Stochastic Multiscale Analysis and Design

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Integrated DEsign Automation Laboratory (*IDEAL*)

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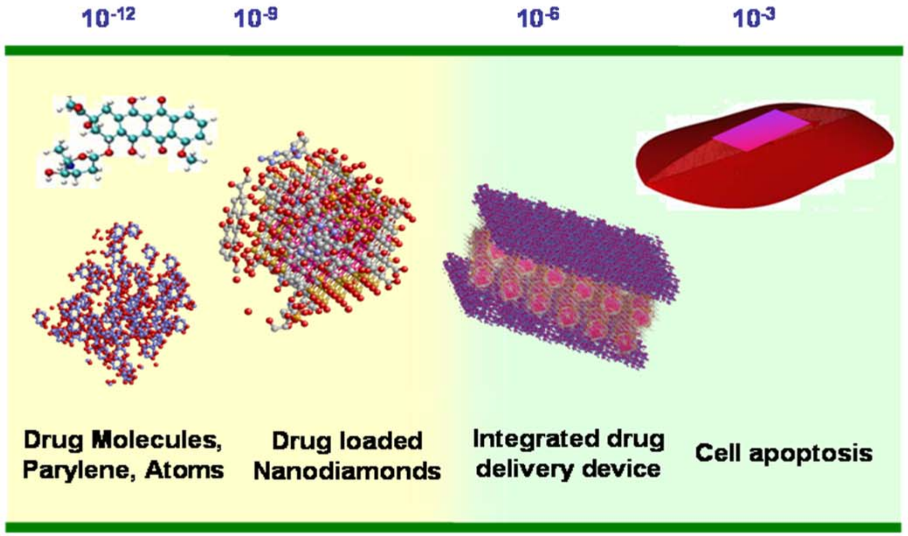
Hierarchical Multiscale Design

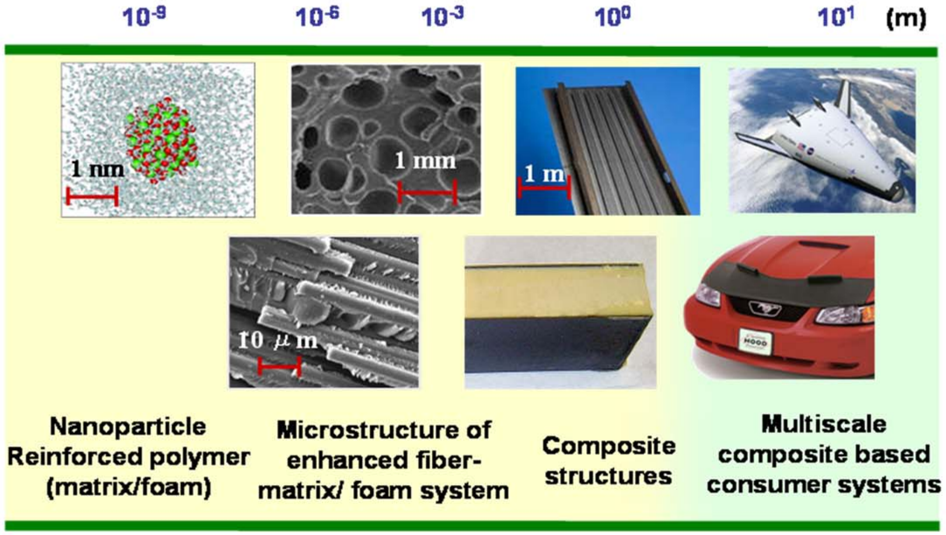
Multiscale Design

Concurrent optimization of hierarchical materials and product designs across multiple scales, accounting for the multiscale nature of physical behavior and manufacturing restrictions.

Bio-Multiscale System for Drug Delivery

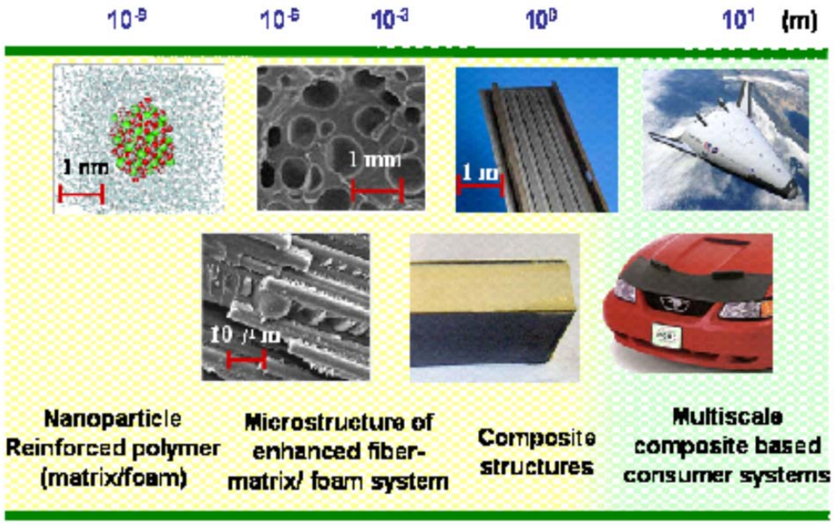


Micro-Nano-Composites Structure

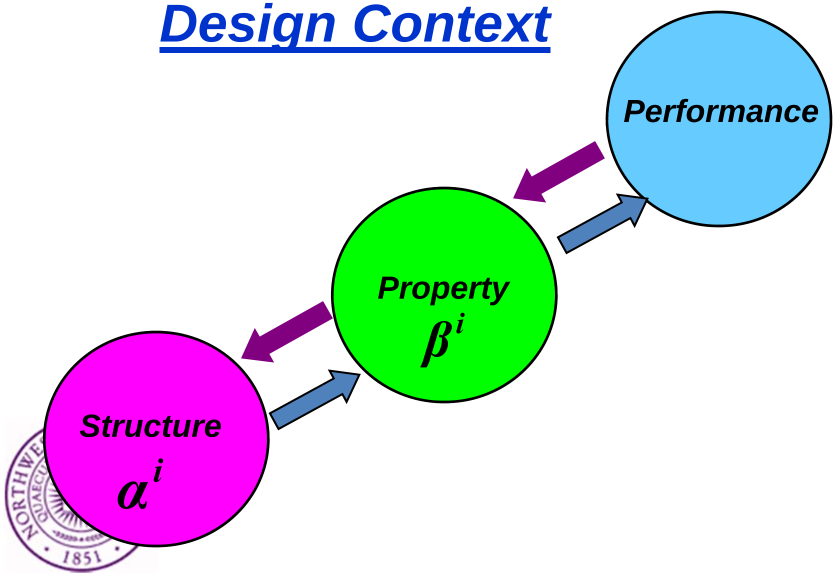


Structure-Property-Performance

Multiscale Micro-Nano-Composites Structure



Design Context



Performance

Property β^i

Structure α^i

Multiscale Design

Example: Nano-Composite Aircraft

Scale	Design Variables (potential)	
4 – atomistic	$\vec{\beta}^4$	Matrix Material Properties
3 – nano	$\vec{\alpha}^3$	Nano-particle volume fraction NP particle size distribution
2 – meso/micro	$\vec{\alpha}^2$ $\vec{\beta}^2$	Composite layer orientation Adhesive material properties
1 – milli	$\vec{\alpha}^1$	Surface texture
0 – macro	$\vec{\alpha}^0$	Wing geometry

Performance: Strength, weight, heat conductivity

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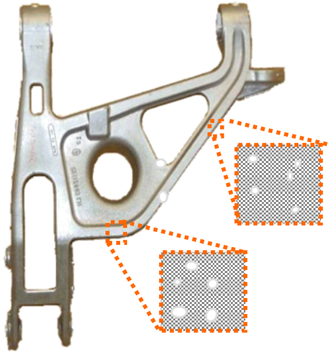
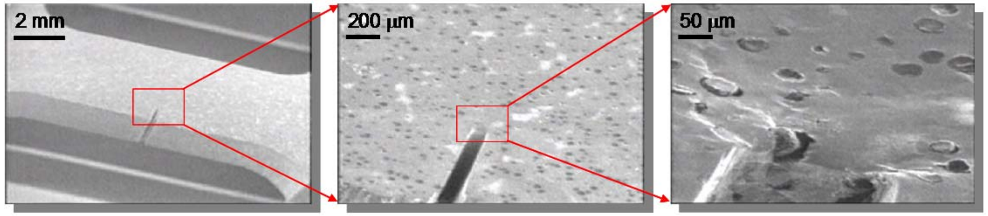
Uncertainty Sources

Type I: Parameterizable variability (Aleatory)

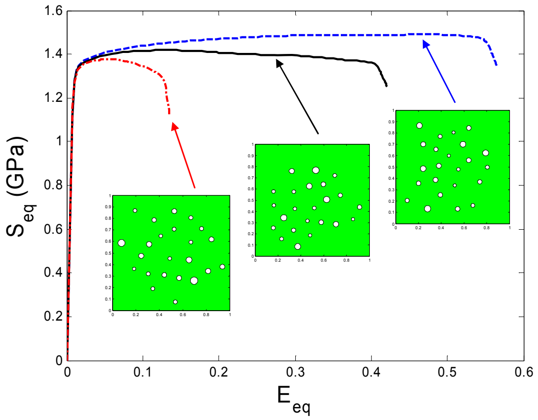
– Uncertainty associated with model parameters, e.g., microstructure, material parameters, loading





Type II: Unparameterizable variability (Epistemic)

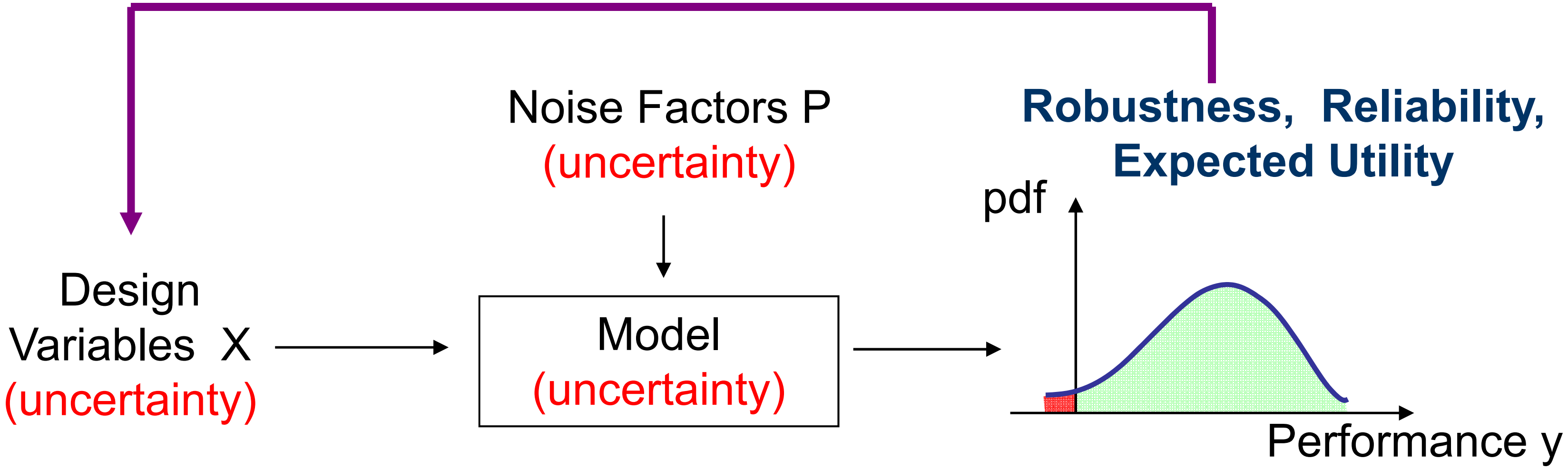
– Uncertainty due to the inadequate statistical descriptors/parameters, or lack of computing power



Type III: Model/method errors (Epistemic)

– Uncertainty caused by lack of knowledge, model simplification/approximation often manifested by homogenization when bridging between scales.

Design under Uncertainty



Noise Factors P
(uncertainty)

Design
Variables X
(uncertainty)

Model
(uncertainty)

Robustness, Reliability,
Expected Utility

pdf

Performance y

- *Uncertainty Representation*
- *Efficient Uncertainty Propagation (robustness & reliability Assessments)*
- *Efficient Probabilistic Optimization*
- *Quantification of Model Uncertainty (model validation)*

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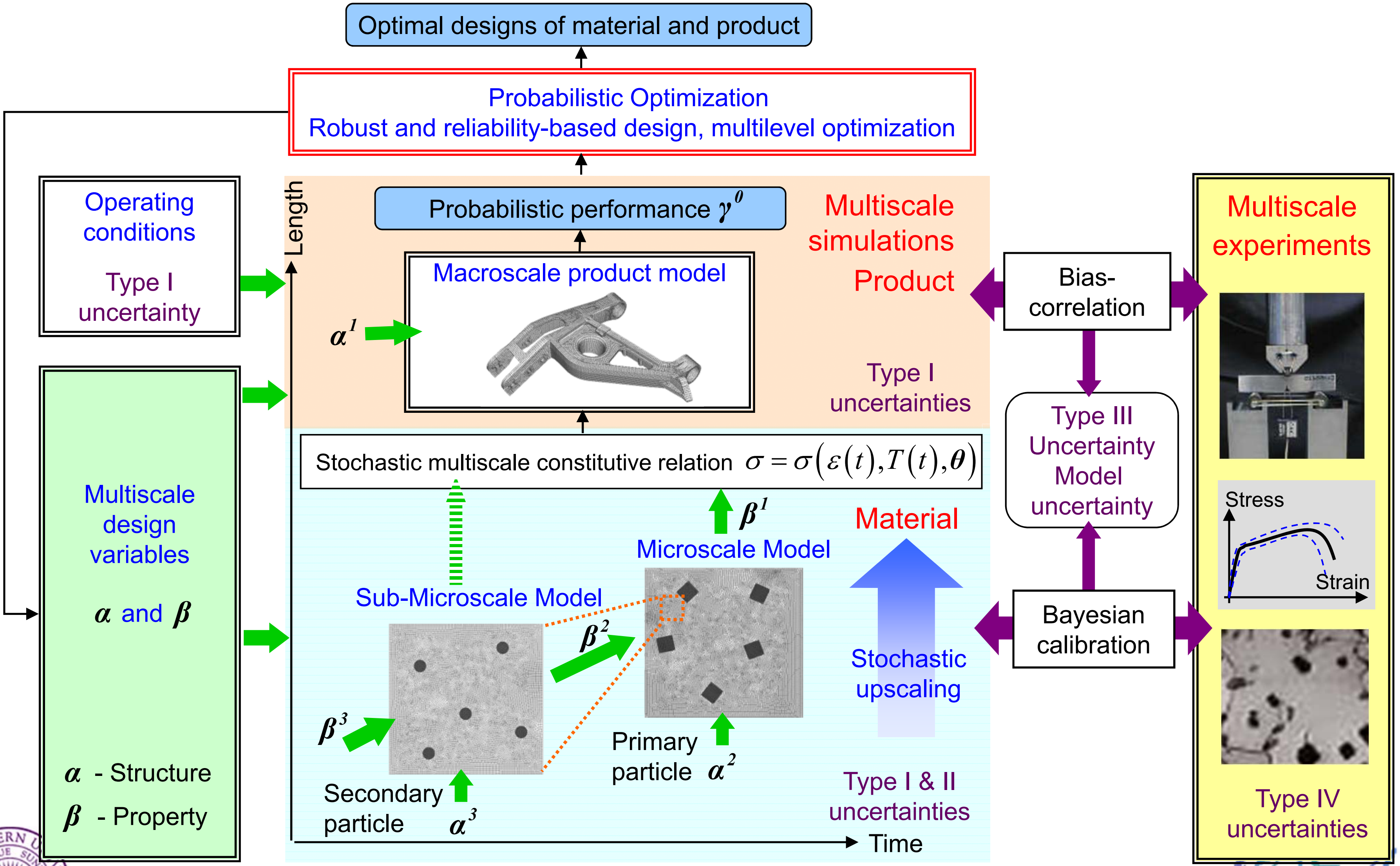
Stochastic Multiscale Computational Design Framework



Optimal designs of material and product

Probabilistic Optimization
Robust and reliability-based design, multilevel optimization

Operating conditions

Type I uncertainty

Multiscale design variables

α and β

α - Structure

β - Property

Probabilistic performance γ^0

Macroscale product model

α^1

Multiscale simulations

Product

Type I uncertainties

Stochastic multiscale constitutive relation $\sigma = \sigma\left(\varepsilon(t), T(t), \theta\right)$

Material

Microscale Model

β^1

Sub-Microscale Model

β^2

β^3

Primary particle α^2

Secondary particle α^3

Stochastic upscaling

Type I & II uncertainties

Bias-correlation

Type III Uncertainty Model uncertainty

Bayesian calibration

Multiscale experiments

Type IV uncertainties

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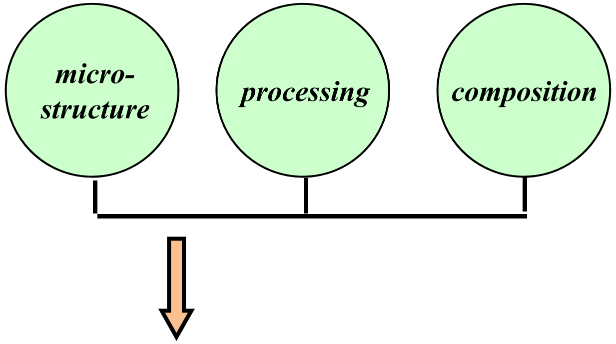
Stochastic Multiscale Analysis and Design Methodology

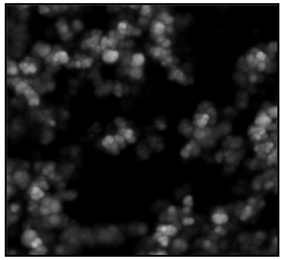
- Predictive stochastic multiscale analysis
  - *Statistical material characterization*
  - *Stochastic constitutive theory (upscaling)*
- Managing complexity in multiscale design
  - *Multilevel optimization (target cascading)*
  - *Hierarchical statistical cause-effect analysis*
- Quantification of model uncertainty
  - *Combining computer simulations & physical experiments*

Statistical Material Characterization

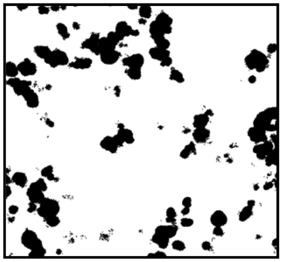
MATERIAL STRUCTURE



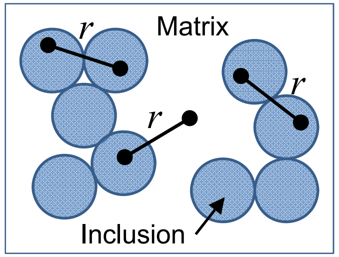
1 SEM Image



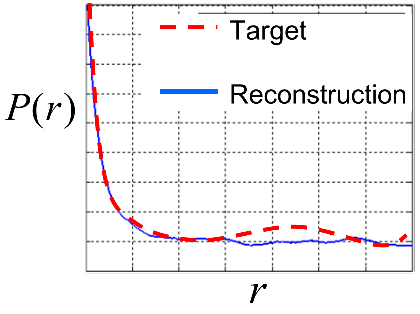
2 Target



3 Point correlation

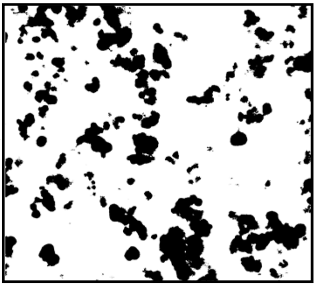


- **1** Microstructure imaging techniques (SEM, TEM, etc.)
- **2** Binary image construction via image processing algorithms
- **3** *n*-point correlation functions (2-point shown)
- **4** Statistically equivalent microstructure reconstruction

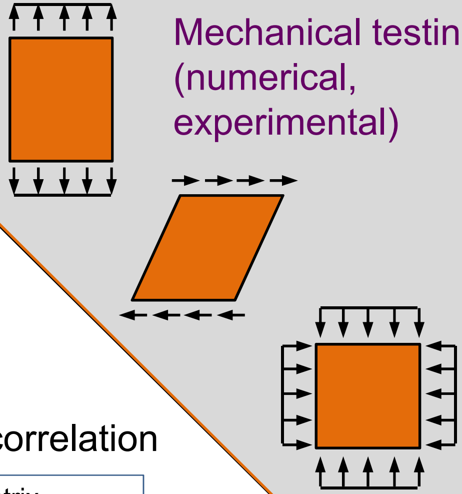


Work primarily conducted by Y. Liu

4 Reconstruction

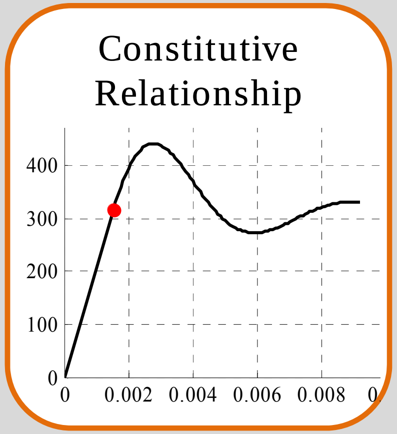


Accuracy lost with simplified statistical description



Mechanical testing (numerical, experimental)

MATERIAL PROPERTY



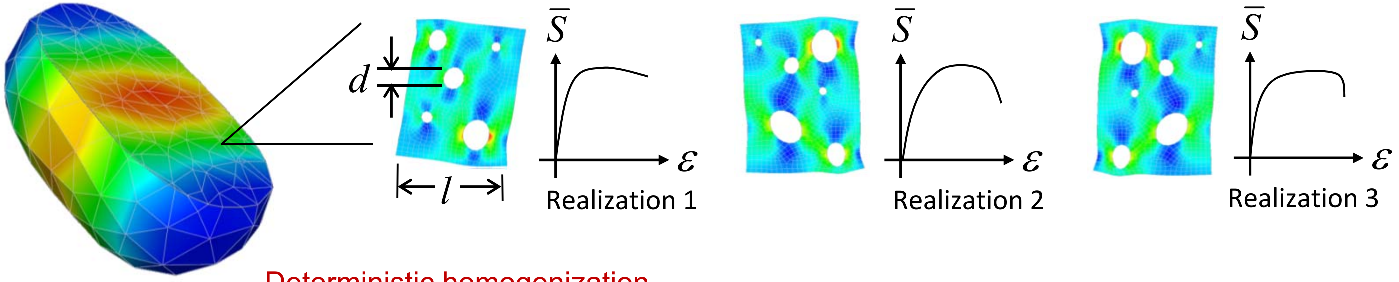
Constitutive Relationship

Stochastic Constitutive Theory

For multiscale analysis, deterministic fine scale simulations create randomness

Macroscale, e.g.

Fine resolution statistical volume element realizations



Deterministic homogenization
(standard constitutive modeling)

$$\langle \mathbf{S}\rangle = f\left(\boldsymbol{\kappa},\langle\boldsymbol{\varepsilon}\rangle,\langle\dot{\boldsymbol{\varepsilon}}\rangle,\langle T\rangle,t,\ldots,SA\right)$$

Fit set of phenomenological constitutive law parameters to SVE simulation results

Treat parameters as multivariate statistical distribution whose data are each realization

Add randomness to constitutive law parameters

$$\langle \mathbf{S}\rangle = f\left[\mathbf{K}(\omega),\langle\boldsymbol{\varepsilon}\rangle,\langle\dot{\boldsymbol{\varepsilon}}\rangle,\langle T\rangle,t,\ldots,SA\right]$$

Specific form of stochastic constitutive theory

$$\mathbf{K}(\theta)\sim f_K\left(\boldsymbol{\kappa},\theta\right)$$

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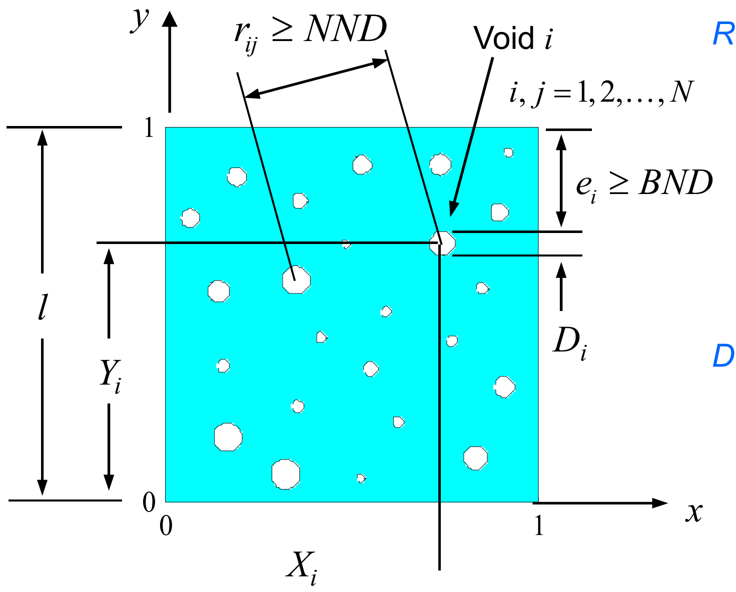
Data-Driven Approach to Stochastic Constitutive Relations

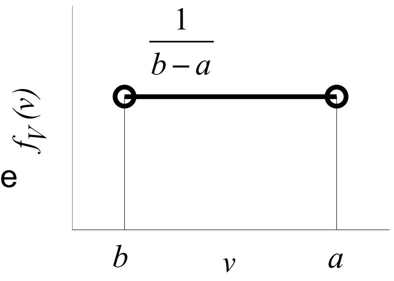
High strength, porous 4330 steel alloy with microstructure *Yin et. al (2008)*



Random parameters (all follow uniform distribution)

v	a	b	Description
N	10	25	Number of particles
D_i	0.02	0.08	Void diameter
NND	0.12	0.1645	Nearest neighbor distance
X_i, Y_i	0.06	0.94	Void center coordinates

Arbitrary uniform distribution



Deterministic parameters

$BND = 0.06$

minimum distance from void to SVE boundary

$l = 1$

SVE simulation domain size

330 SVE simulations
(30 minutes apiece)

Phenomenological Constitutive Model – Bamann Chiesa Johnson *Bammann et. al (1996), McVeigh & Liu (2008)*

$$\sigma(\boldsymbol{\kappa}, \varepsilon) = (1-\phi)\left[\kappa_1 + \kappa_2 \tanh(\kappa_3 \varepsilon)\right]$$

Damage a quadratic function of effective strain

$$\phi = \phi_0 + \kappa_4 \varepsilon + \kappa_5 \varepsilon^2$$

$$\sigma\left[\mathbf{K}(\theta), \varepsilon\right] = \left[1 - \left(\phi_0 + \underline{\mathrm{K}_4}\varepsilon + \underline{\mathrm{K}_5}\varepsilon^2\right)\right]\left[\underline{\mathrm{K}_1} + \underline{\mathrm{K}_2} \tanh\left(\underline{\mathrm{K}_3}\varepsilon\right)\right]$$

Via **stochastic constitutive theory**, the 5 constitutive model parameters are assumed to have some unknown joint distribution

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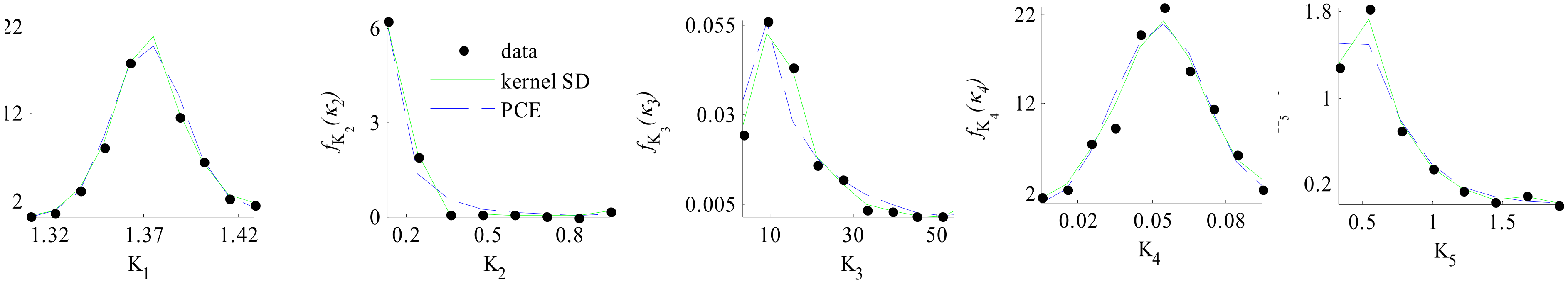
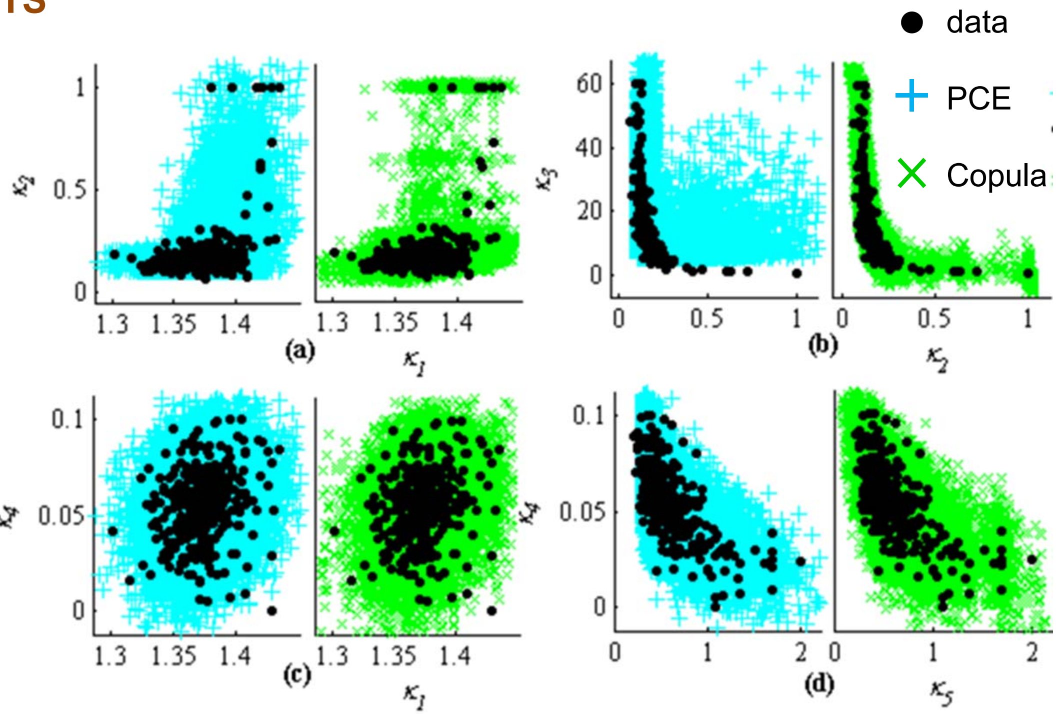
Capturing Correlations of Coefficients in Stochastic Constitutive Relation

MARGINAL PROBABILITY DISTRIBUTIONS



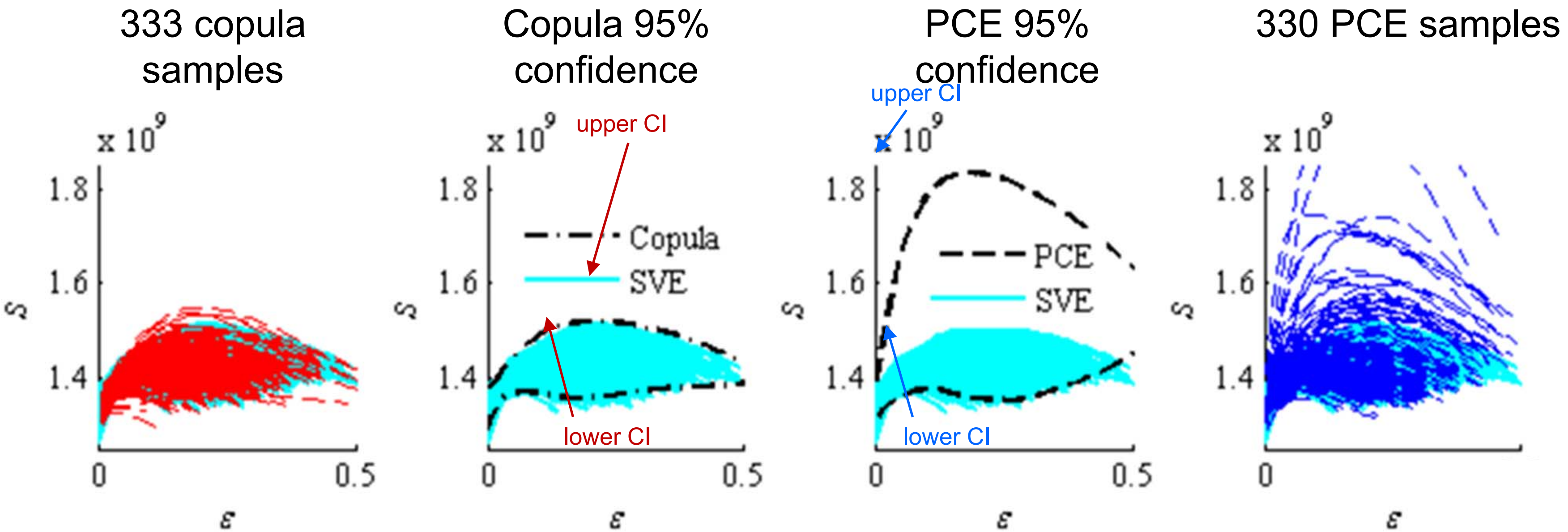
SELECTED BIVARIATE SCATTER PLOTS



- Copula approach (Schweizer and Wolff, 1981) links arbitrary marginal CDFs to multivariate dependence structures through correlation measure that depends on the copula type.
- Polynomial chaos for non-Gaussian processes used to quantify joint statistical distribution

Prediction of Stochastic Constitutive Relation

CONSTITUTIVE BEHAVIOR CONFIDENCE



- **Copula method better captures the constitutive behavior observed in the sample of SVE simulations**
- **PCE method provides a highly conservative estimate on the upper bound of constitutive behavior.**

Greene M.S., Liu, Y., Chen, W., Liu, W.K., “Computational Uncertainty Analysis in Multiresolution Materials via Stochastic Constitutive Theory”, CMAME, 200, 309-325, 2011.

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Stochastic Multiscale Analysis and Design Methodology

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  - *Statistical material characterization*
  - *Stochastic constitutive theory (upscaling)*

- Managing complexity in multiscale design
  - *Multilevel optimization (target cascading)*
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- Quantification of model uncertainty
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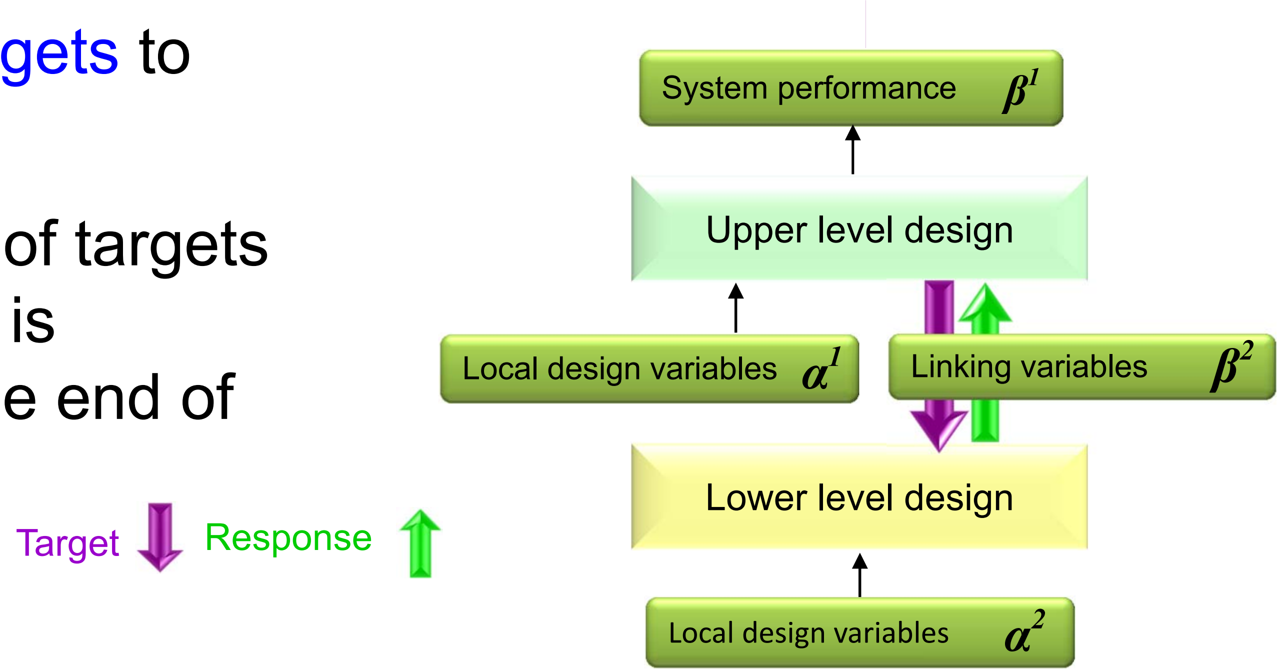
Multilevel Optimization for Multiscale Design

Multi-level optimization is used for designing multiscale systems across various scales and disciplines.

- Cascading targets to lower level
- Convergence of targets and response is achieved at the end of the process



- Analytical Target Cascading (ATC) (*Kim et. al., 2003*)
- Probabilistic ATC (PATC) (*Kokkolaras et al. 2004; Liu et al. 2005*)
- PATC with correlated subsystems (*Xiong et al. 2009*)

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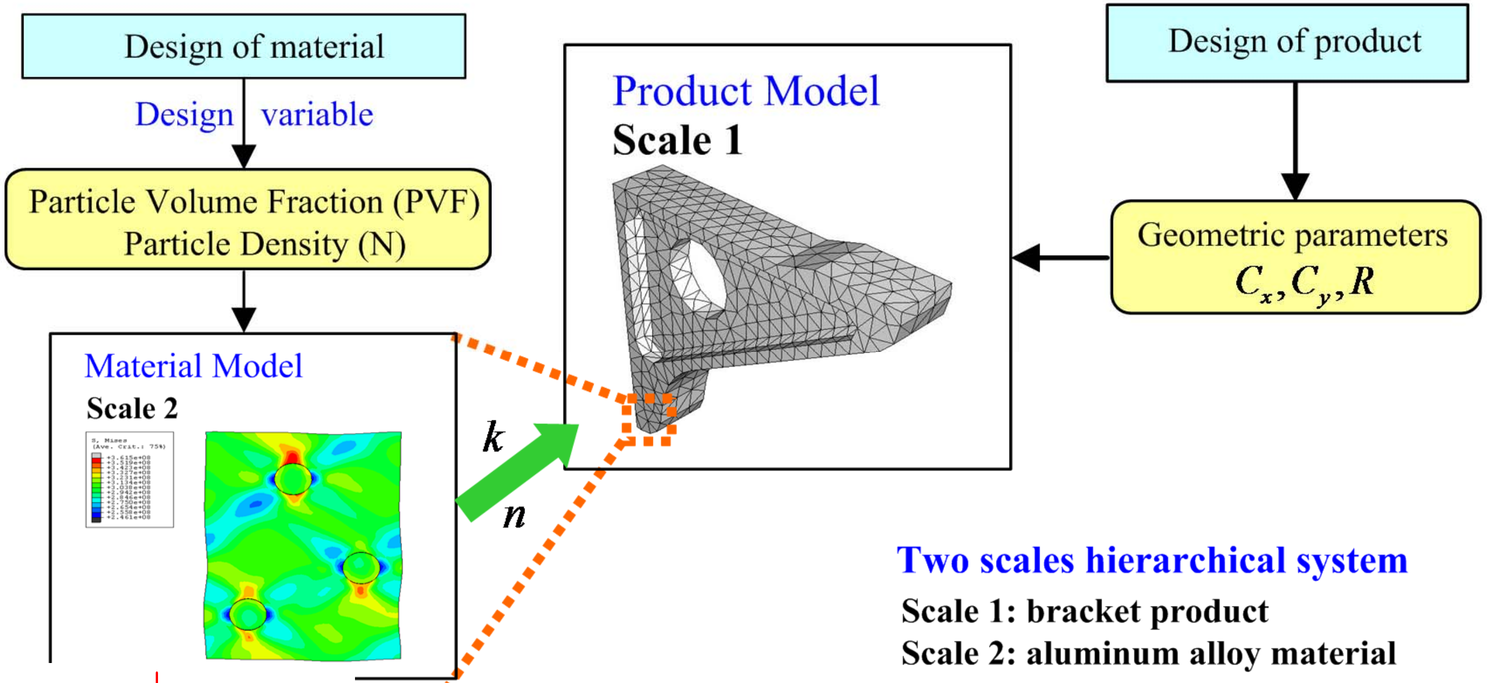
Example - Multiscale Bracket Design



Design of material

Design variable

Particle Volume Fraction (PVF)
Particle Density (N)

Material Model
Scale 2

k

n

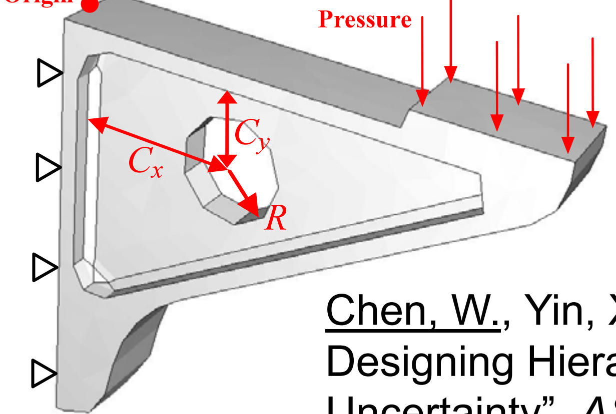
Product Model
Scale 1

Design of product

Geometric parameters
C_x, C_y, R

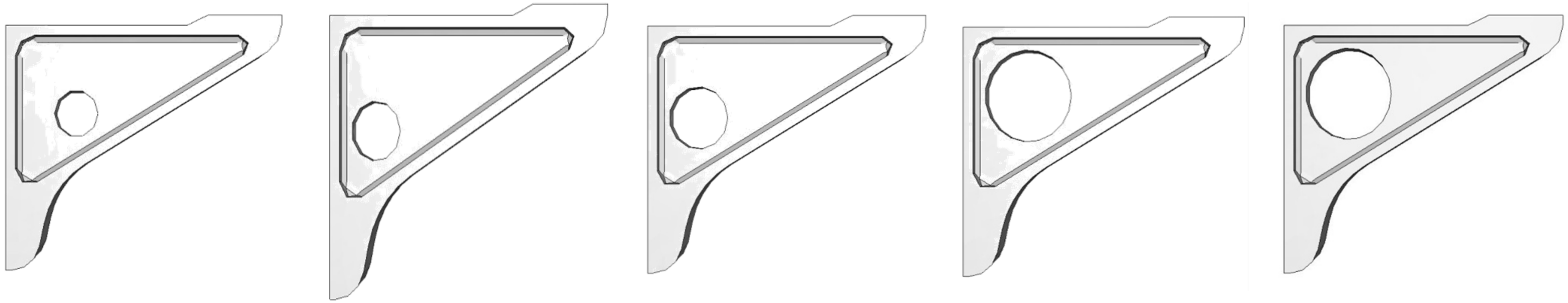
Two scales hierarchical system

Scale 1: bracket product
Scale 2: aluminum alloy material



Chen, W., Yin, X., Lee, S., and Liu, W. K., "A Multiscale Design Methodology for Designing Hierarchical Multiscale Systems Considering Random Field Uncertainty", *ASME Journal of Mechanical Design,* 2010.

Multiscale Design Solutions

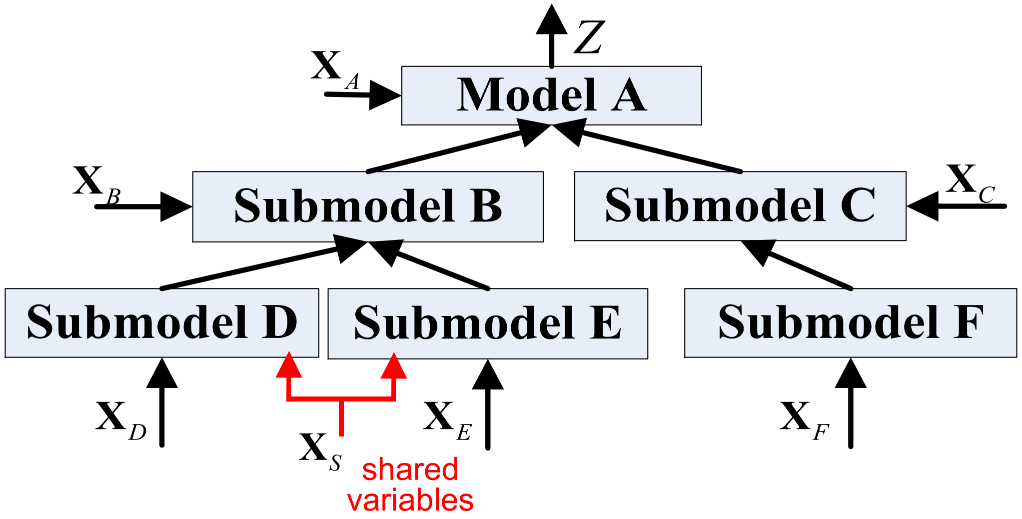


Material microstructure solutions (PVF_3, N_3)

S_c (GPa)	0.258	0.260	0.265	0.269	0.270
(PVF_3, N_3)	0.0390, 3.0000	0.0343, 3.0000	0.0300, 3.8098	0.0300, 3.8163 0.0300, 6.1924 0.0418, 4.0944 0.0500, 4.9826 0.0300, 3.7667 0.0300, 3.7787 0.0300, 3.8429 0.0524, 5.0095 0.0300, 3.7285 0.0300, 3.8964	0.0300, 3.7297 0.0789, 3.0000 0.1095, 6.0229 0.0300, 4.0143 0.0435, 4.8733 0.0632, 3.0000 0.0705, 4.1363 0.0832, 5.2942 0.0986, 5.5558 0.0478, 7.0000

- Unique solutions for small S_c; Multiple solutions of material microstructure for large S_c
- New aluminum alloy achieves reduction of stress concentrations by re-distribution of loads after yielding in the plastic range

Hierarchical Statistical Sensitivity Analysis (HSSA) Method



Features:

(1) SSA is applied to submodels at each level with top-down sequence;

(2) The global *Statistical Sensitivity Index (SSI)* are aggregated from the local SSA at each level.

(3) Aggregation formulation considers submodel dependencies

Yu, L., Yin, X., Arendt, P., Chen, W., Huang, H-Z., "A Hierarchical Statistical Sensitivity Analysis Method for Multilevel Systems with Shared Variables", ASME Journal of Mechanical Design, 2010

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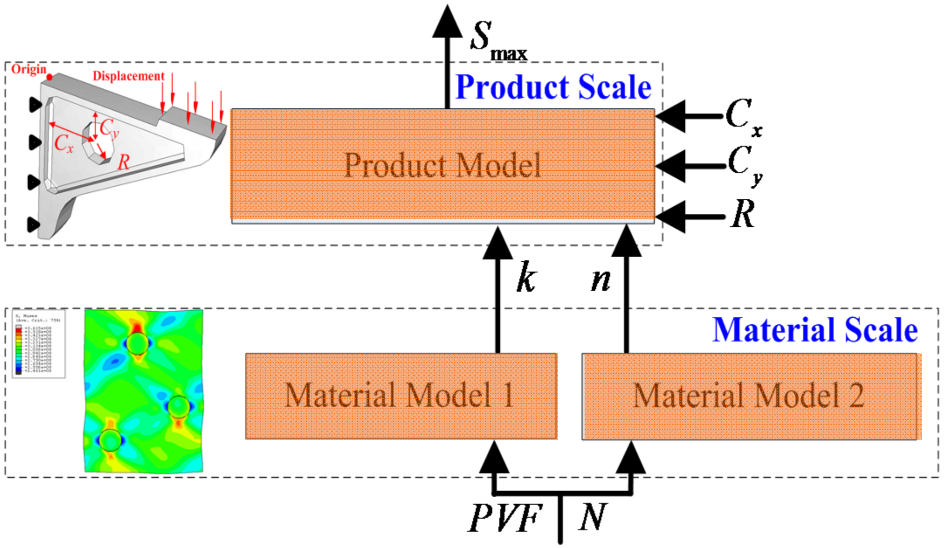
HSSA Results



S_{max}

Product Scale

Product Model

C_x

C_y

R

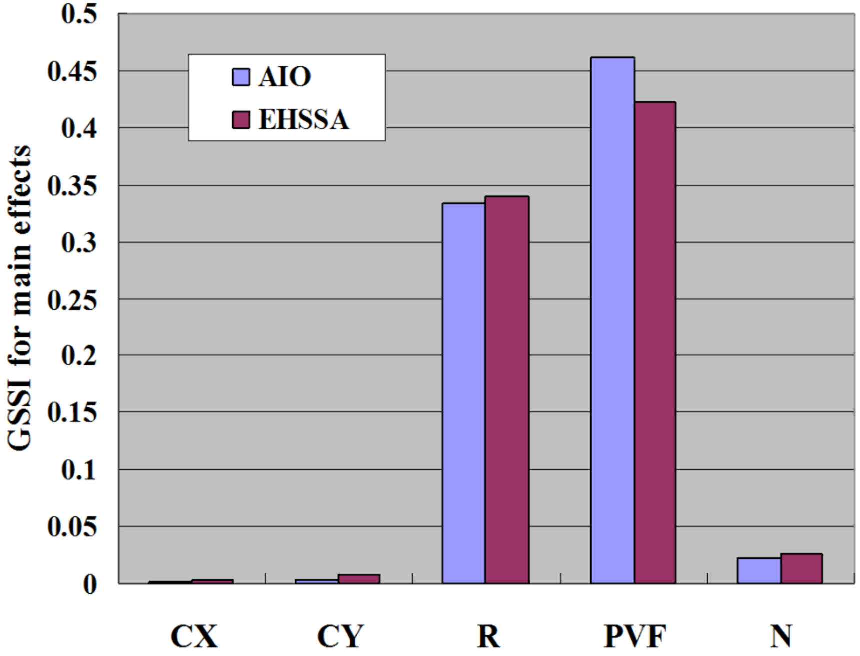
k n

Material Scale

Material Model 1

Material Model 2

PVF | N



$SSI_R + SSI_{PVF} > 0.75$

Chen, W., Yin, X., Lee, S., and Liu, W. K., "A Multiscale Design Methodology for Designing Hierarchical Multiscale Systems Considering Random Field Uncertainty", *ASME Journal of Mechanical Design,* 2010.

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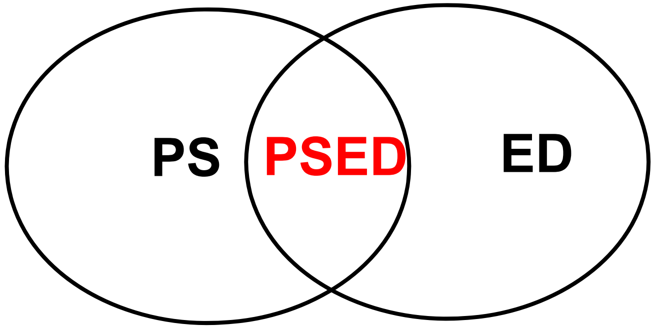
Predictive Science & Engineering Design Cluster

- Predictive Science (PS) - the application of verified and validated computational simulations to predict the response of complex systems, particularly in cases where routine experimental tests are not feasible.
- Engineering Design (ED) - the process of devising a system, component or process to meet desired needs.



- Certificate Requirements: 3 core courses + 2 electives
  - Modeling, Simulation, and Computing
  - Computational Design
  - PS&ED 510 Seminar

http://psed.tech.northwestern.edu/

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Dynamic Energy Dissipation for Earthquake Protection, PSED Cluster 2009-2010

Graduate Student Fellows:
GEORGE FRALEY
STEVEN GREENE

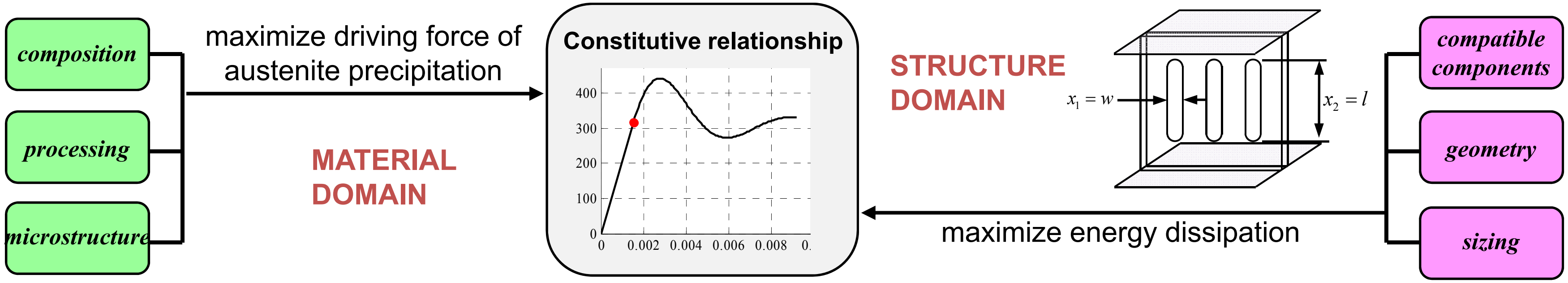
Faculty Advisors:
WEI CHEN, WING KAM LIU
GREG OLSON

Academic Disciplines:
MECHANICAL ENGINEERING, CIVIL ENGINEERING
MATERIALS SCIENCE & ENGINEERING

June 03, 2010

RESEARCH OBJECTIVE

Integrate contemporary materials and structure analysis & design principles to create products with better functionality as ***passive energy dissipation*** devices. Through exploring the codependent physics in the material (nano, micro) and continuum (meso, macro) domains, automated design techniques utilize experimental data, structural concepts, and atomistic and continuum simulations to consider mutual design issues across disparate scales in length and time. The end mission of the project is to use the integrated design approach to unlock new devices for earthquake protection, with a specific focus on historic buildings.



composition

processing

microstructure

maximize driving force of austenite precipitation

MATERIAL DOMAIN

Constitutive relationship

STRUCTURE DOMAIN

maximize energy dissipation

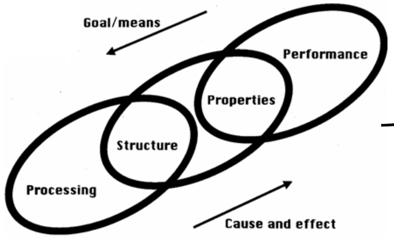
compatible components

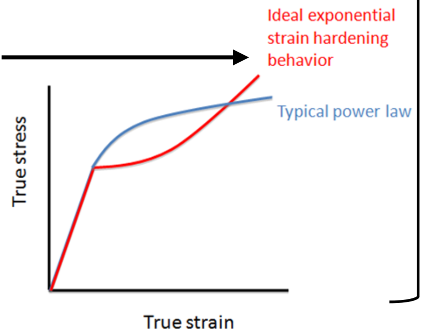
geometry

sizing

BENCHMARK PROBLEM

- Preliminary material and structural design of slit steel damper
- Optimal combination of material & geometry sought
- Dissipation occurs through metal yielding
- Material/structure integration through constitutive relationship

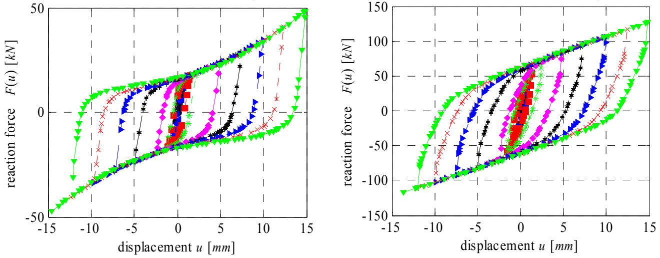




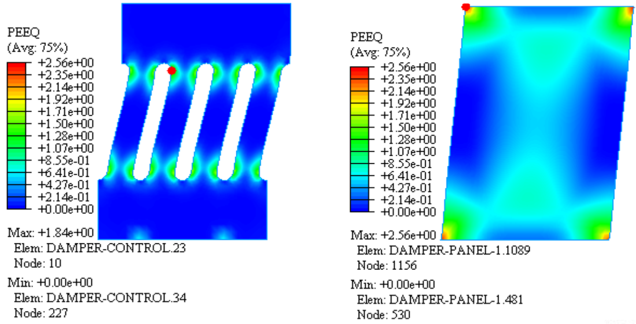
Class of secondary hardened Martensitic steel is considered to exploit transformation plasticity.
Materials design provides optimal constitutive relationship for energy dissipation

Structural design produces solid shear panel, confirmed by literature, due to highest plastic strain from mobilized shear deformation

Sample Design **Optimal Design**



Cyclic loading hysteris loop



Equivalent plastic strain field

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Metal-Polymer Laminate Composite: Modeling and Design, PSED Cluster 2010-2011

Graduate Student Fellows:
Jiayi Yan, Ying Li, Yang Li

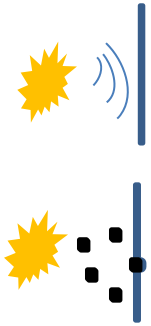
Faculty Advisors:
WEI CHEN, WING KAM LIU
GREG OLSON, CATE BRINSON

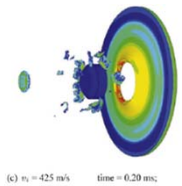
Academic Disciplines:
MECHANICAL ENGINEERING
MATERIALS SCIENCE & ENGINEERING

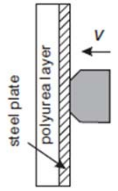
Mar 19 , 2011

RESEARCH OBJECTIVE

The rapid development of industry in recent decades greatly raises the demand of high-performance structural materials to survive severe mechanical loadings. Our objective is to provide some insight to materials behavior of Metal Polymer laminates composites, and come up with novel designs. With impact resistance improved and other advantages maintained, such designed materials will have a board spectrum of applications, including aircrafts, automobiles, armors, electronic devices and helmets.

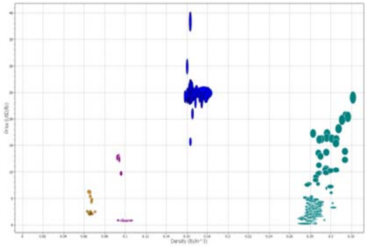






MATERIAL SELECTION

The properties of composites significantly depend on their constitutive components. To obtain some insight from existing MPLCs, we need to relate their general properties to materials selection. Based on the desirable performance, we will make a list of primary and secondary properties taken into account with comprehensive consideration. We will follow the ideas from Ashby and use CES EduPack.

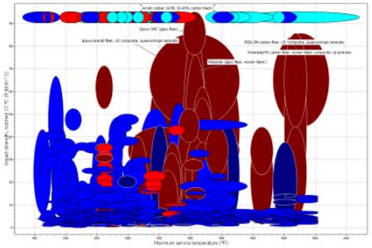


Metal
Al alloy
Mg alloy
Steel
Ti alloy
…

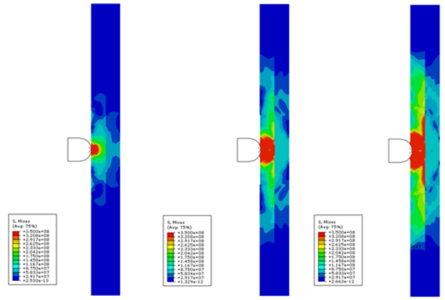
Tensile strength
Ductility
Density
Cost
Modulus

Polymer
Polyurea
PC
…

Tensile strength
Ductility
Density
Cost
Modulus



FINITE ELEMENT SIMULATION



Stress wave propagation under round-nosed projectile

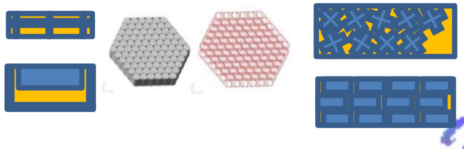
FUNCTION-ORIENTED OPTIMIZATION

Divide the structure into functional layers

- Shielding layer
- Supporting layer
- Anti-trauma layer

↓

Concept design of each layer



↓

Adjust ratio of each functional layer

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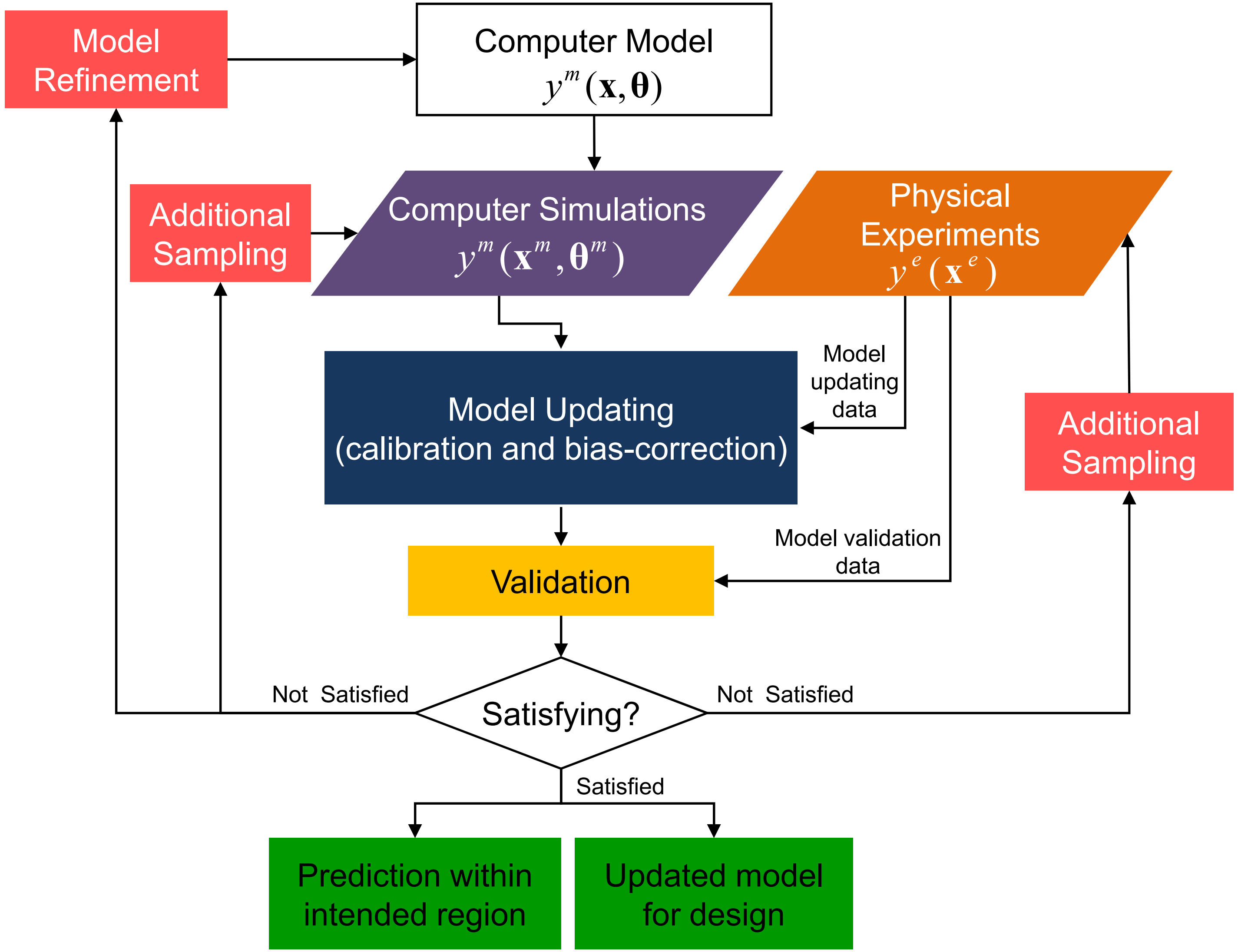
Stochastic Multiscale Analysis and Design Methodology

- Predictive stochastic multiscale analysis
  - *Statistical material characterization*
  - *Stochastic constitutive theory (upscaling)*

- Managing complexity in multiscale design
  - *Multilevel optimization (target cascading)*
  - *Hierarchical statistical cause-effect analysis*

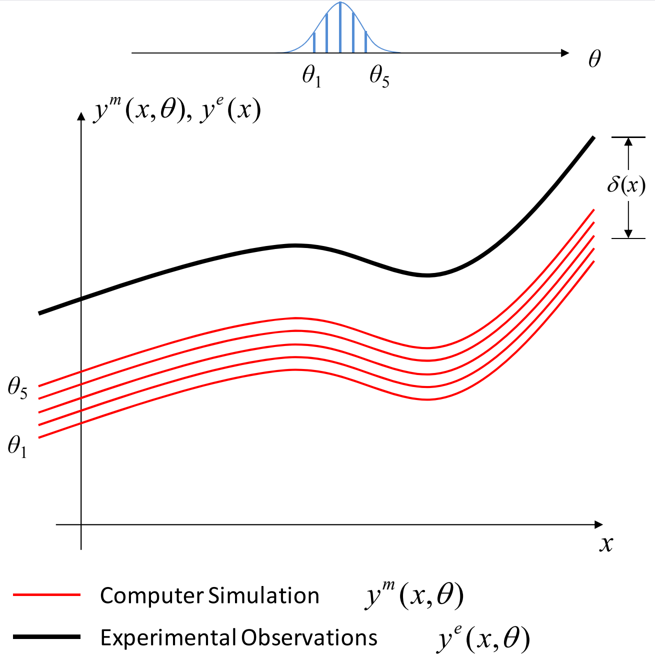
- Quantification of model uncertainty
  - *Combining computer simulations & physical experiments*

Model Updating and Uncertainty Quantification



Xiong, Y., Chen, W., Tsui, K-L., and Apley, D., "A Better Understanding of Model Updating Strategies in Validating Engineering Models", *Journal of Computer Methods in Applied Mechanics and Engineering*, 198 (15-16), pp. 1327-1337, March 2009.

Bias Correction and Calibration



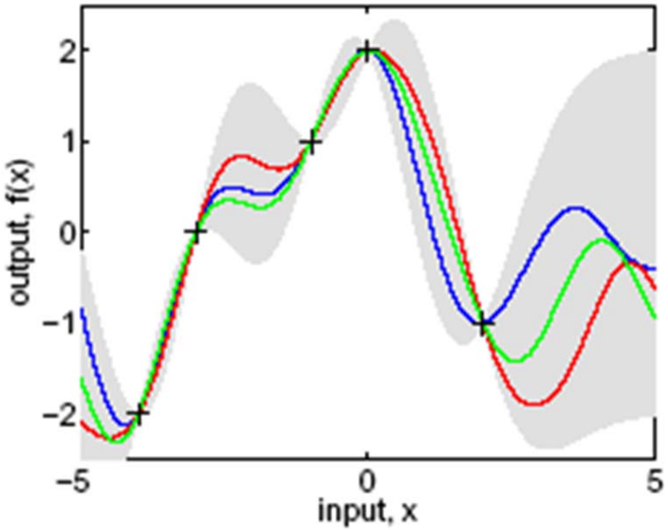
$$\underbrace{y^e\overbrace{(\mathbf{x})}^{\text{Variable Inputs}}}_{\text{Experimental Prediction}} = \overbrace{y^m(\mathbf{x},\underbrace{\boldsymbol{\theta}}_{\text{Unknown Parameters}})}^{\text{Computer Model}} + \underbrace{\delta(\mathbf{x})}_{\text{Bias Correction Function}} + \overbrace{\varepsilon}^{\text{Experimental Error}}$$

Kennedy and O'Hagan (2001)

Gaussian Processes (GP) for Lack of Data

- Representation assuming the function is a multivariate normal distribution
- Reflects uncertainty between sample points
- Written as:

$$f(x) \sim \mathcal{GP}(m(x), K(x, x'))$$



Example of a Gaussian metamodel (Rasmussen and Williams 2006 p. 15)

Mean of the Gaussian process

$$m(x) = h(x)\enclose{circle}{\beta}$$

β: Parameters for polynomial regression of the mean

h(*x*): Polynomials used to represent the mean

Hyperparameters $\beta \quad \sigma^2 \quad \omega$

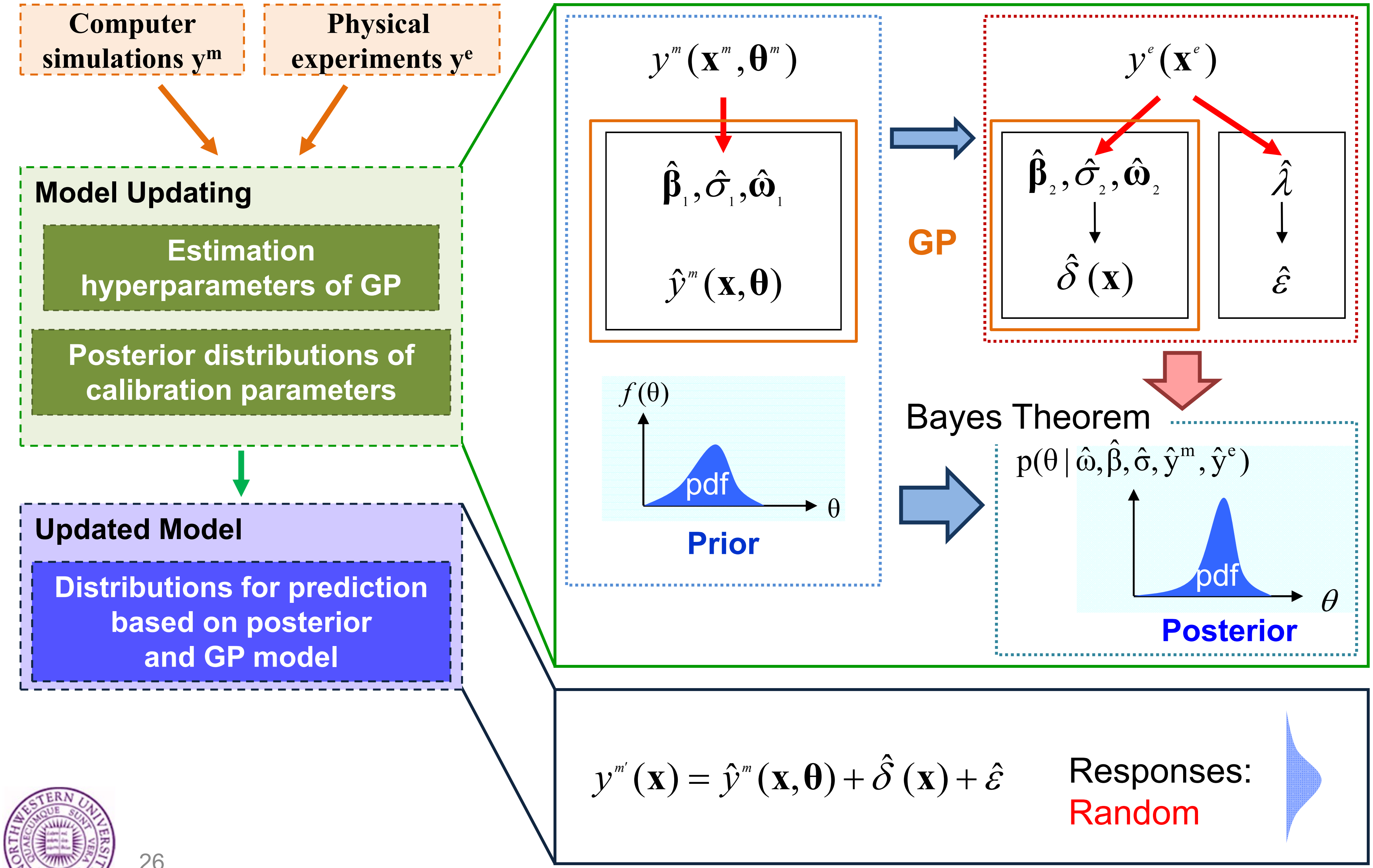
Covariance function of the Gaussian process

$$K(x, x') = r(x - x')$$

$$r(x - x') = \enclose{circle}{\sigma^2} \exp\left(-\sum_{i=1}^{d} \enclose{circle}{\omega_i} (x - x')^2 \right)$$

Correlation of the distance between two points, *x* and *x'*

Modular Bayesian Approach



Computer simulations y^m

Physical experiments y^e

Model Updating

Estimation hyperparameters of GP

Posterior distributions of calibration parameters

Updated Model

Distributions for prediction based on posterior and GP model

$y^m(\mathbf{x}^m,\boldsymbol{\theta}^m)$

$\hat{\boldsymbol{\beta}}_1,\hat{\sigma}_1,\hat{\boldsymbol{\omega}}_1$

$\hat{y}^m(\mathbf{x},\boldsymbol{\theta})$

GP

$y^e(\mathbf{x}^e)$

$\hat{\boldsymbol{\beta}}_2,\hat{\sigma}_2,\hat{\boldsymbol{\omega}}_2$

$\hat{\delta}(\mathbf{x})$

$\hat{\lambda}$

$\hat{\varepsilon}$

Prior

Bayes Theorem

$p(\theta \mid \hat{\omega},\hat{\beta},\hat{\sigma},\hat{y}^m,\hat{y}^e)$

Posterior

$$y^{m'}(\mathbf{x}) = \hat{y}^m(\mathbf{x},\boldsymbol{\theta}) + \hat{\delta}(\mathbf{x}) + \hat{\varepsilon}$$

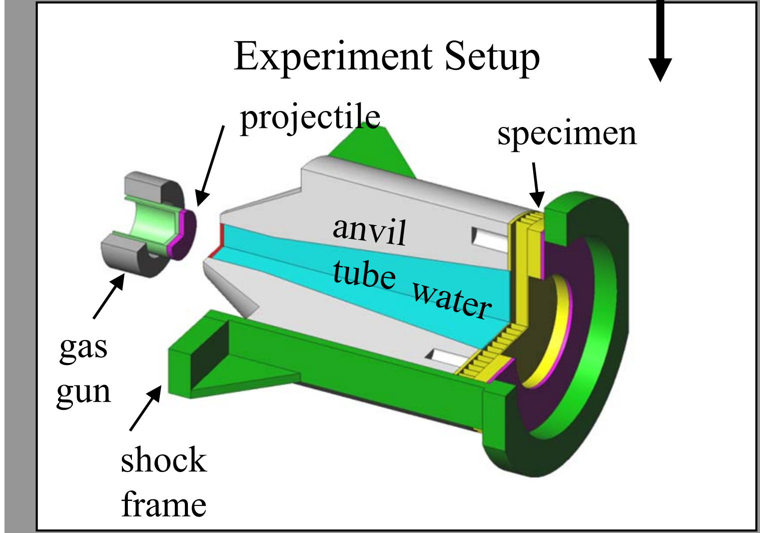
Responses: Random

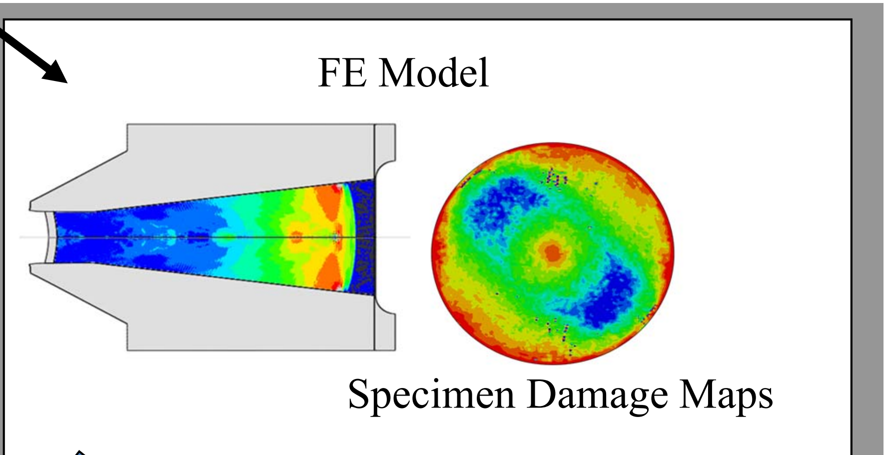
Kennedy and O'Hagan (2001) and termed by Bayarri et al (2007)

Blast Resistant
Fiber Reinforced Plastic (FRP) Sandwich

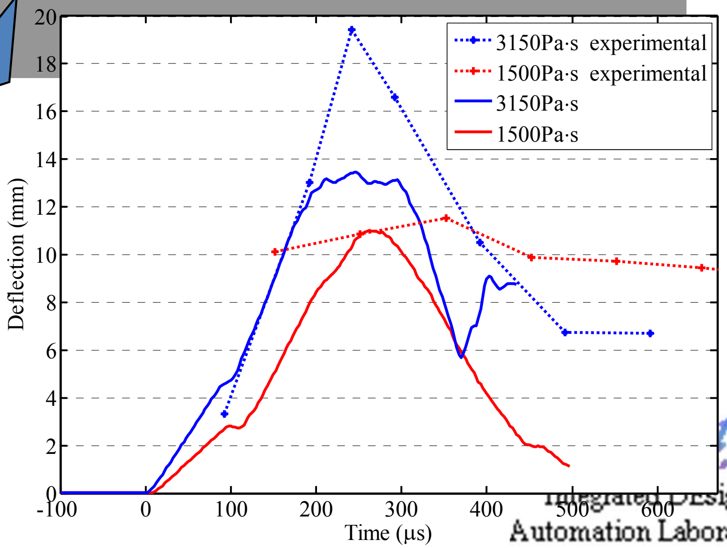
x (known inputs)

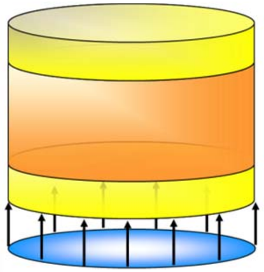
Flyer plate thickness and velocity, and **time**





Assume well calibrated model





Displacement

$u^m = y^m(x,\theta)$

$u^e = y^e(x)$

Collaboration with Prof. H. Espinosa

Figures provided by Ravi Bellur Ramaswamy

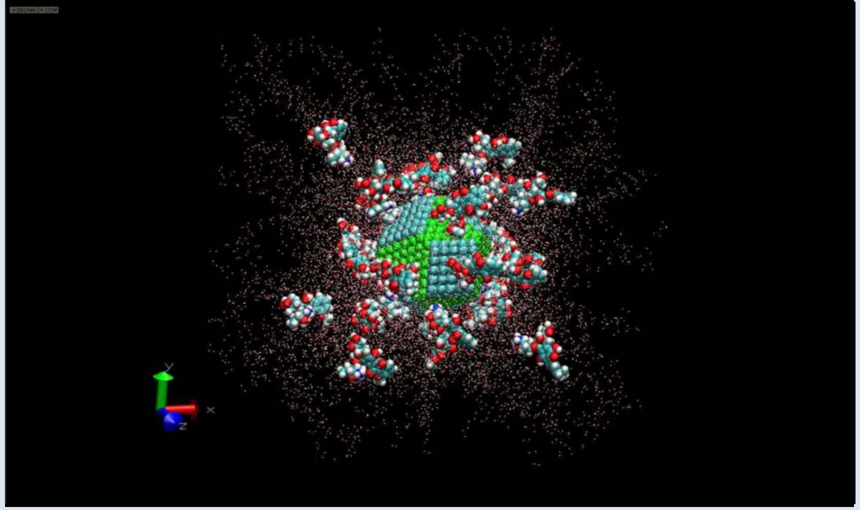
Nanodiamond (ND) Drug Delivery System

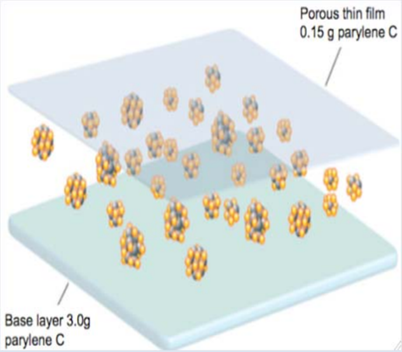
θ

(unknown but fixed inputs)

% of Atoms on Surface of ND for Drug Attachment

MD Simulations



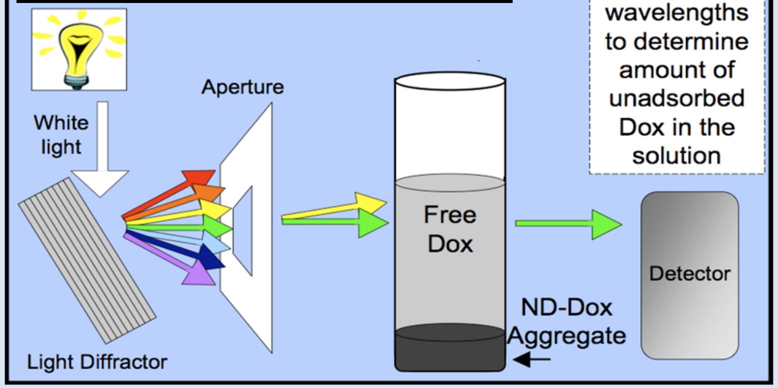


x

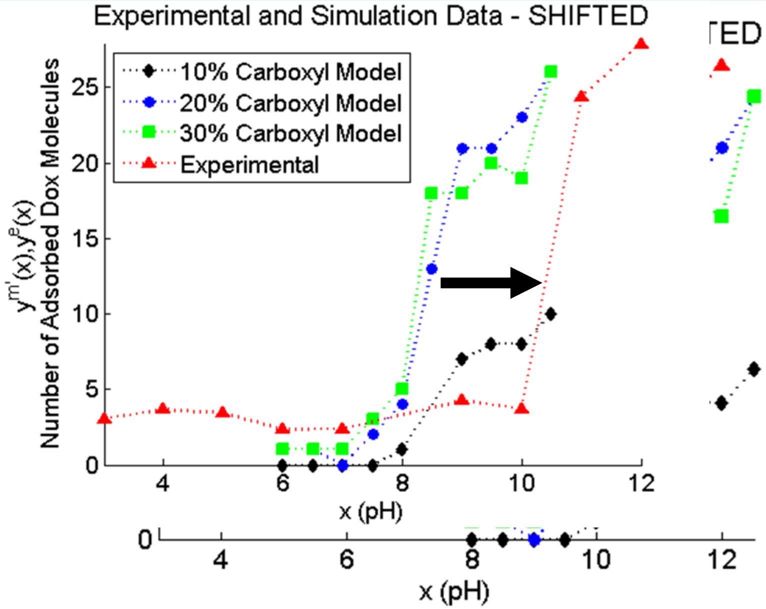
(known inputs)

pH

Physical Experiments



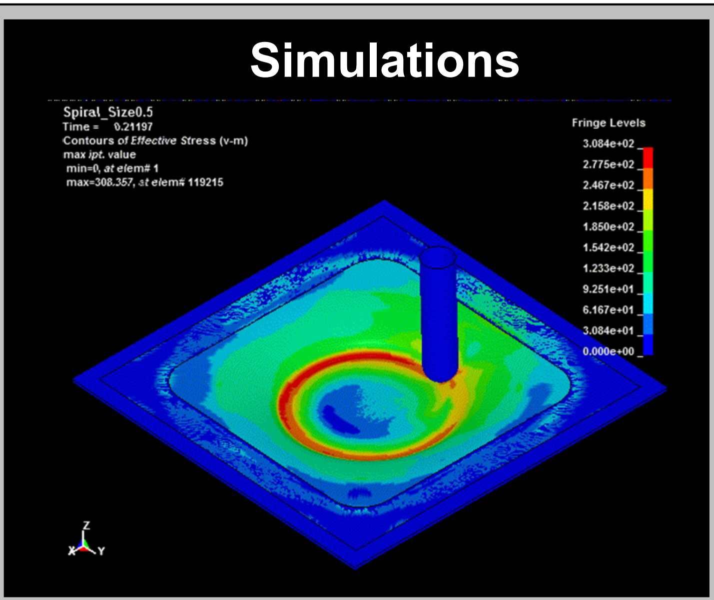
Measure light wavelengths to determine amount of unadsorbed Dox in the solution



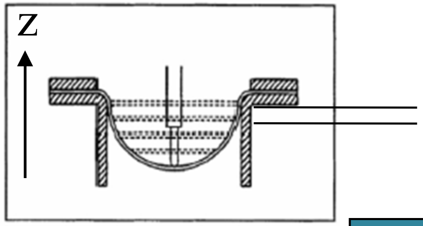
Collaboration with Prof. W. K. Liu and Prof. D. Ho

Incremental Forming Process

Experiments



Simulations



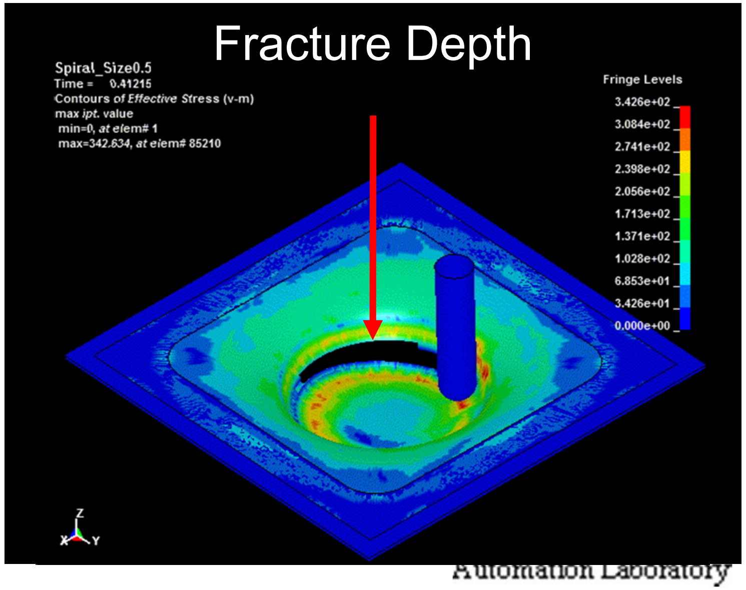
x
(known inputs)

Δz

θ
(unknown but fixed inputs)

m – damage evolution

β – weakening parameter



Fracture Depth

Collaboration with Prof. Jian Cao

Observations

1. Model calibration/updating insights into the computer model
   - Discrepancy function – capture missing physics
   - Calibration parameters – accurate identification is needed to be used in larger simulation system

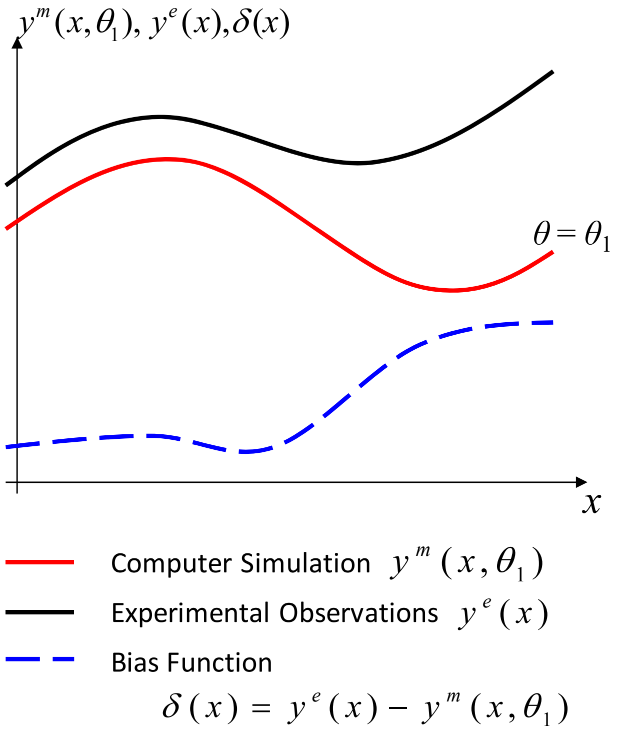
2. Implementation of modular Bayesian process suffered from:
   - Computationally expensive posterior distribution
   - Confounding between calibration parameters
   - Confounding between bias function and calibration parameters

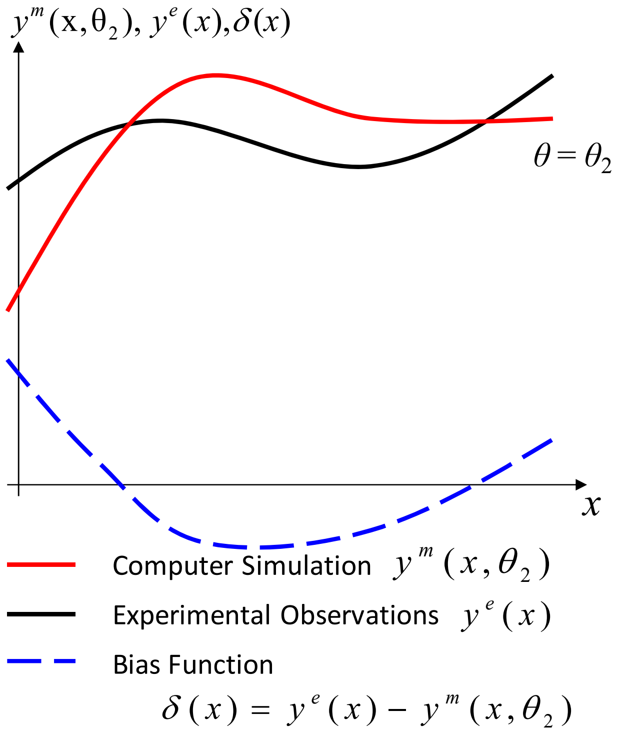
Identifiability in Model Updating

Identifiability (Lancaster 2004)

A System is not identifiable if different values of the model parameters are equally probable

$$y^e(\mathbf{x}) = y^m(\mathbf{x},\boldsymbol{\theta}) + \delta(\mathbf{x}) + \varepsilon$$



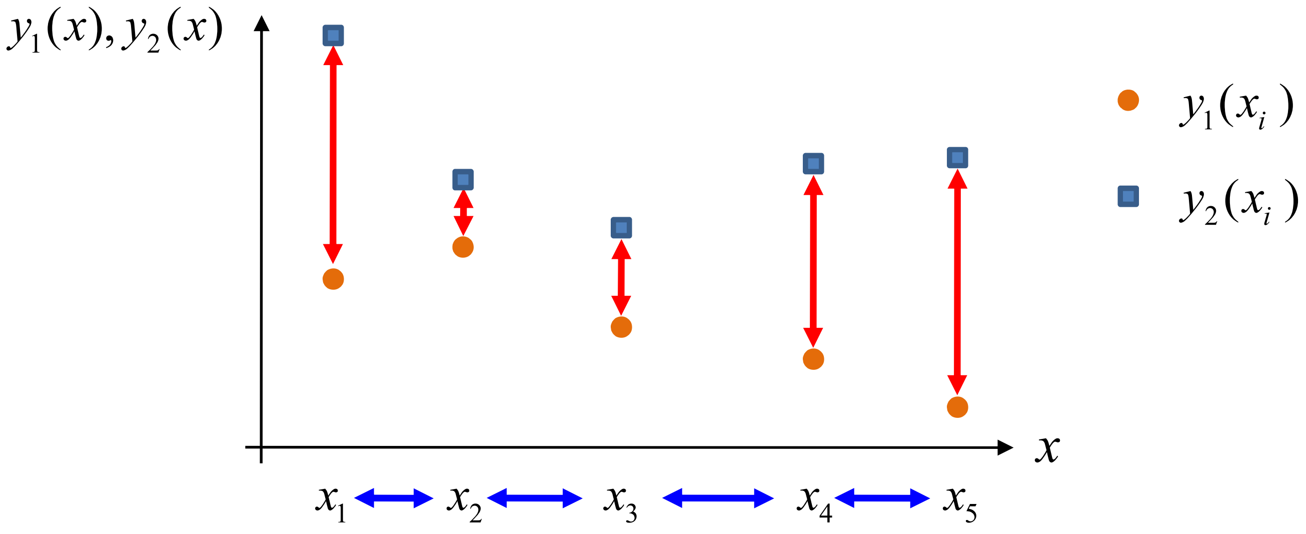


Two equally plausible solutions for θ and bias function

Multi-Response Calibration and Bias Correction

Multiple Response Gaussian Process (MR GP)

$$\mathrm{vec}(\mathbf{y}(\mathbf{x})) \sim GP(\mathrm{vec}(\mathbf{H}\boldsymbol{\beta}), \boldsymbol{\Sigma} \otimes \mathbf{R}(\mathbf{x},\mathbf{x}))$$



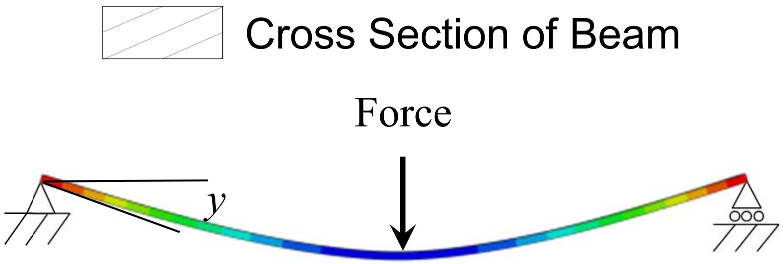
Define MR GP for computer simulations and bias function

$$\mathrm{vec}\left(\mathbf{y}^m(\mathbf{x},\boldsymbol{\theta})\right) \sim GP\left(\mathrm{vec}(\mathbf{H}_1(\mathbf{x},\boldsymbol{\theta})\boldsymbol{\beta}_1), \boldsymbol{\Sigma}_1 \otimes \mathbf{C}_1\{(\mathbf{x},\boldsymbol{\theta}),(\mathbf{x},\boldsymbol{\theta})\}\right)$$

$$\mathrm{vec}\left(\boldsymbol{\delta}(\mathbf{x})\right) \sim GP\left(\mathrm{vec}(\mathbf{H}_2(\mathbf{x})\boldsymbol{\beta}_2), \boldsymbol{\Sigma}_2 \otimes \mathbf{C}_2\{\mathbf{x},\mathbf{x}\}\right)$$

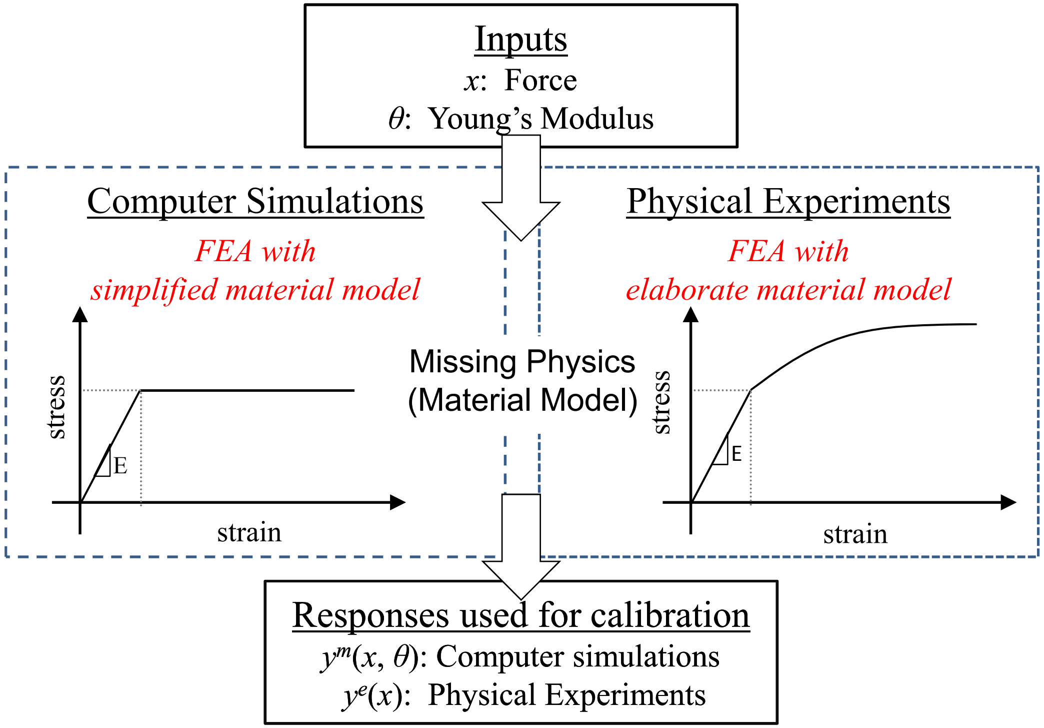
MR GP Based on Conti and O'Hagan (2010)

Simply Supported Beam Example



Objective: Find Young's modulus (θ) and missing physics of the physical experiments

Problem: Identifiability



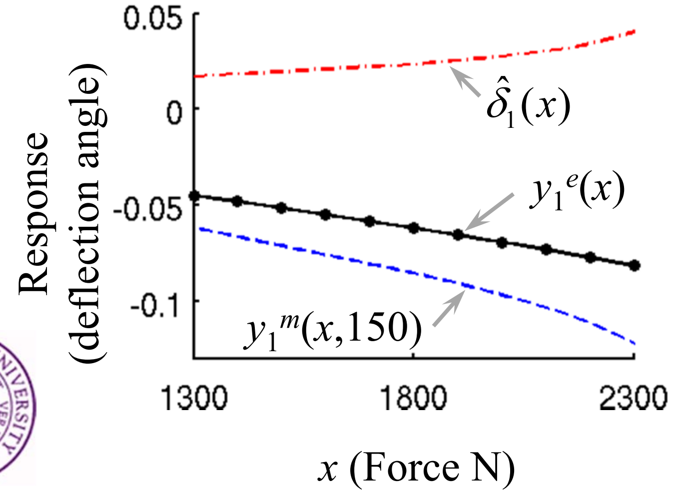
Inputs
x: Force
θ: Young's Modulus

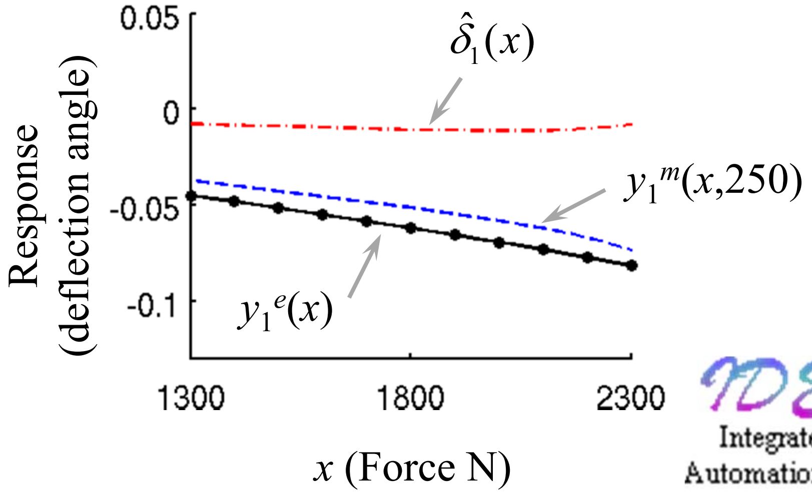
Computer Simulations
FEA with simplified material model

Physical Experiments
FEA with elaborate material model

Missing Physics (Material Model)

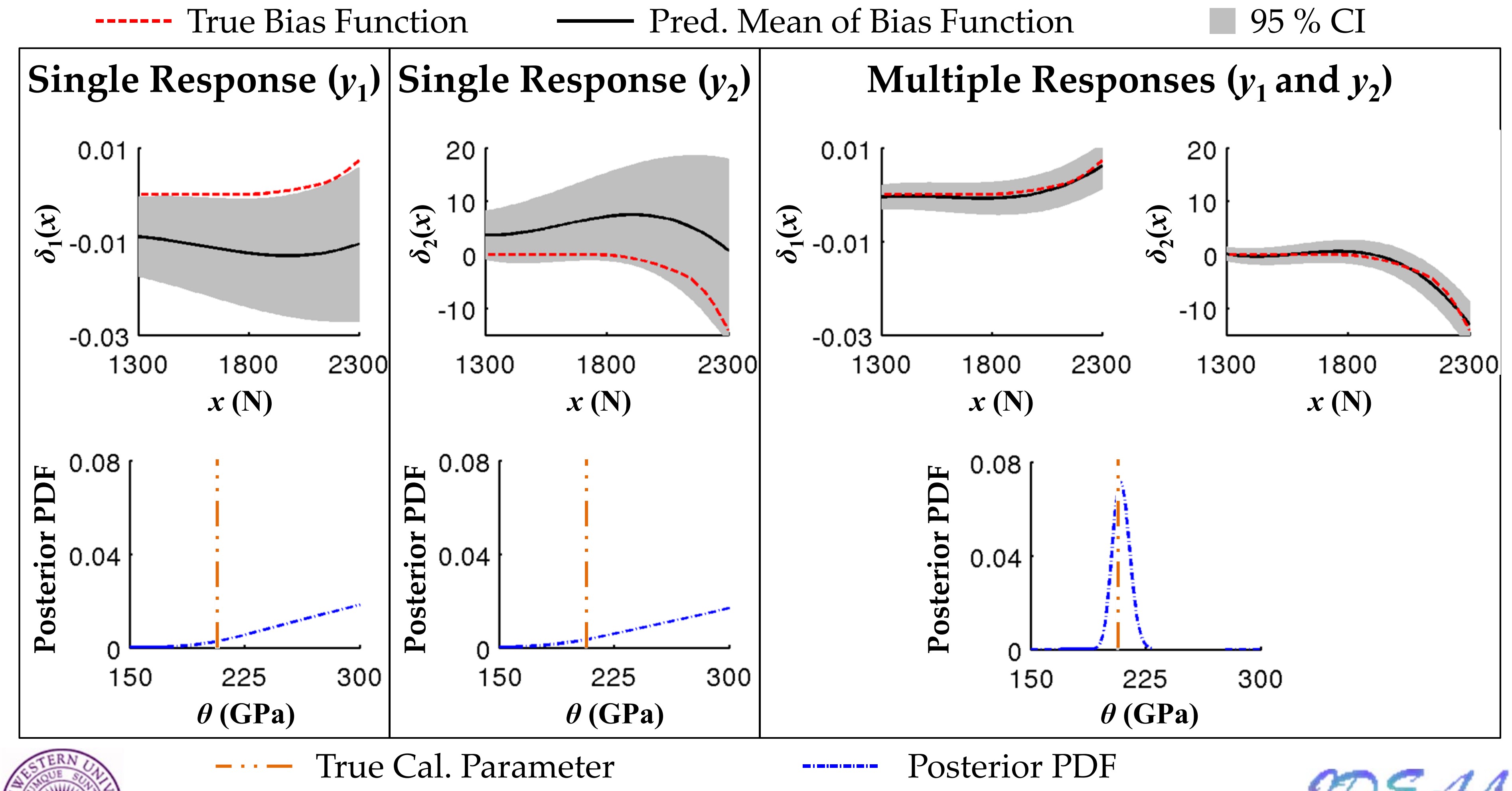
Responses used for calibration
$y^m(x, \theta)$: Computer simulations
$y^e(x)$: Physical Experiments





Simply Supported Beam Calibration

y_1: Angle of deflection at the end of the beam (radians)
y_2: Internal energy (Joules)



Note experimental prediction is not shown because it is accurate in all cases for the amount of experimental data used.

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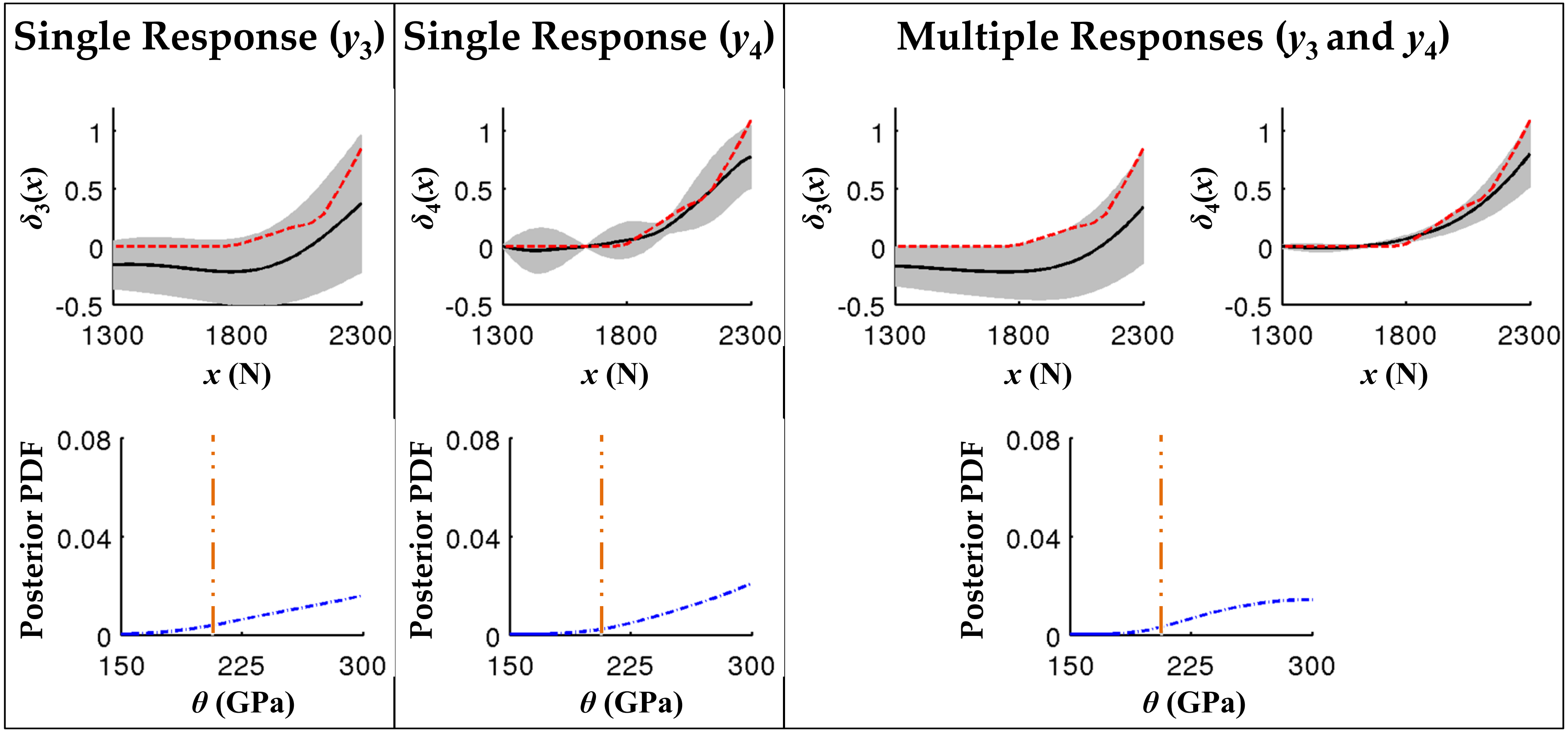
Calibration with Different Responses

y_3: Total strain at the midpoint of the beam (mm)

y_4: Plastic strain at the midpoint of the beam (mm)

------- True Bias Function —— Pred. Mean of Bias Function ▨ 95 % CI



–·– True Cal. Parameter -·-·-·- Posterior PDF

Benefits of Designed Experiments for Calibration

Computer Model:

$$y_1^m(x,\theta) = \sin(\theta x)$$

$$\theta \in [1,4] \quad x \in [0,\pi]$$

Experimental Function:

$$y_1^e(x) = \sin(\theta_{\text{true}} x) + 0.1e^x - 0.05x^2 + \varepsilon_1$$

$$\varepsilon_1 \sim N(0,\lambda \mathbf{I}) \qquad \theta_{\text{true}} = 3.1 \qquad \lambda = 0$$

Initial Data Set

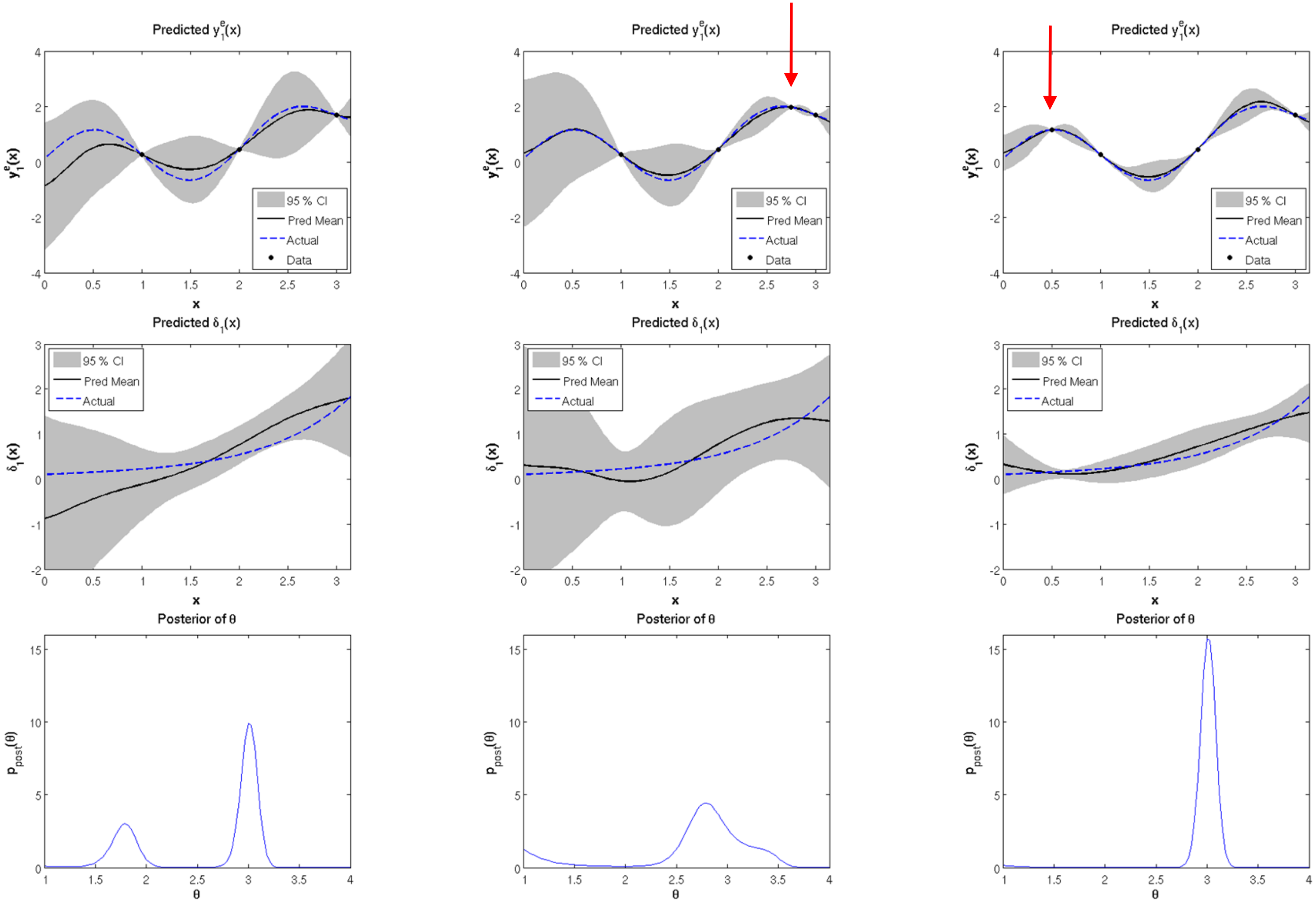
Add x = 2.75

Add x = 0.5

Experimental Prediction

Bias Function

Posterior θ



Closure – Research Challenges

- Stochastic multiscale analysis
  - How to identify critical macroscopic property/performance that are sensitive to microscopic variability – value of information, resource allocation in uncertainty management.
  - We don't know what is critical until we model it correctly
  - Capture the right correlation (space, time) to gain the usefulness of data

- Stochastic multiscale design
  - How to efficiently build constitutive relations for a range of design
  - Concurrent topology and material design

- Quantification of model uncertainty
  - Criterion for identifiability prior to experiments
  - Design of experiments for improved identifiability

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