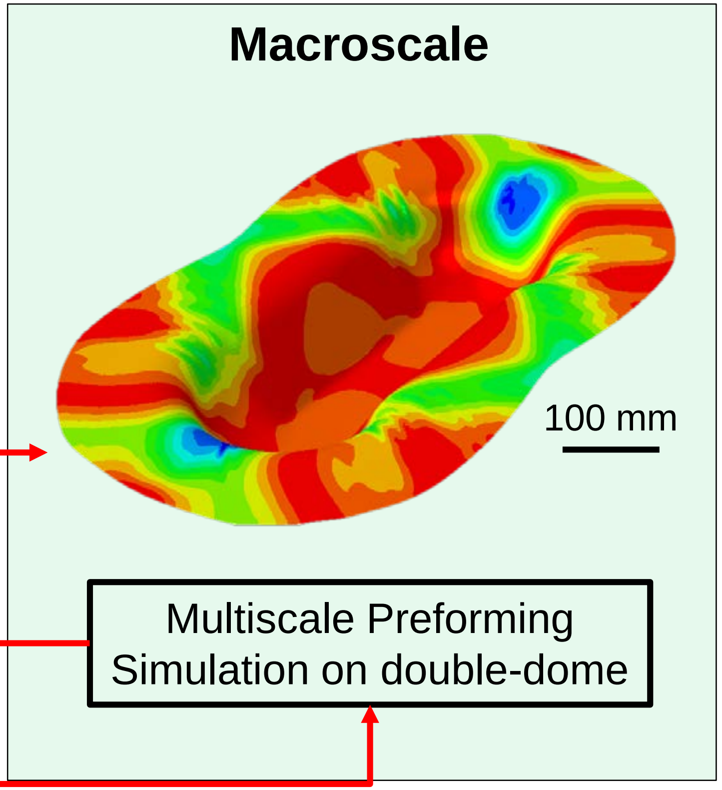
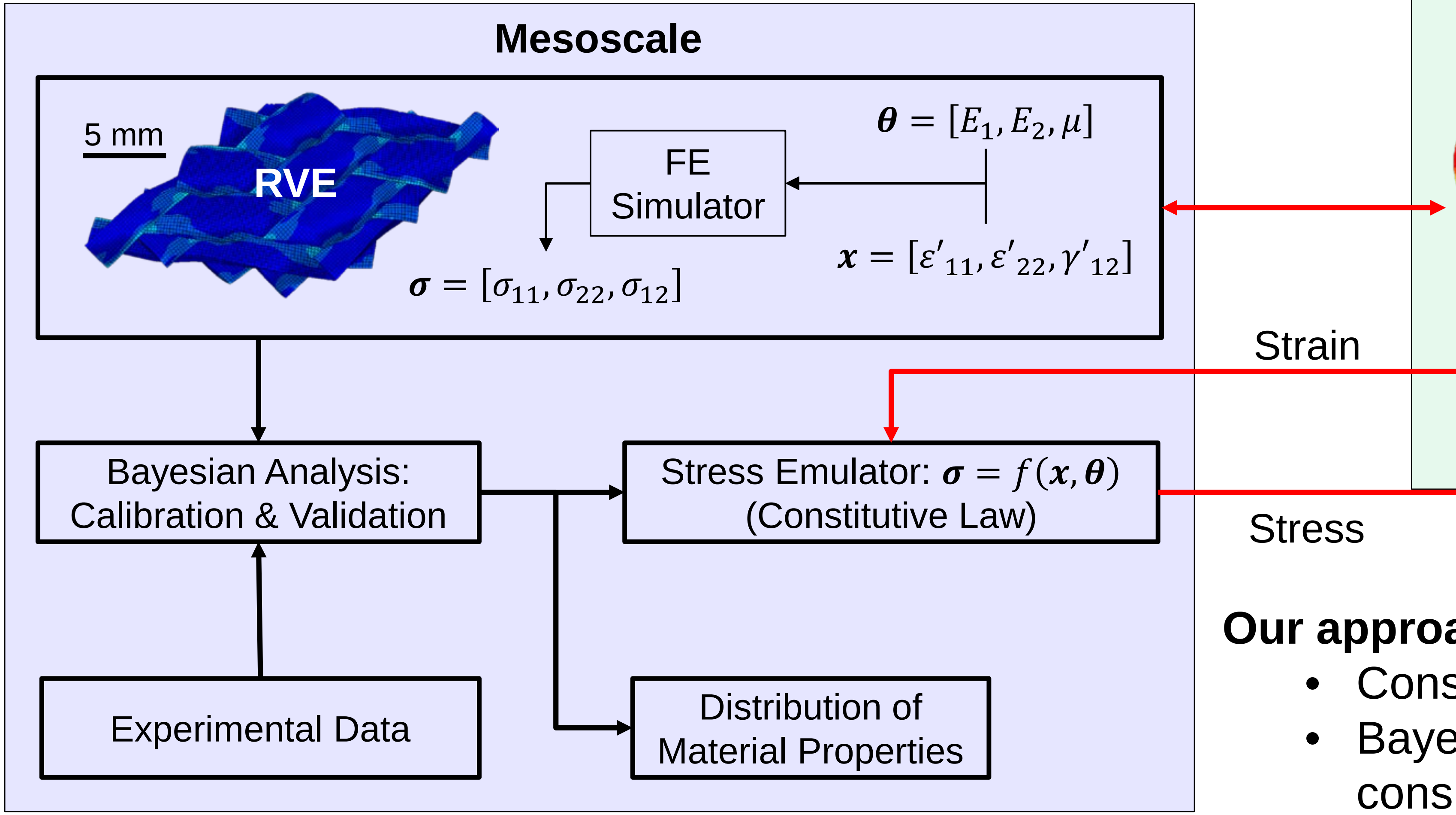
# Bayesian-Calibrated Material Model With Tension-Shear Coupling

**Prior works:**
- Neglect mesoscale tension-shear coupling
- Least-squares calibration or neglecting the potential model bias






**Our approach:**
- Considers tension-shear coupling
- Bayesian-calibrated while considering potential biases

# Bayesian Analysis of Computer Simulators

**A Bayesian framework enables:**

$$z(\boldsymbol{x}) = \eta(\boldsymbol{x}, \boldsymbol{\theta}) + \delta(\boldsymbol{x}) + \varepsilon$$

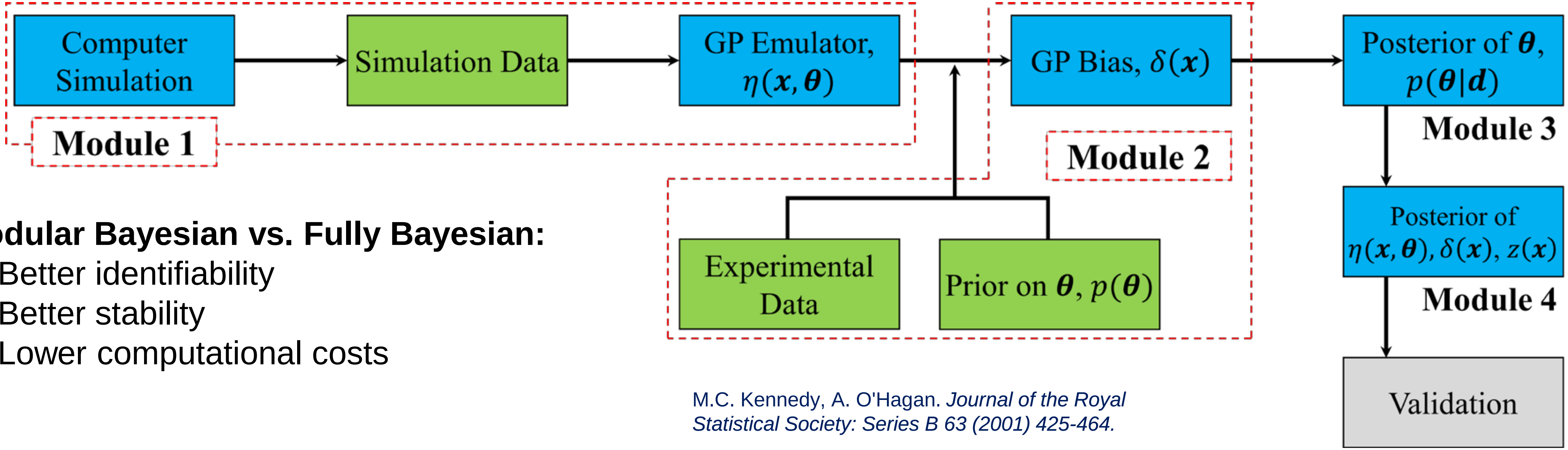
($i$) Considering various uncertainty sources

($ii$) Obtaining posterior joint distributions as opposed to a single value

($iii$) Considering potential simulator discrepancy.

| | |
|---|---|
| $z(\boldsymbol{x})$: | True Physical (Preforming) Process |
| $\eta(\boldsymbol{x}, \boldsymbol{\theta})$: | FE (low fidelity) Simulator |
| $\boldsymbol{x}$: | Controllable Inputs, $[\varepsilon'_{11}, \varepsilon'_{22}, \gamma'_{12}]$ |
| $\boldsymbol{\theta}$: | Calibration Parameters, $[E_1, E_2, \mu]$ |
| $\delta(\boldsymbol{x})$: | Discrepancy Function |
| $\varepsilon$: | White noise |

**Sources of Uncertainty:**
- Parameter Uncertainty
- Model Discrepancy
- Interpolation Uncertainty
- Experimental Uncertainty




**Modular Bayesian vs. Fully Bayesian:**
- Better identifiability
- Better stability
- Lower computational costs

M.C. Kennedy, A. O'Hagan. *Journal of the Royal Statistical Society: Series B 63 (2001) 425-464.*

# Posterior of the Calibration Parameters

**Fitting $\eta(\boldsymbol{x}, \boldsymbol{\theta})$:**

- Replacing the simulator with a multi-response Gaussian process (MRGP) metamodel that predicts $\boldsymbol{\sigma} = [\sigma_{11}, \sigma_{22}, \sigma_{12}]$ as a function of $\boldsymbol{x} = [\varepsilon'_{11}, \varepsilon'_{22}, \gamma'_{12}]$ and $\boldsymbol{\theta} = [E_1, E_2, \mu]$.

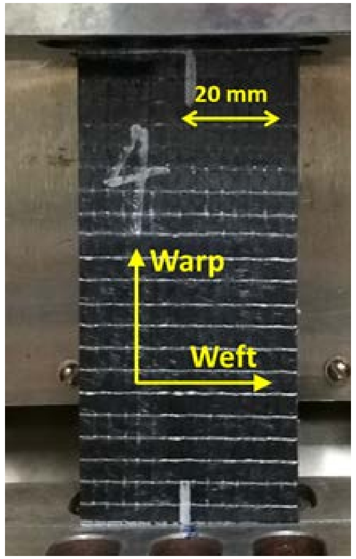
**Priors:**

- $\delta(\boldsymbol{x})$: Smooth Gaussian process
- $\boldsymbol{\theta}$: Uniform distribution

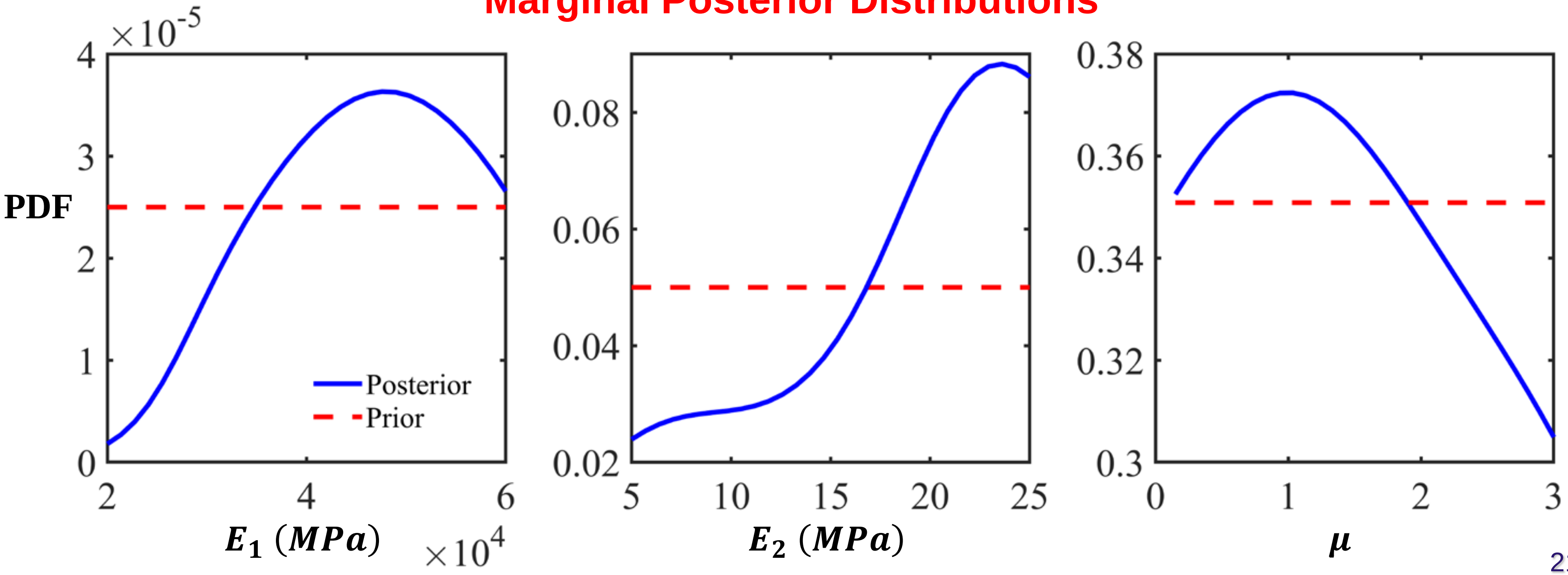
**Input Ranges:**

- $\boldsymbol{x}$: $-0.02 \leq \varepsilon'_{11}, \varepsilon'_{22} \leq 0.02$ $0 \leq \gamma'_{12} \leq 1$
- $\boldsymbol{\theta}$: $20 \leq E_1 \leq 60\ GPa$ $5 \leq E_2 \leq 25\ MPa$ $0.15 \leq \mu \leq 3$

**Setup: Uniaxial Tension**



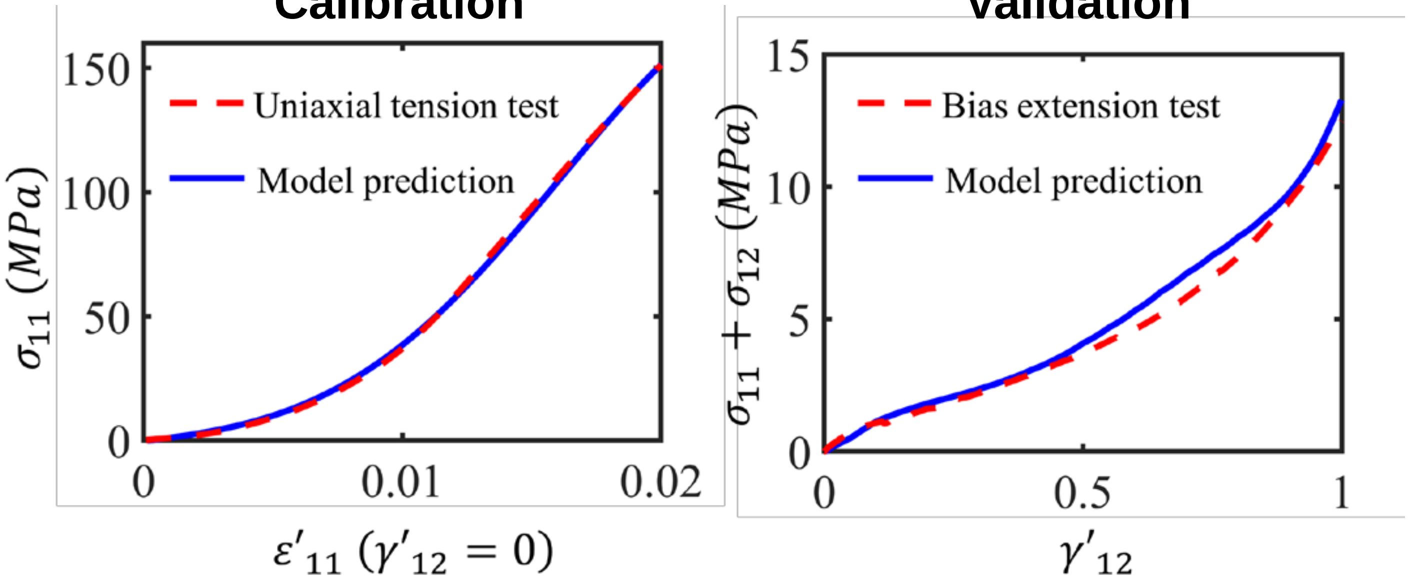

**Marginal Posterior Distributions**

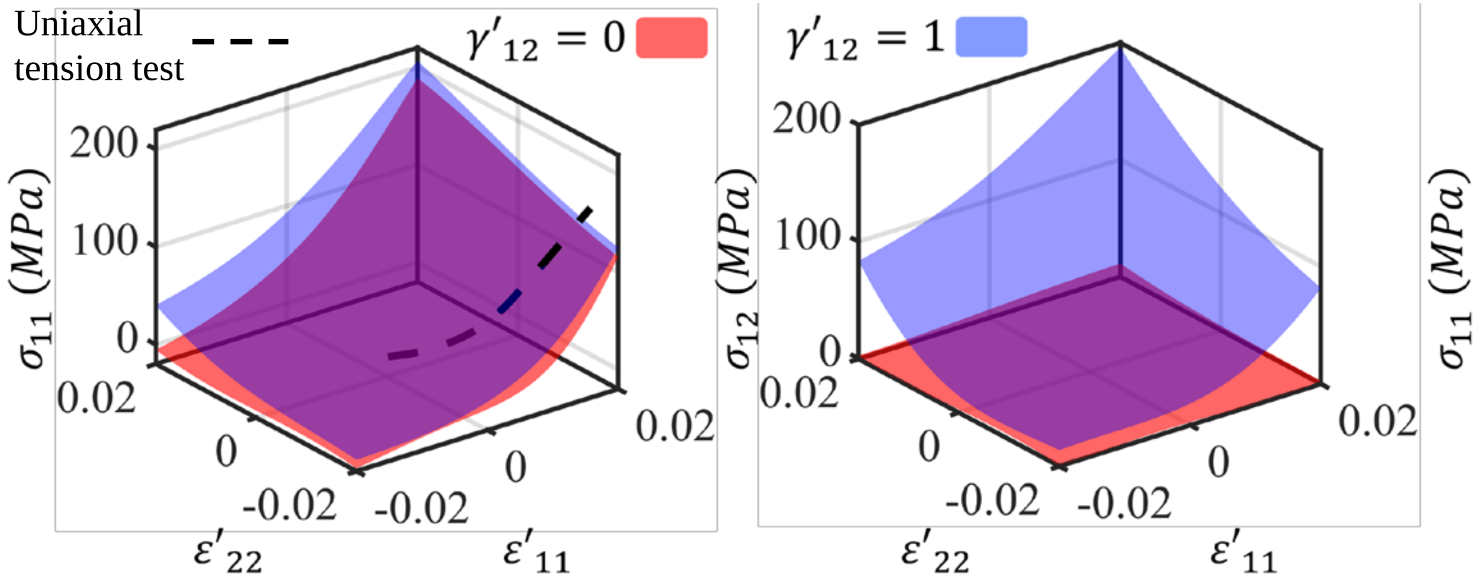


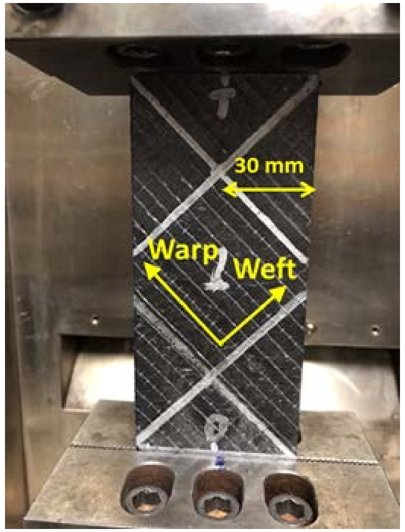
# Posterior of Stress Predictions

- **Calibration** is done via the uniaxial tension test.
- **Validation** is done via the bias extension test.

- Posterior of stresses are readily available at any strain state.



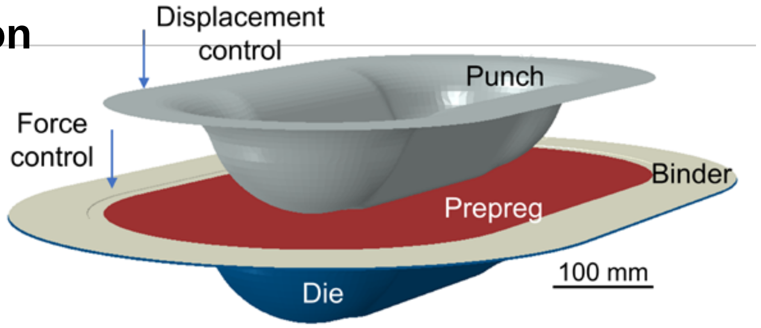



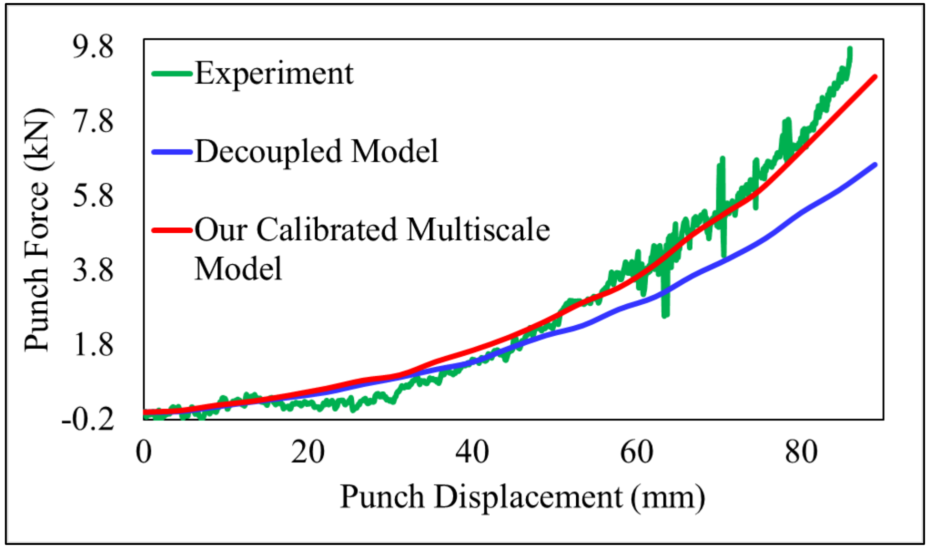

**Setup:**
**Bias Extension**

# Final Validation: Macroscale Simulation

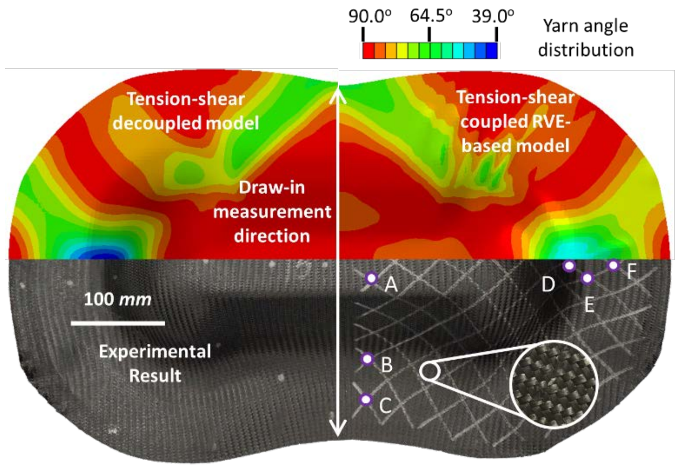
- The calibrated and validated emulator is used as the **constitutive law** in the macroscale simulations.

**Simulation Setup**




- Our predictions of **punch force** and **yarn angle** are compared against experiments.

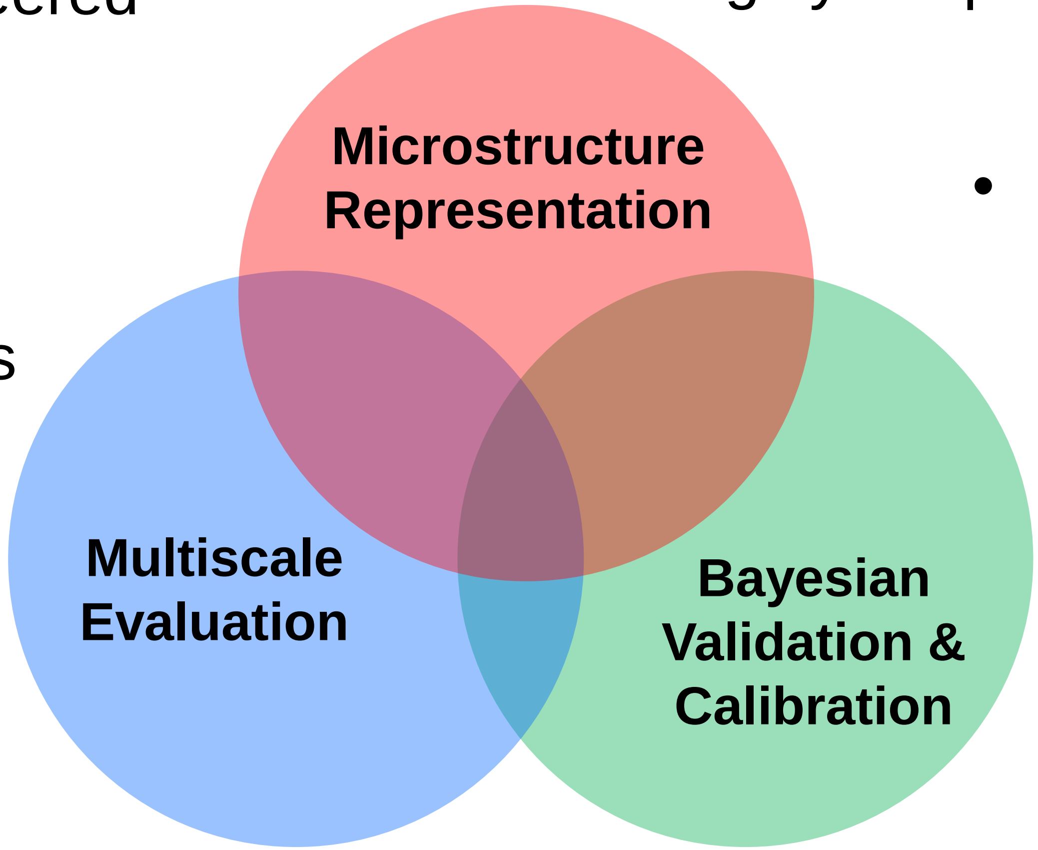



**Yarn angle comparison**

| Comparison | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| Multiscale model | **86º** | **88º** | 73º | **54º** | **57º** | **67º** |
| Decoupled model | 89º | 89º | **71º** | 40º | 45º | 65º |
| Experiment | 80º | 88º | 71º | 49º | 56º | 66º |

# Closure

- Material systems are complex engineered
- Design and manufacturability are highly coupled in materials design.
- Big data and lack of data co-exist in materials informatics.
- Stochasticity plays a critical role in materials behavior prediction




- Various sources of spatiotemporally varying uncertainty sources should be considered in multiscale materials.
- Linear & nonlinear dimensionality reduction can provide significant speed-ups.

# Model UQ in Materials – Challenges (SAMSI NUMS Working Group)

- **UQ of Microstructures**
  - How do we properly characterize location dependent and scale-coupled heterogamous material micro-/meso-/nano-structure?
  - When is (microstructural) uncertainty important to consider in multiscale systems?
  - Dimension reduction and active subspace for vector valued, time-dependent, and space-dependent QoI
  - UQ when inferring 3D microstructures with 2D images
  - Physics-aware machine learning of processing-structure relations
- **Emulators in Multiscale Modeling**
  - Time-dependent and path dependent surrogates
  - Surrogates that maintain conservation properties
  - Dimension reduction and active subspace of surrogate inputs and outputs
  - Data fusion from multi-fidelity simulations
- **Multiscale Model Calibration and UQ**
  - Spatially varying calibration parameters in the presence of model bias
  - Form of discrepancy function
  - Can “calibrated” material parameters be extrapolative ?
  - How to pass model UQ from lower scale to higher scale?
  - Strategies for improving  model “identifiability”
  - Design of multi-scale data collection
  - Concurrent design of experiments and computer simulations

# Acknowledgment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AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
UNITED STATES AIR FORCE

INTERNATIONAL INSTITUTE FOR NANOTECHNOLOGY
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# Related Publications


Bostanabad, R., Zhang, Y., Li, X., Kearney, T., Brinson, L. C., Apley,  D., Wing K., and Chen, W., "Computational Microstructure Characterization and Reconstruction: Review of the State-of-the-art Techniques", Progress in Materials Science, 95, June 2018.

Bostanabad, R., Liang, B., Gao, J., Liu, W-K., Cao, J., Zeng, D., Su, X., Xu, H., Li, Y., and Chen, W. (2018). "Uncertainty Quantification in Multiscale Simulation of Woven Fiber Composites". Computational Methods in Applied Mechanics and Engineering , 338(8), 2018.

Chen, Z., Huang, T., Shao, Y., Li, Yang, Xu, H., Avery, K., Zeng, D., Chen, W., and X. Su, "Multiscale Finite Element Modeling of Sheet Molding Compound (SMC) Composite Structure based on Stochastic Mesostructure Reconstruction", Composite Structures, 188, 25–38, 2018.

Zhang, W., Bostanabad, R., Liang, B., Su, X., Zeng, D., Bessa, M., Wang, Y., Chen, W., and Cao, J., " A Numerical Bayesian-Calibrated Characterization Method for Multiscale Prepreg Preforming Simulations with Tension-Shear Coupling", Composite Science and Technology, in press.

Bessaa, M.A., Bostanabad, R., Liu, Z., Apley, D.W., Brinson, C., Chen, W., and Liu, W-K, "A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality", Computer Methods in Applied Mechanics and Engineering, 320, 633-667, 2017.