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Calibration, Propagation, and Validation of Model Discrepancy Across Experiments

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Motivation: Predictions Under Uncertainty

We need to make predictions that incorporate both parametric and model form uncertainties

- Predictions may be interpolatory or extrapolatory
- Central to high-consequence modeling and simulation activities

Here, we focus on non-intrusive methods to support black-box simulations

- Perform predictions under uncertainty with explicit discrepancy models
- Explore challenges from algorithmic and deployment perspectives

Calibration of Computer Models

Experimental data = model output + error

$$d(x_i) = M(\boldsymbol{\theta}, x_i) + \varepsilon_i$$

- $\boldsymbol{\theta}$ = variables to be calibrated
- x = scenario or configuration variables
  - Represent different experimental settings at which data is taken (temperature, pressure, etc)
- $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ = i.i.d. measurement/observation error

Often, even with calibration, the agreement between the data and the model is not very close. This can be due to model form error, also called model discrepancy or structural error

$$\Rightarrow \quad d(x_i) = M(\boldsymbol{\theta}, x_i) + \delta(x_i) + \varepsilon_i$$

Goal: Make predictions in the presence of parametric and model form uncertainties under different experimental conditions

Philosophical and Implementation Issues

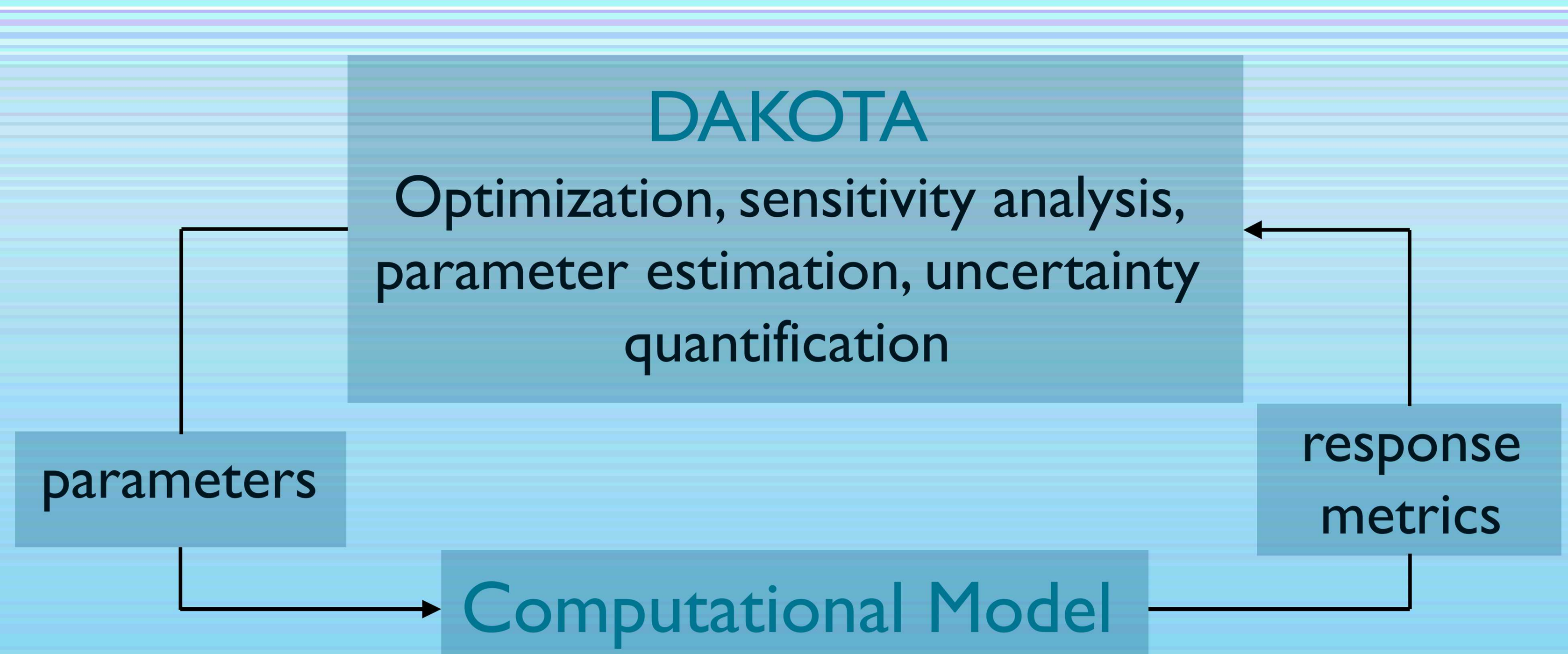
- How do we estimate δ?
  - Simultaneous versus sequential optimization of discrepancy and calibration parameters
- What model form is appropriate for δ?
- How can we understand if there is significant confounding (non-identifiability) between our estimates of $\boldsymbol{\theta}$ and δ?
- How can we appropriately use δ to improve the predictive capability of the model?
- How do we capture and propagate extrapolation uncertainty?
  - In the model form
  - In the parameters
  - In the discrepancy

How do we make the answers to these questions general?

DAKOTA

Explore and predict with confidence.

Automate typical parameter variation studies with advanced methods and a generic interface to your simulation



Discrepancy Formulation in Dakota

Sequential calibration of model parameters and model discrepancy

- Parameters $\boldsymbol{\theta}$ are calibrated to experimental data $d(x)$
- Discrepancies are calculated
  - For each scalar response

$$\delta(x_i) = d(x_i) - M(\boldsymbol{\theta}, x_i)$$

  - For each field response

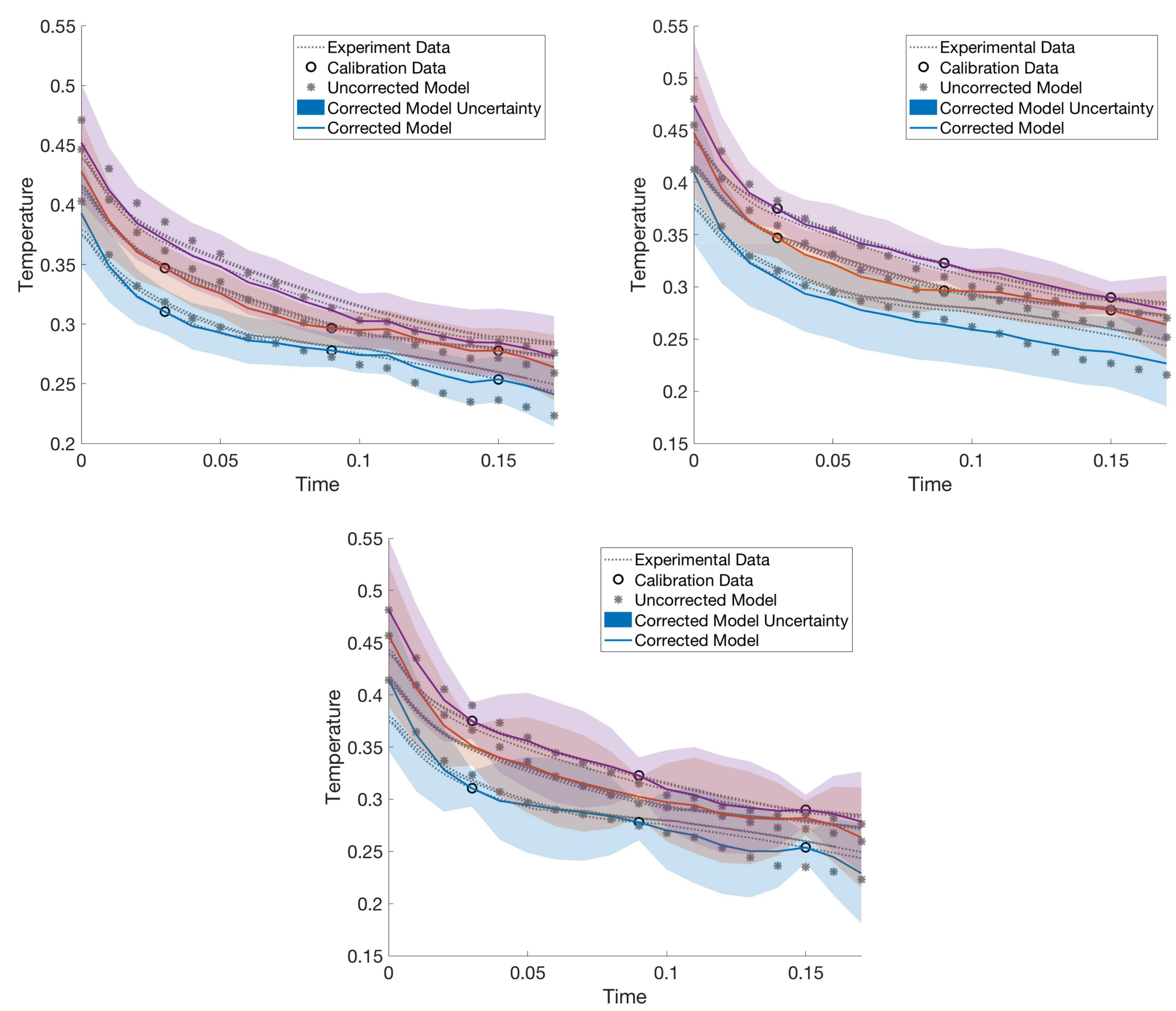
$$\delta(t_i, x_j) = d(t_i, x_j) - M(t_i, \boldsymbol{\theta}, x_j)$$

- Prediction variance can also be computed

Example: Thermal Battery Calibration

We wish to use a single model for temperature calculations for any initial condition

- Calibrate $\boldsymbol{\theta}$ to experimental data
  - Model is an emulator with 7 parameters
  - Three cases of "leave one out" calibration
  - One experiment of each type
  - $\pi(\boldsymbol{\theta}) \sim \mathcal{U}$ and $(d|\boldsymbol{\theta}) \sim \mathcal{N}$
- Calculate discrepancies and calibrate discrepancy model



Discrepancy model corrected some areas better than others, but experimental data is contained within the prediction intervals of the corrected model

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Explicit Discrepancy Calibration

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