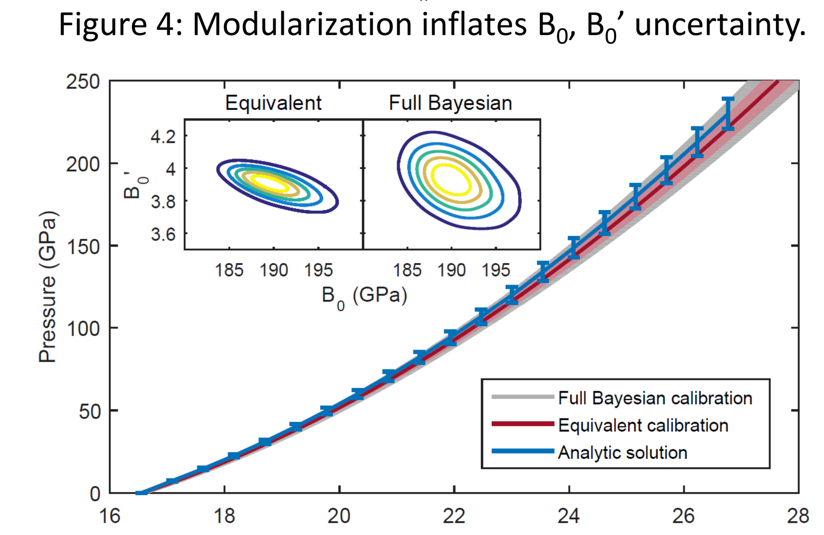

Figure 5: Full BMC compared to analytic solution and equivalent BMC with a reduced set of uncertainties used in the historical approach.

References:

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

Brynjarsdóttir, J., & O'Hagan, A. (2014). Learning about physical parameters: The importance of model discrepancy. *Inverse Problems*, *30*(11).