Uncertainty Quantification and Parameter Inference for Material Models Using a Bayesian Paradigm

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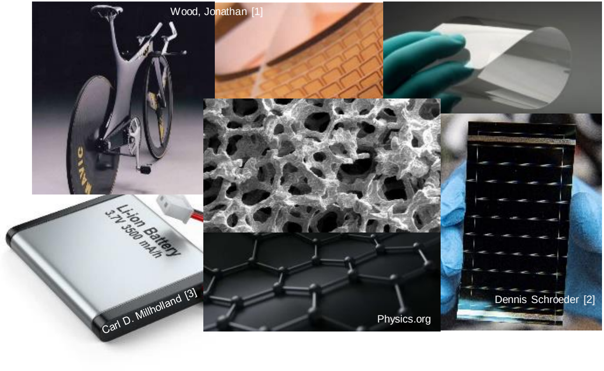
Materials Science Advancing Technology

Technology advancements enabled by the discovery and design of new materials



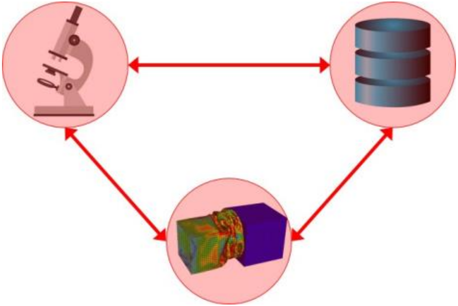
The discovery and design of new materials is also often the bottleneck in advancing technology

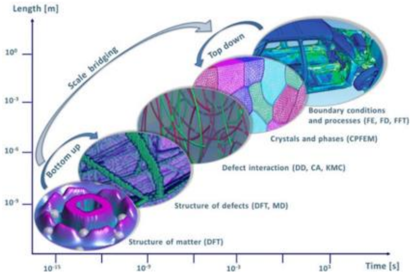
ICME for the Discovery and Design of New Materials

Integrated Computational Materials Engineering (ICME):

Integration of materials information, experiment, and computational tools across length and timescales.

Processing ↔ Microstructure ↔ Properties ↔ Performance





Raabe, Dierk, et al. "Multi-scale modeling in materials science and engineering." (2009) [4].

ICME for the Discovery and Design of New Materials

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Integration of materials information, experiment, and computational tools across length and timescales.

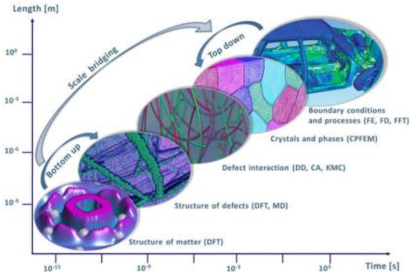
Processing ↔ **Microstructure** ↔ **Properties** ↔ **Performance**

Benefits

- Model linkages account for mechanisms at various scales
- Reduced cost of time and resources
- Accelerated materials development

Challenge

- Establishing a statistical design confidence from deterministic models



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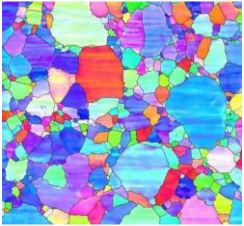
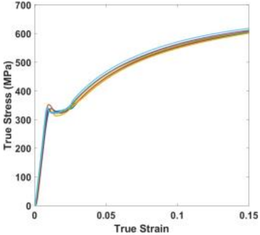
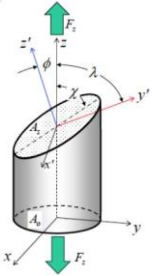
Sources of Uncertainty in Materials Modeling

- Parameter uncertainty
- Noisy/inconsistent experimental data
- Model-form uncertainty
- **Sample to sample variability**
  - Microstructure dictates material behavior
  - Randomness creates sample-to-sample variability
  - Each sample has a unique true underlying property value due to its unique microstructure
  - There is a single true underlying property of the material







UQ for materials science and ICME

Principled approaches for UQ critical to reliably develop and deploy new and improved materials within the ICME paradigm.

Objective

Demonstrate a generalized framework for UQ for predictions of material behavior which considers various sources of uncertainty and is easily adaptable to important problems in materials modeling.

UQ	→ Bayesian inference
Sample-to-Sample Variability	→ Random Effects Model
Model Discrepancy	→ Gaussian Process
Exemplar Demonstration	→ Crystal Plasticity Modeling

Bayesian formalism for statistical inference

Statistical Inference

The goal of recovering information about unknown components, or parameters, $\boldsymbol{\theta}$ of a probability model from observed data, **y**, while accounting for associated uncertainty.

The Bayesian Paradigm for Inference

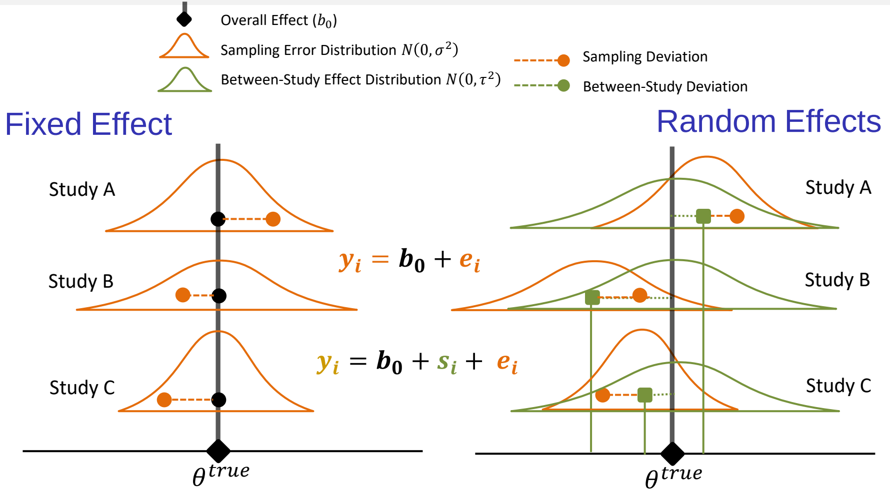
Directly defining and updating beliefs about unknown quantities conditionally on observed data

$$\pi(\theta \mid y) = \frac{f(y \mid \theta)\pi(\theta)}{\int_{\Theta} f(y \mid \theta)\pi(\theta) d\theta} \propto f(y \mid \theta)\pi(\theta)$$

Markov Chain Monte Carlo

MCMC simulation methods are state of the art for generating approximate samples from the posterior distributions.

Statistical models for multiple studies/experiments



- All studies share a **common mean**.
- Deviations due to **sampling variance**

- The **means of the studies** are distributed about the **overall mean**.
- **Deviations** not strictly due to **sampling variance**

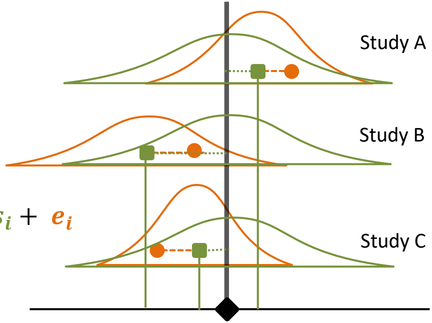
Nakagawa et. al [5]

Random Effects Model for UQ in Materials Science

- Reflects the natural structure of a class of problems in materials modeling and simulation
- In materials testing, it is not uncommon to see experimental deviations test-to-test which cannot be attributed strictly to sampling error.

Random Effects

$$y_i = b_0 + s_i + e_i$$



- The **means of the studies** are distributed about the **overall mean**.
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A hierarchical random effects model DAG

DAG: directed acyclic graph. Arrows → direction of conditional dependence

Effects

- The 'true' underlying state of nature, θ, is the *overall effect*.

A Hierarchical Random Effects Structure

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Effects

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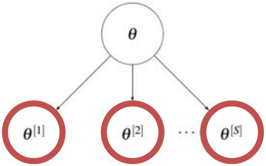
- The data are collected from samples that, due to heterogeneity, have been generated under a different state, $\theta^{[s]}$, which are *random effects*.



A Hierarchical Random Effects Structure

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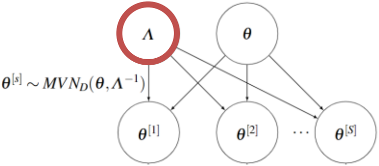
Effects

- The 'true' underlying state of nature, θ, is the *overall effect*.
- The data are collected from samples that, due to heterogeneity, have been generated under a different state, $\theta^{[s]}$, which are *random effects*.
- $\theta^{[s]}$ connected to θ by a MVN distribution

$$\theta^{[s]} \sim MVN_D(\theta, \Lambda^{-1})$$

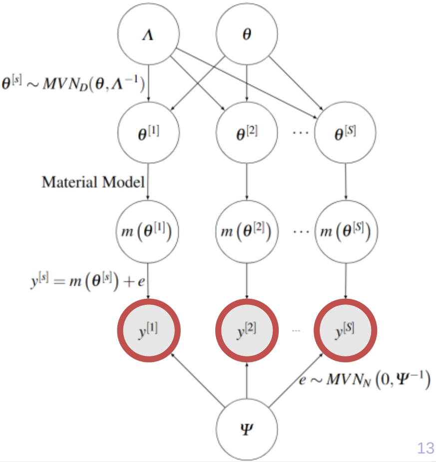


A Hierarchical Random Effects Structure

DAG: directed acyclic graph. Arrows → direction of conditional dependence

Model for the Data

- The model for the observations
  - $y^{[s]} = m(\theta^{[s]}) + e$



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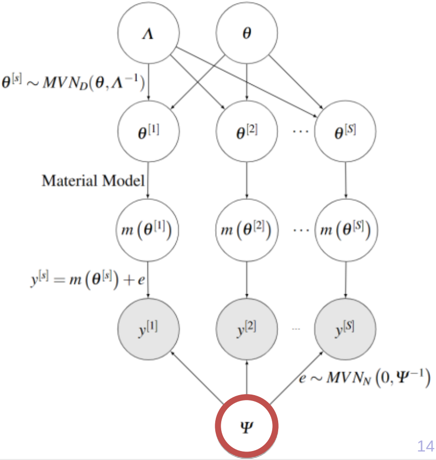

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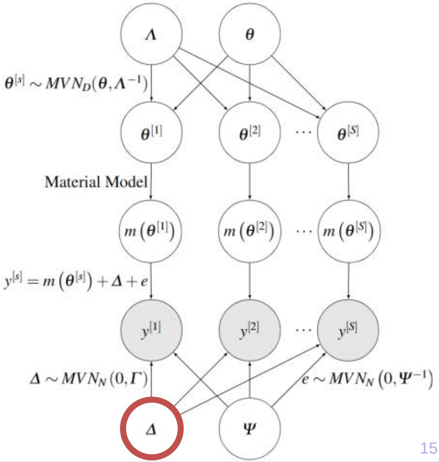
Model for the Data

- The model for the observations
  - $y^{[s]} = m(\theta^{[s]}) + e$
  - $e \sim MVN_N(0, \Psi^{-1})$
- With added **model discrepancy** term
  - $y^{[s]} = m(\theta^{[s]}) + \Delta + e$
  - $\Delta \sim MVN_N(0, \Gamma)$



A Hierarchical Random Effects Structure

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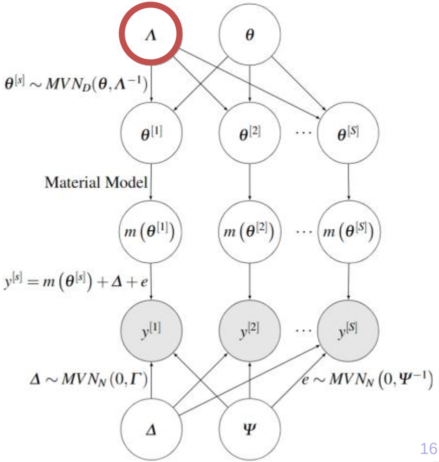
Prior Modeling for Λ

- Wishart Distribution: probability distribution on positive-definite matrices
  - $\boldsymbol{\Lambda} \sim \boldsymbol{Wish_D}(\boldsymbol{V_o}, \boldsymbol{v_o})$
  - Complex relationship between hyperparameters and features of the distribution
  - A flexible alternative is to model a decomposition of the precision matrix instead



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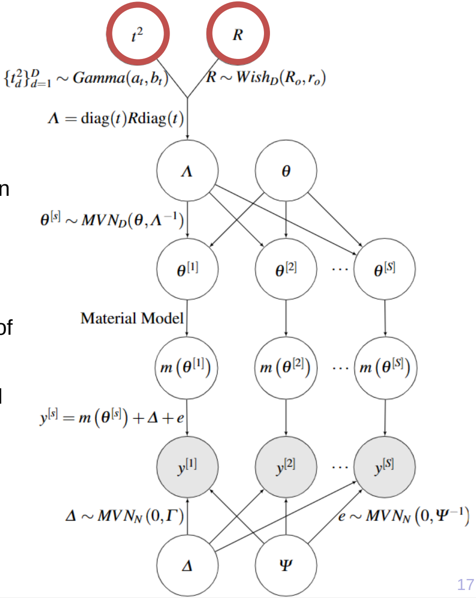
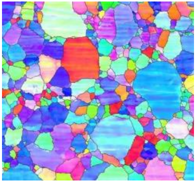
  - $\Lambda \sim Wish_D(V_o, v_o)$
  - Complex relationship between hyperparameters and features of the distribution
  - A flexible alternative is to model a decomposition of the covariance matrix instead
  - $\Lambda = \text{diag}(t) R \text{diag}(t)$

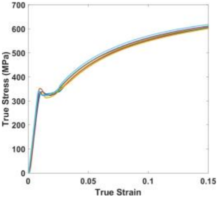


Exemplar Problem: Crystal Plasticity

Crystal Plasticity (CP) Modeling:

Used to predict mechanical behavior of polycrystalline materials such as the stress-strain response and texture evolution under specific modes of deformation.

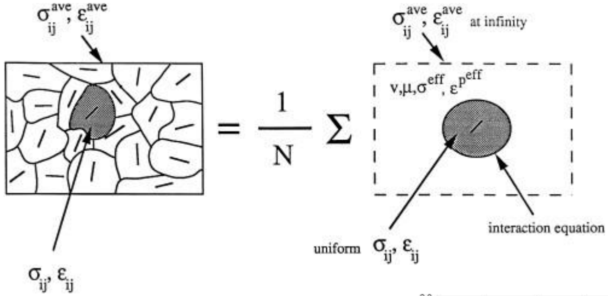




- CP models vary greatly in complexity
- High-fidelity models appealing for scientific inquiry
  - too expensive for UQ
- Reduced-order, homogenized, mean-field models well-suited for UQ
- Often have some systematic model discrepancy
- Inference and prediction important in this setting

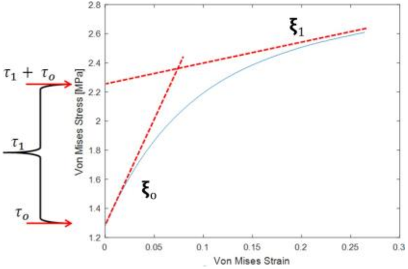
Phenomenological VPSC CP Model

Tome & Lebensohn [6]



The evolution of the CRSS with deformation is described in VPSC by the Voce Law

$$\hat{\tau}^{\alpha} = \tau_0^{\alpha} + \left(\tau_1^{\alpha} + \xi_1^{\alpha}\Gamma\right)\left(1 - \exp\left\{-\Gamma\left|\frac{\xi_0^{\alpha}}{\tau_1^{\alpha}}\right|\right\}\right)$$

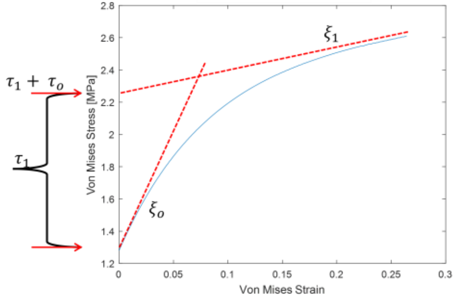


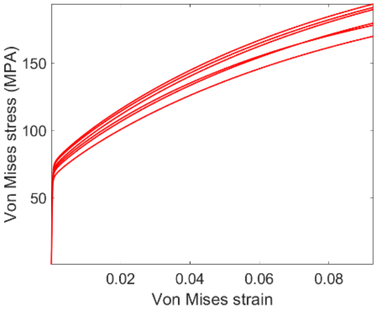
Inference Problem

Voce Parameters: $\theta := (\tau_0, \tau_1, \xi_0, \xi_1)$

Constraints: $C(\theta) = (\tau_0, \tau_1, \xi_0 - \xi_1) > 0$

mimic hardening behavior for the room-temperature deformation of copper





Simulated calibration data from the physics-based elasto-viscoplastic FFT model

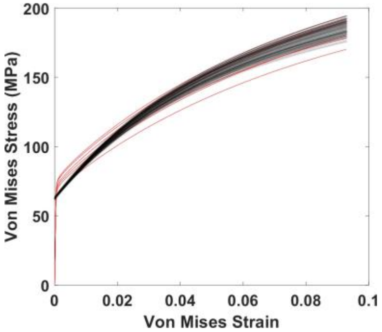
VPSC – missing physics for the elastic region of deformation → model discrepancy

Importance of Accounting for Model Discrepancy

If model discrepancy ignored- **bias** is introduced in the inference and consequently in predictions

*Kennedy and O'Hagan (2001) [7] laid out a hierarchical framework for doing inference for reduced order models with discrepancy.

$$y = m(\theta) + \Delta + e$$



Analysis of the VPSC model with model discrepancy not accounted for.

Gaussian Processes to Model Discrepancy

A **Gaussian Process (GP)** can be used to define a prior over functions and is characterized by a mean function and covariance function

$$\Delta \sim GP\,(\mu, c)$$

Δ may be represented with a prior mean function $\mu(x) = 0$

$$\Delta(x_1), \ldots, \Delta(x_N) \sim MVN_N(\mathbf{0}, C)$$

$$C = \mathrm{Cov}\left(\left(\Delta(x_1), \ldots, \Delta(x_N)\right)^T, \left(\Delta(x_1), \ldots, \Delta(x_N)\right)^T\right)$$

The covariance between the process at any two points is related to the covariance function,

$$c\left(x_i, x_j\right) = \mathrm{Cov}\left(\Delta(x_i), \Delta(x_j)\right)$$

Covariance structure controls correlation scale and smoothness of stochastic process

Prior Modeling

Careful choice of the covariance structure is needed to specify a sufficiently informative prior process for the discrepancy Δ

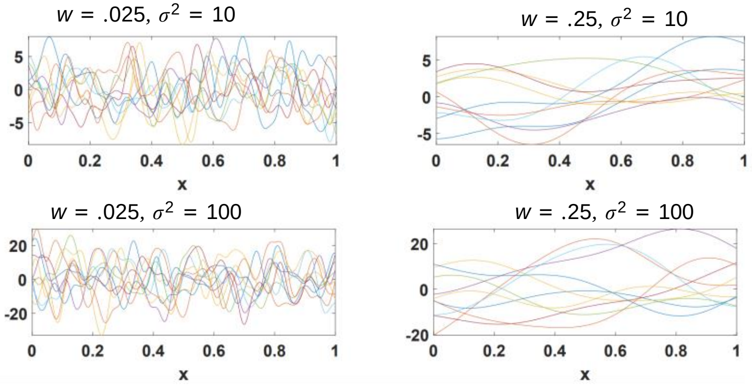
Prior Modeling of the Discrepancy

Example covariance function, the squared exponential,

$$\mathrm{Cov}\left(\Delta(x_i), \Delta(x_j)\right) = c(x_i, x_j) = \sigma^2 \exp\left\{-\frac{1}{2}\left(\frac{x_i - x_j}{w}\right)^2\right\}.$$

Hyperparameters

- Length scale, w, & variance, σ^2



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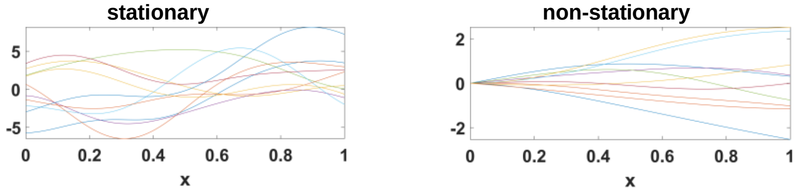
Stationarity

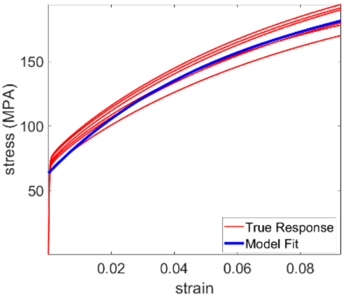
Covariance function depends only on the distance between inputs and is independent of their relative location.



Discrepancy Prior for the VPSC CP Model

Prior knowledge about Δ

VPSC expected to capture the plastic region nearly perfectly and the elastic region not at all



Discrepancy Prior for the VPSC CP Model

Prior knowledge about Δ

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Elastic Region

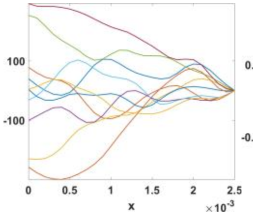
Model discrepancy is the greatest at $x = 0$ & decreases to 0 at the elastic-plastic transitio

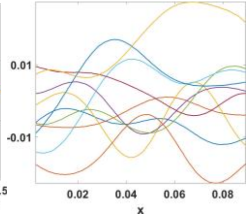
- **Constrained non-stationary** covarianc function

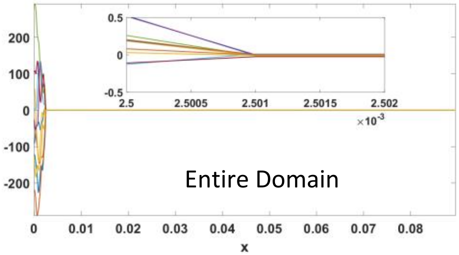
Plastic Region

Model discrepancy is expected to remain constant at nearly 0 for the plastic region

- **Stationary squared-exponential** covariance function



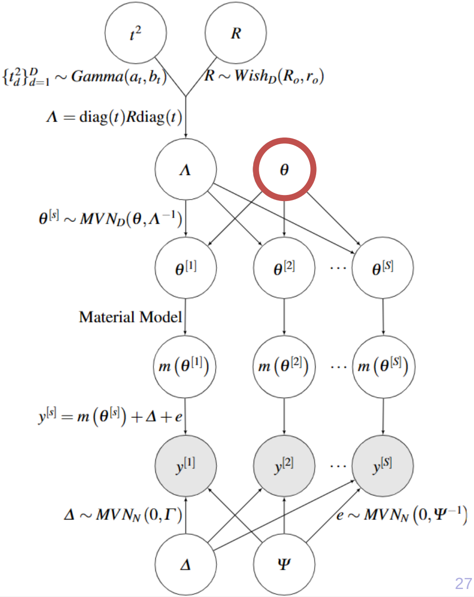




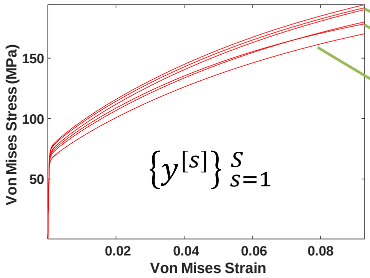
Prior Modeling of θ

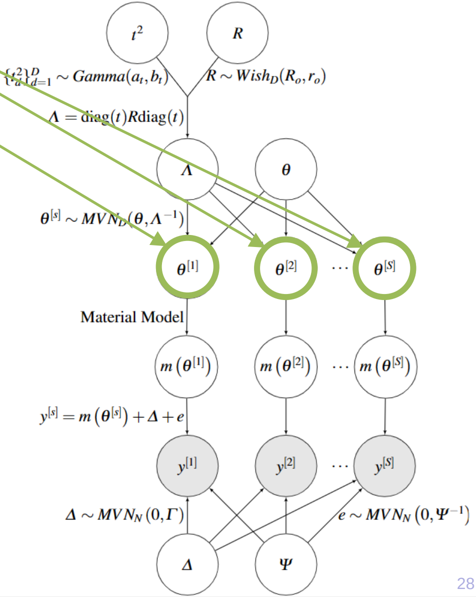
The degree to which the prior choice affects posterior uncertainty depends on

- How informative the prior is
- How much information the data contain about the unknown parameters



Prior Modeling of θ

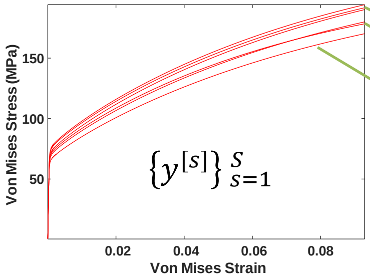


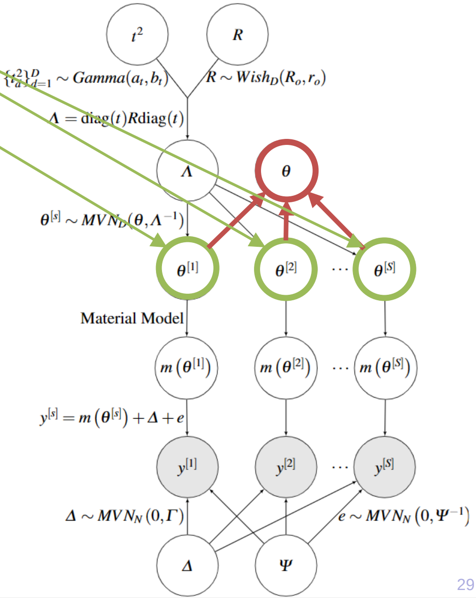


Materials Applications

- Much information available about random effects, $\theta^{[s]}, s = 1, \ldots, S$

Prior Modeling of θ

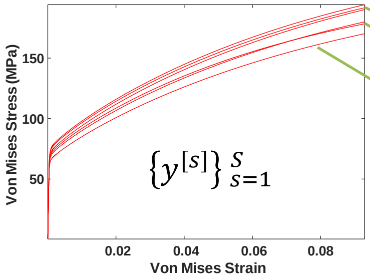


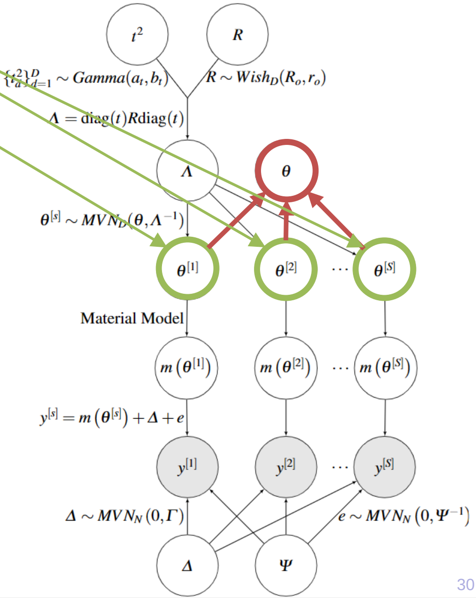


Materials Applications

- Much information available about random effects
- Information propagated in hierarchy to θ is quite small

Prior Modeling of θ



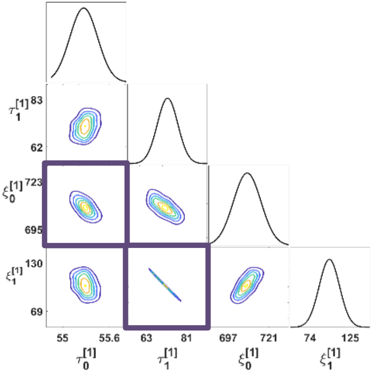


Materials Applications

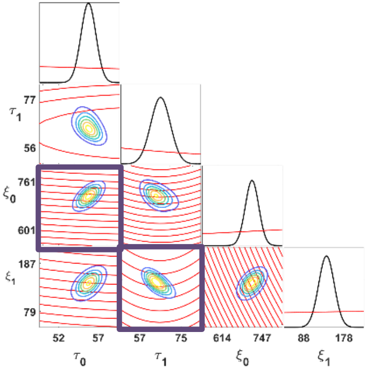
- Sensitivity to the choice of $\pi(\theta)$
- **Diffuse** priors chosen for θ

Bivariate Kernel Density Estimates

1.2×10^5 samples produced, 2×10^4 discarded as burn-in. Adaptive algorithm used to overcome high parameter correlations

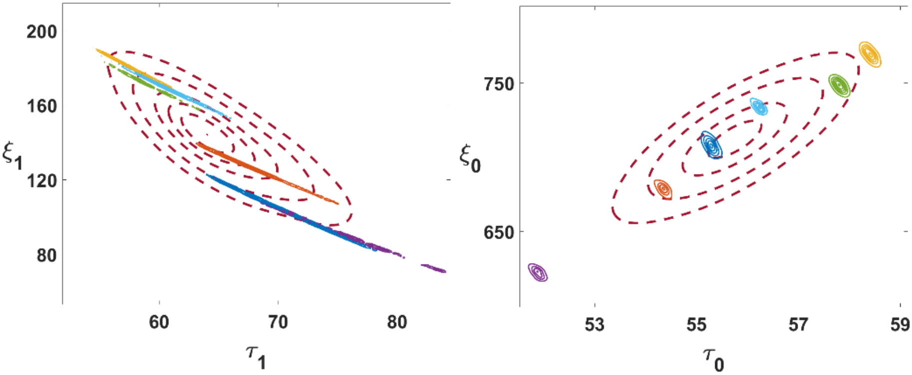


Representative Random Effect



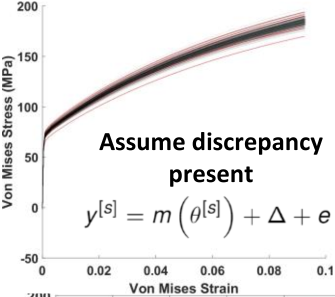
Overall Effect

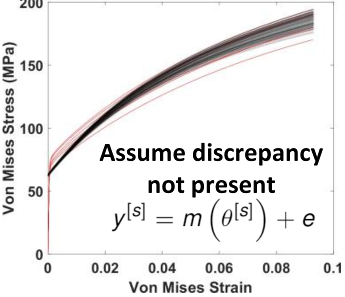
Marginal Posterior Contours

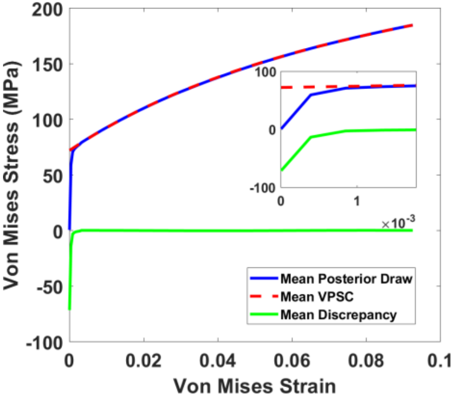


Insight: The highest reduction in uncertainty will be achieved by testing more samples rather than further trying to decrease the measurement noise for each single trajectory.

Posterior Uncertainty Propagated to Model Output







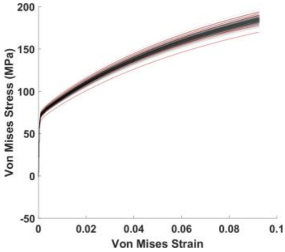
The point-wise posterior mean, the VPSC model evaluated at the posterior mean parameter values and the mean discrepancy are shown with an inset showing the elastic region.

Summary

A framework for UQ for materials modeling was demonstrated in a CP example.

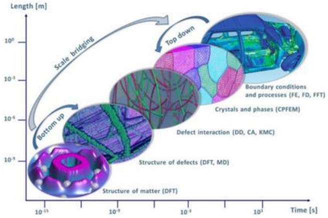
UQ accounting for:

- Parameter uncertainty
- Observation error
- Sample-to-sample variability
- Model discrepancy



Implications for ICME

- Reliable use of fast reduced-order, phenomenological (etc.) models
- True material properties are inferred from variable experimental data
- Uncertainty can be propagated in model linkages for processing → performance predictions
- Supports reliable design and discovery of new materials



Raabe [4].

Thank You

Ricciardi, Denielle E., Oksana A. Chkrebtii, and Stephen R. Niezgoda. "Uncertainty Quantification for Parameter Estimation and Response Prediction: Generalizing the Random Effects Bayesian Inferential Framework to Account for Material and Experimental Variability." *Integrating Materials and Manufacturing Innovation* 8 (2019): 273-293.

Ricciardi, Denielle E., Oksana A. Chkrebtii, and Stephen R. Niezgoda. "Uncertainty quantification accounting for model discrepancy within a random effects Bayesian framework." Integrating Materials and Manufacturing Innovation 9 (2020): 181-198.

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Supplemental Slide I: When to Include Discrepancy

Include when...

- The model is missing physics, resulting in systematic discrepancy between the model output and the observations
- There is strong prior knowledge about the misfit between the model and true process
- Identifiability

$$\Delta(x) = \zeta(x) - m(x, \theta).$$

May exclude when...

- No systematic discrepancy is expected
- The model is flexible enough to fit the data
- The model is empirical in nature, where parameters do not have physical significance since the parameter estimates will be strongly biased and HPIs may not cover the true parameter values

Supplemental Slide II: Modeling Discrepancy

Observations of the physical system, y_n, at independent variable inputs, $\mathbf{x} = \{x_1, \cdots, x_N\}$, are centered around some true value, $\zeta(x_n)$, with independent Gaussian observation errors, e_n,

$$y_n = \zeta(x_n) + e_n, \qquad n = 1, \cdots, N.$$

Assume some model of the physical system, $m(\cdot)$, which accepts a vector of input parameters θ and is evaluated at variable inputs $\mathbf{x} = \{x_1, \cdots, x_N\}$,

$$m(\mathbf{x}, \theta).$$

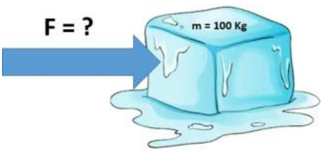
We can link the model to the true system, by incorporating the discrepancy, Δ,

$$\zeta(\mathbf{x}) = m(\mathbf{x}, \theta) + \Delta(\mathbf{x}).$$

Relating the model to the observations:

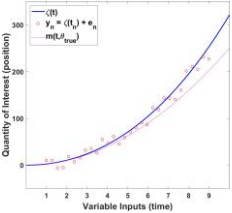
$$y_n = m(x_n, \theta) + \Delta(x_n) + e_n, \qquad n = 1, \cdots, N$$

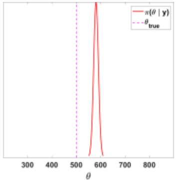
Toy Example for Discrepancy



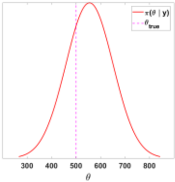
Model of behavior: $m(t,\theta) = \frac{1}{2}\left(\frac{\theta}{\text{mass}}\right)t^2$

True behavior: $\zeta(t) = \frac{1}{2}\left(\frac{\theta_{true}}{\text{mass}\cdot\exp(-\lambda t)}\right)t^2$





No Discrepancy

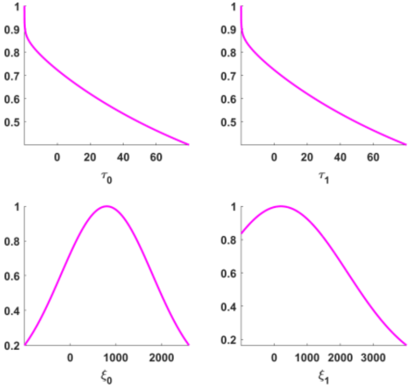


With Discrepancy

Supplemental Slide IV: Priors

Priors

Parameter	Model	$\mathbb{E}_\theta$	$\mathbb{V}_\theta$	a_{shape}	b_{rate}
τ_0	Gamma	70	5000	.98	.014
τ_1	Gamma	70	5000	.98	.014
ξ_0	Normal	1800	1×10^6	–	–
ξ_1	Normal	600	1×10^6	–	–
δ^2	Gamma	10	100	1	.1
Δ	MVN_N	0	Γ	–	–
R	$Wishart_D$	$(D+2)\cdot\mathbb{I}_D$	$(D+2)\cdot 1_D + (D+2)\cdot\mathbb{I}_D$	–	–
t_d^2	Gamma	10	100	1	.1



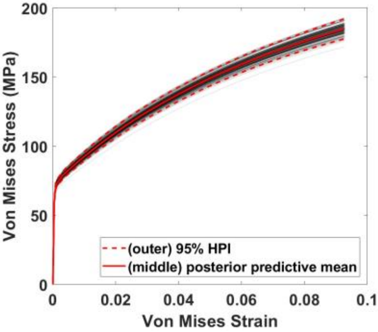
Supplemental Slide V: Constitutive Model

$$\dot{\varepsilon}^p = \sum_\alpha m^\alpha \dot{\gamma}^\alpha = \dot{\gamma}_0 \sum_\alpha m^\alpha \left(\frac{m^\alpha : \sigma^\alpha}{\tau_0^\alpha} \right)^n$$

α: slip systems
τ_0: initial threshold stress
m: Schmid tensor
$\dot{\varepsilon}^p$: deviatoric plastic strain rate
σ: stress
$\dot{\gamma}^\alpha$: local shear rate on slip system α
$\dot{\gamma}_0$: reference shear rate
n: rate-sensitivity exponent

Supplementary Slide VI: Inference and Prediction

Inference



Prediction