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Reduction of Epistemic Uncertainty in Multifidelity Simulation-Based Multidisciplinary Design

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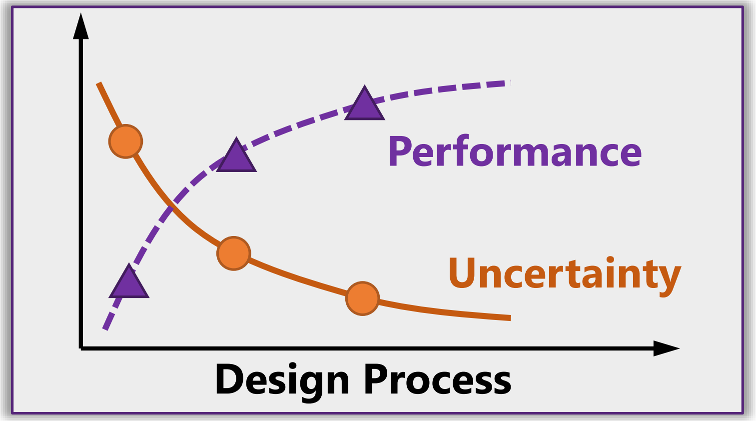
Simulation-Based Design under Uncertainty

SIMULATION-BASED DESIGN



- An information-seeking and learning **process**
- **Aleatory uncertainty**
  Due to natural/physical randomness; irreducible
- **Epistemic uncertainty**
  Due to lack of data and/or knowledge; reducible

SOURCES OF UNCERTAINTY THAT AFFECT MODEL PREDICTION

- Epistemic Uncertainty
  - **Model bias**
  - **Parameter uncertainty**
    Due to naturally fixed but unknown model parameters
  - **Interpolation uncertainty**
    Due to lack of data
  - **Numerical uncertainty**
    Due to numerical implementations of a model
- Aleatory Uncertainty
  - **Input variability**
    Operating conditions; manufacturing …
  - **Experimental variability**

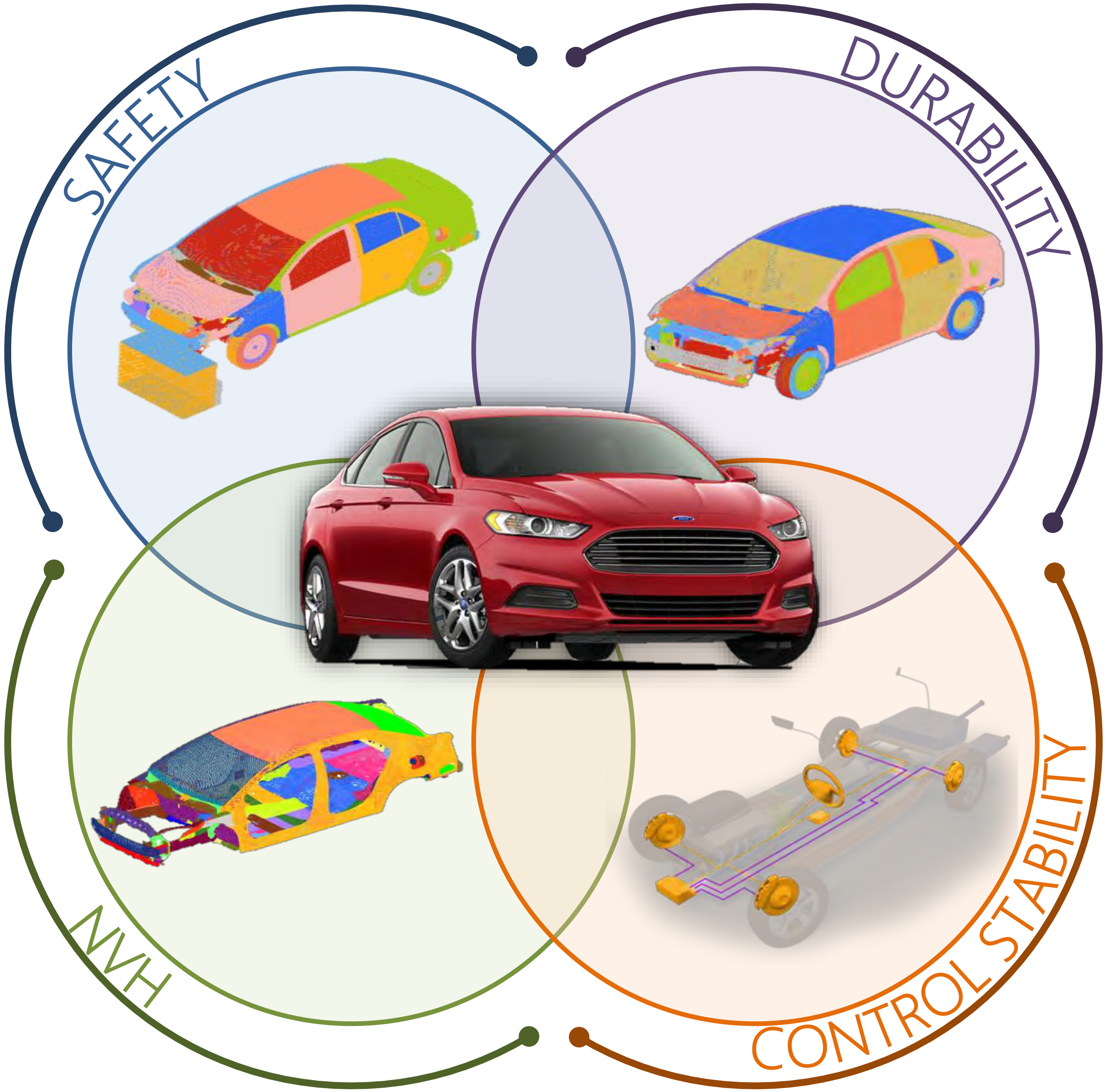
DESIGN UNDER UNCERTAINTY

To achieve a design that is insensitive to uncertainties

- Kennedy & O'Hagan, J. Roy. Stat. Soc. B, 63(3), 2001

Multidisciplinary Design Optimization (MDO)

- **Requires analyses in multiple disciplines**
  Involves multiple subsystems and/or components



- Fusion SE 2014 image from Ford Motor Co
- FEA model images provided by Dr. Lei Shi, Shanghai Jiao Tong University
- Control system image from StabiliTrak

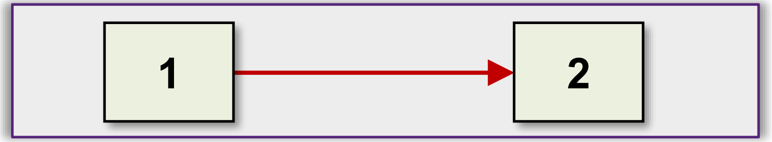
Multidisciplinary Design Optimization (MDO)

- **Requires analyses in multiple disciplines**
  Involves multiple subsystems and/or components

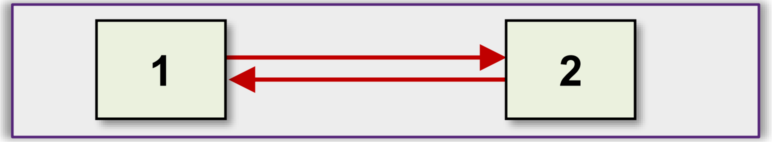
- **CHALLENGE #1**
  Coupling in analysis and UQ

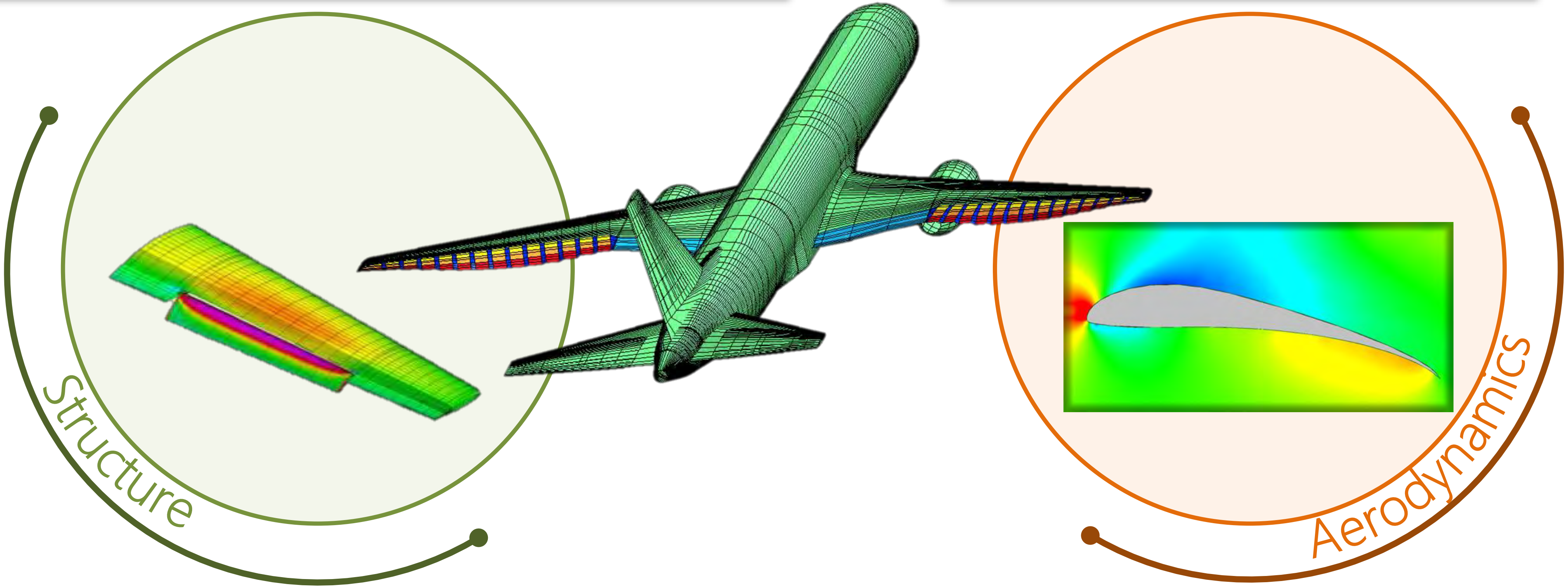
- **CHALLENGE #2**
  Dynamic decision making in resource allocation

- **Interdisciplinary couplings**
  - Feed-forward Coupling



  - Feedback Coupling



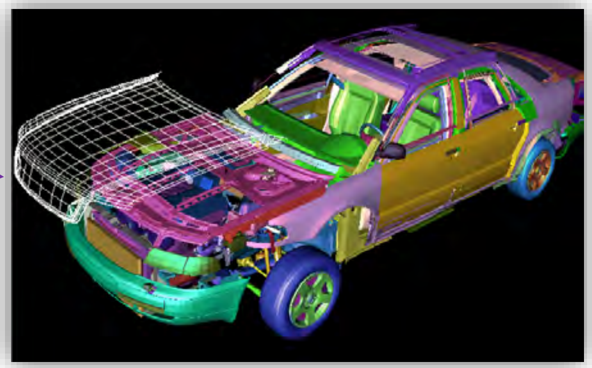


Multiple Models with Different Levels of Fidelity

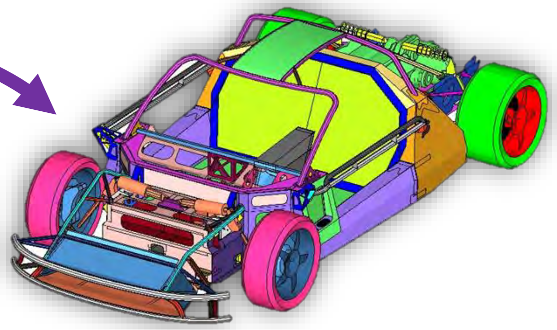
CHALLENGE #3
Heterogenous information from different sources (multifidelity simulations and experiments)

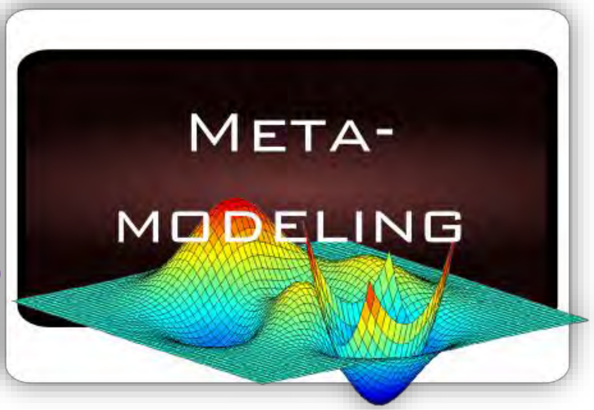
"High-fidelity" experiment test

"High-fidelity" physics-based CAE model



"Intermediate-fidelity" physics-based CAE model





"Intermediate-fidelity" surrogate model

"Low-fidelity" simplified handbook equations

$$2m_c v_1^2 = \frac{1}{2}(2m_c + m_t)v_2^2 + E_{\text{structural}}$$

$$2m_c v_1^2 = \frac{1}{2}(2m_c + m_t)\left(\frac{2m_c v_1}{2m_c + m_t}\right)^2 + E_{\text{structural}}$$

$$E_{\text{structural}} = 2m_c v_1^2 - \frac{2m_c^2 v_1^2}{2m_c + m_t}$$

$$E_{\text{structural}} = 2m_c v_1^2\left(1 - \frac{m_c}{2m_c + m_t}\right)$$

Research Topics

Model-Fusion for Combining Heterogeneous Information

- Both hierarchical and nonhierarchical rankings of fidelity

Managing Couplings and Information Complexity

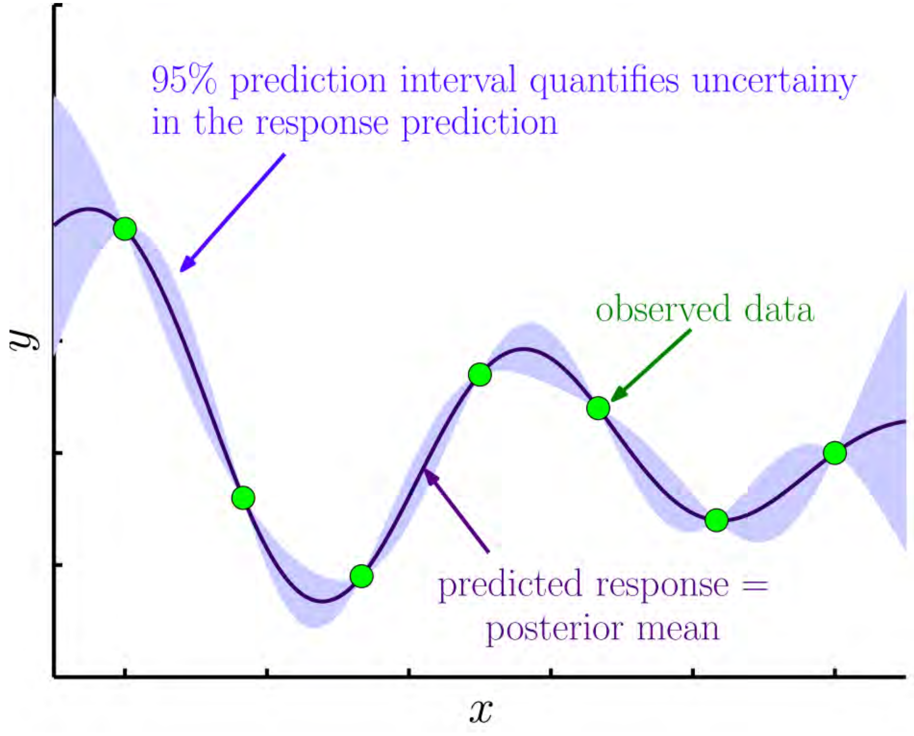
- Multidisciplinary statistical sensitivity analysis (MSSA)
- Multidisciplinary uncertainty analysis (MUA)

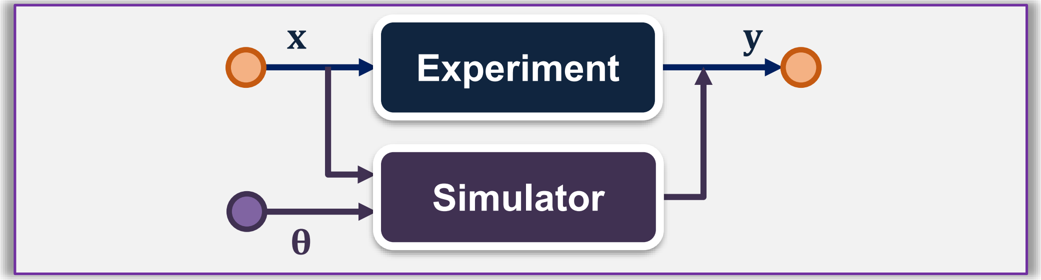
Resource Allocation for Reducing Epistemic Uncertainty in MDO

- How to design paths of information seeking actions
- Decision making meta-optimization problem

Spatial Random Process Based Model Uncertainty Quantification

- Any pair of random variables, $Y(\mathbf{x})$ and $Y(\mathbf{x}')$, is spatially correlated
- Example: *Gaussian Process*
  - $Y(\mathbf{x}) \sim GP\left(m(\mathbf{x}), V(\mathbf{x},\mathbf{x}')\right)$
  - $m(\mathbf{x}) = \mathbf{h}(\mathbf{x})^T \boldsymbol{\beta}, \quad V(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left\{-\sum_k \omega_k \left(x_k - x_k'\right)^2\right\}$

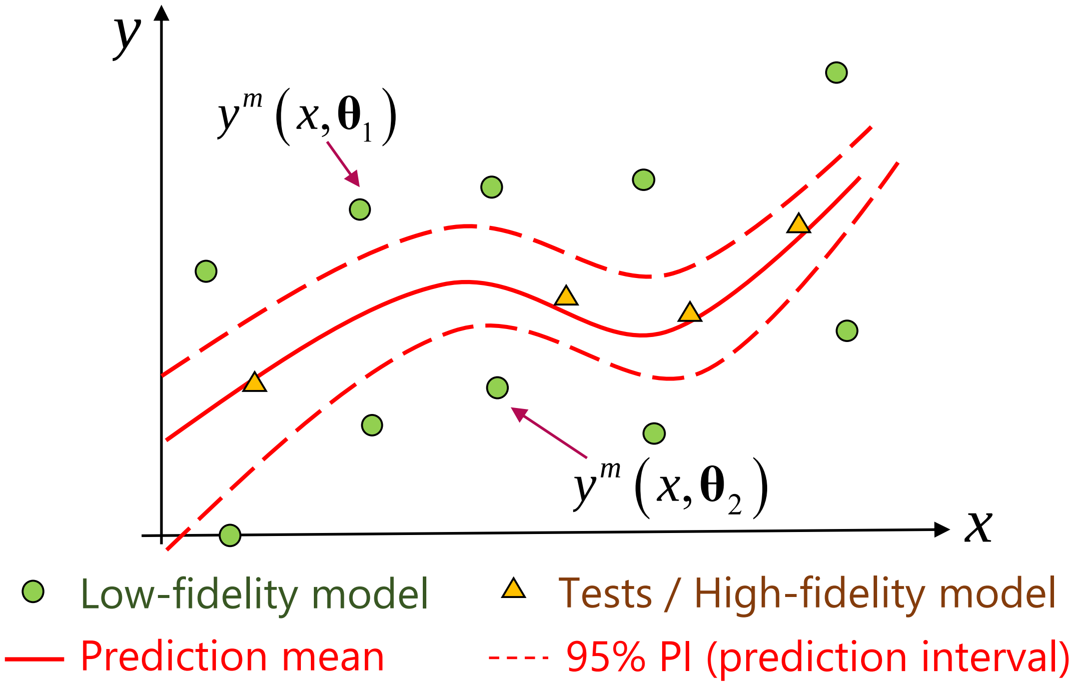




Experiment Model Experimental Error

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

Inputs Bias Function



TOPIC 1
Model Fusion for Combining Heterogeneous Information

Chen, S., Jiang, Z., Yang, S., Apley, D., and Chen, W., "**Nonhierarchical Multi-model Fusion Using Spatial Random Processes**", *International Journal for Numerical Methods in Engineering*, 10.1002/nme.5123, 2015.

Existing Multi-Model Fusion Techniques

Ng, L. W. –T. & M. Eldred, 2012; A. Narayan, D. Xiu, et al., 2014

- Apply low-fidelity information to construct the approximation space for a high-fidelity surrogate and then compute a high-fidelity reconstruction for model prediction.
- Using stochastic allocation with generalized polynomial chaos approach.

Kennedy & O'Hagan, 2000; Qian, P. Z. & C. J. Wu, 2008; Goh, Bingham, et al. 2013

- Assume the higher-fidelity model to be approximated by its next lower-fidelity model with a discrepancy, and then construct a multi-model sequential updating framework.
- Apply spatial random process (SRP) to surrogate the responses from different models.

Common Assumption

- The fidelity levels of the simulation models can be clearly identified and then preliminarily ordered for a hierarchical model updating.

Lack of Clear Ranking of Model Fidelity in Real Applications

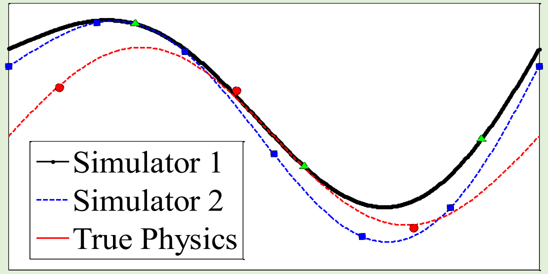
Competitive Simulation Models

- Financial predictive models developed by different commercial companies.

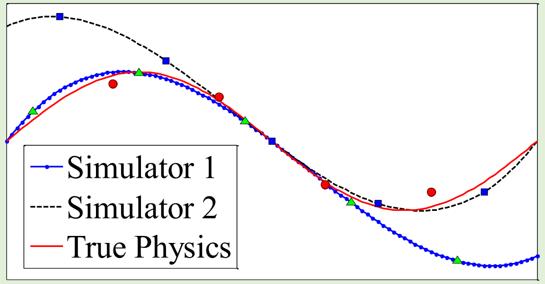
- Climate models arising from different research groups.

Complicated Fidelity Models

- The levels of mode fidelity are such closely similar that cannot be ranked.



- The levels of mode fidelity change over the whole design space.



Goal of this work: Develop model fusion techniques with uncertainty quantification for combining information from multiple models without a clear ranking of fidelity.

Three Spatial Random Process (SRP) based Approaches

Approach 1: Weighted Sum

$$y^t(\mathbf{x}) = y^e(\mathbf{x}) - \varepsilon = \sum_i \rho^{\{i\}} y^{m\{i\}}(\mathbf{x}) + \delta(\mathbf{x})$$

Assumption: Independency between simulations and the discrepancy function

$$\text{Cov}\left(y^{m\{i\}}(\mathbf{x}), \delta(\mathbf{x})\right) = 0, \quad \forall i$$

$y^t(\mathbf{x})$:	True response
$y^e(\mathbf{x})$:	Experimental response
$y^{m\{i\}}(\mathbf{x})$:	i^{th} simulation model
$\delta(\mathbf{x})$:	Discrepancy function
ε:	Experimental error

Approach 2: Each Model Individually Corrected

$$y^t(\mathbf{x}) = y^e(\mathbf{x}) - \varepsilon = y^{m\{i\}}(\mathbf{x}) + \delta^{\{i\}}(\mathbf{x})$$

Assumption: Independency between the discrepancy function and the true response

$$\text{Cov}\left(y^t(\mathbf{x}), \delta^{\{i\}}(\mathbf{x}')\right) = 0, \quad \forall i$$

Approach 3: Fully-Correlated Multi-Response

$$y^t(\mathbf{x}) = y^e(\mathbf{x}) - \varepsilon = y^{m\{i\}}(\mathbf{x}) + \delta^{\{i\}}(\mathbf{x})$$

Assumption: Simulation models and the discrepancy functions follow the same spatial correlation function

Multi-model Fusion Procedure (Illustration of Approach 1)

Covariance Calculation

$$\mathrm{Cov}\left(y^{m\{i\}}(\mathbf{x}), y^{m\{j\}}(\mathbf{x}')\right) = e_i^T \mathbf{\Sigma}^m e_j R^m(\mathbf{x}, \mathbf{x}')$$

$$\mathrm{Cov}\left(y^{e}(\mathbf{x}), y^{m\{i\}}(\mathbf{x}')\right) = \boldsymbol{\rho}^T \mathbf{\Sigma}^m e_i R^m(\mathbf{x}, \mathbf{x}')$$

Data Integration via MVN (**multivariate normal dist)**

MRGP for Models

Covariance Calculation

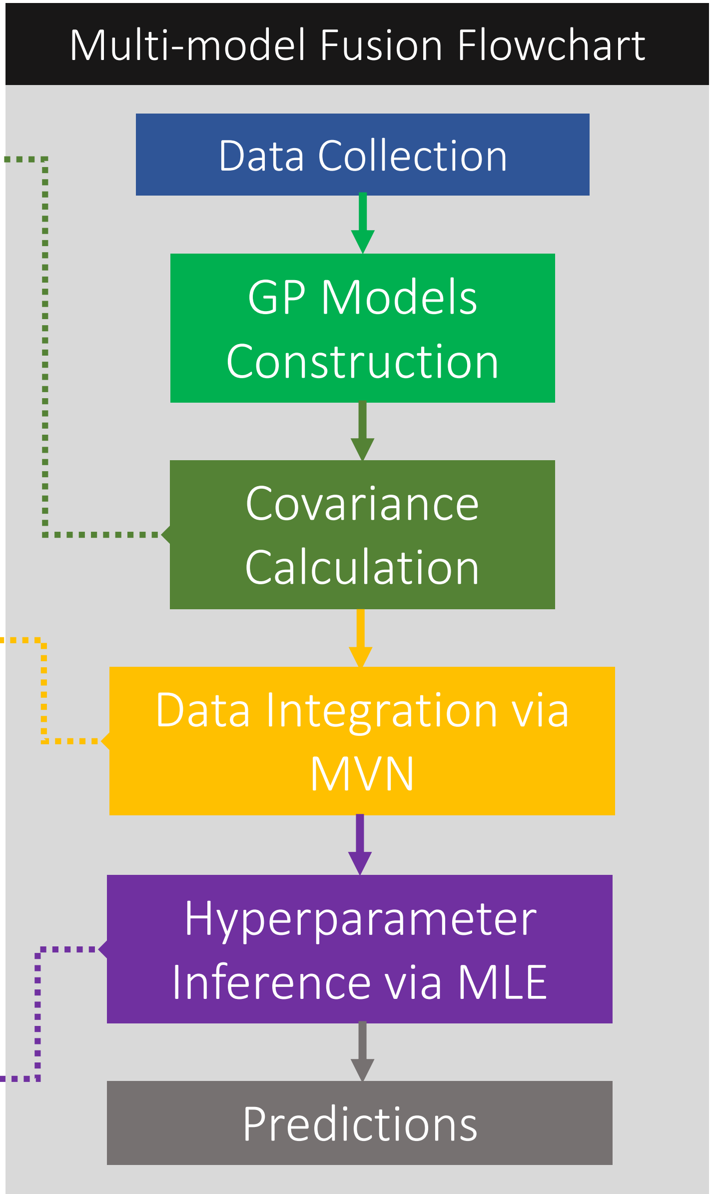
$$\begin{bmatrix} \mathbf{d}^M \\ \mathbf{d}^e \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{H}^M \\ \mathbf{H}^e \end{bmatrix} \boldsymbol{\beta}, \begin{bmatrix} \mathbf{V}_m(\mathbf{X}^M, \mathbf{X}^M) & \mathbf{V}_{me}(\mathbf{X}^M, \mathbf{X}^e) \\ \mathbf{V}_{em}(\mathbf{X}^e, \mathbf{X}^M) & \mathbf{V}_e(\mathbf{X}^e, \mathbf{X}^e) \end{bmatrix} \right)$$

Data Collection

GP for Experiment Test

Hyperparameter Inference via MLE

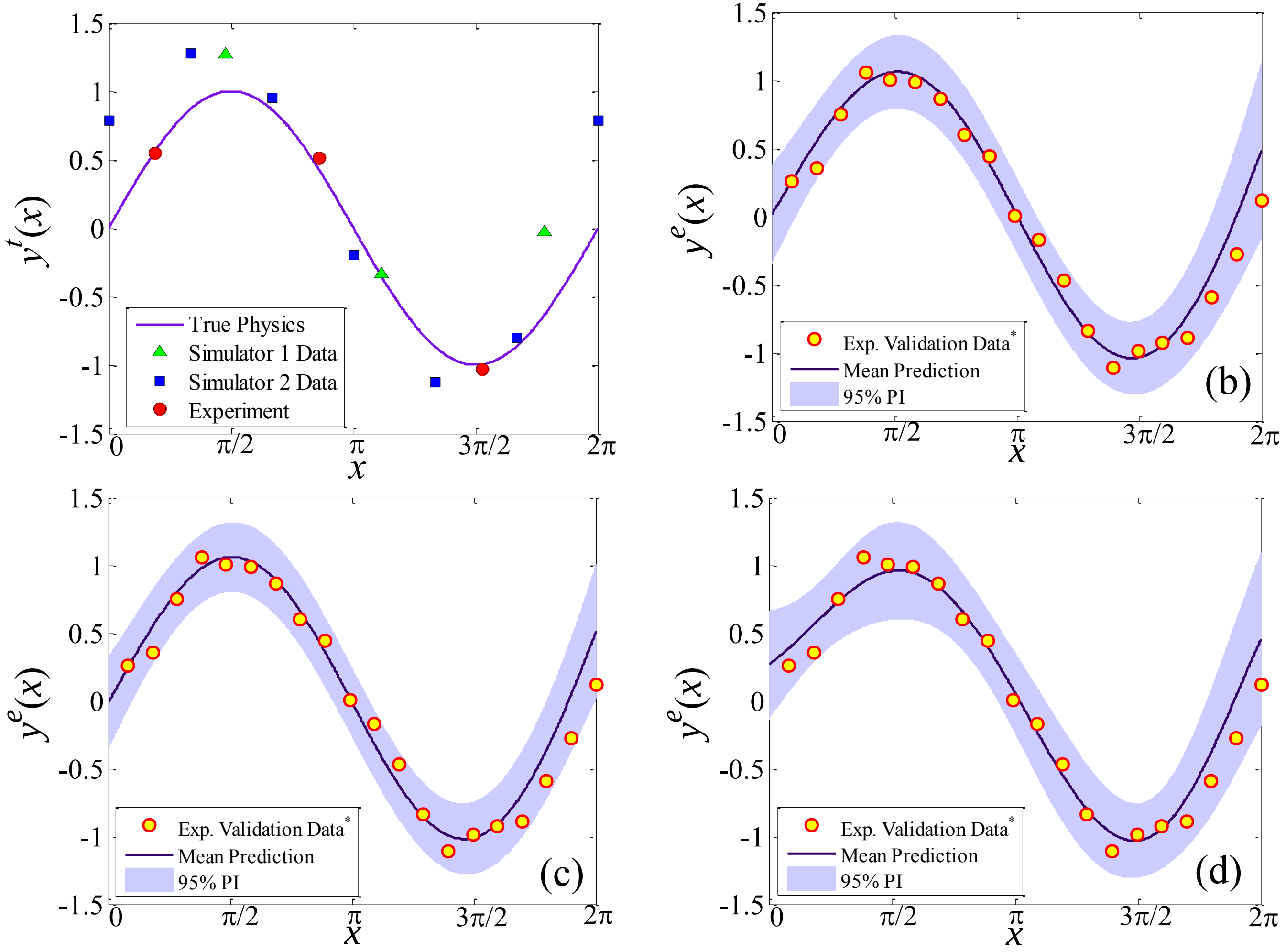
$$L(\boldsymbol{\phi}|\mathbf{d}) \propto |\mathbf{V_d}|^{-1/2} \exp\left\{-(\mathbf{d}-\mathbf{H}\boldsymbol{\beta})^T \mathbf{V_d}^{-1} (\mathbf{d}-\mathbf{H}\boldsymbol{\beta})/2\right\}$$



Example 1: Similar Model Fidelity

The fidelity levels of simulator 1 and 2 are similar.

3 samples from Simulator 1, 7 samples from Simulator 2, 3 observations from experiment



	Approach 1	Approach 2	Approach 3
RMSE	0.1530	0.1636	0.1573
u-pooling	0.0805	0.0786	0.0924

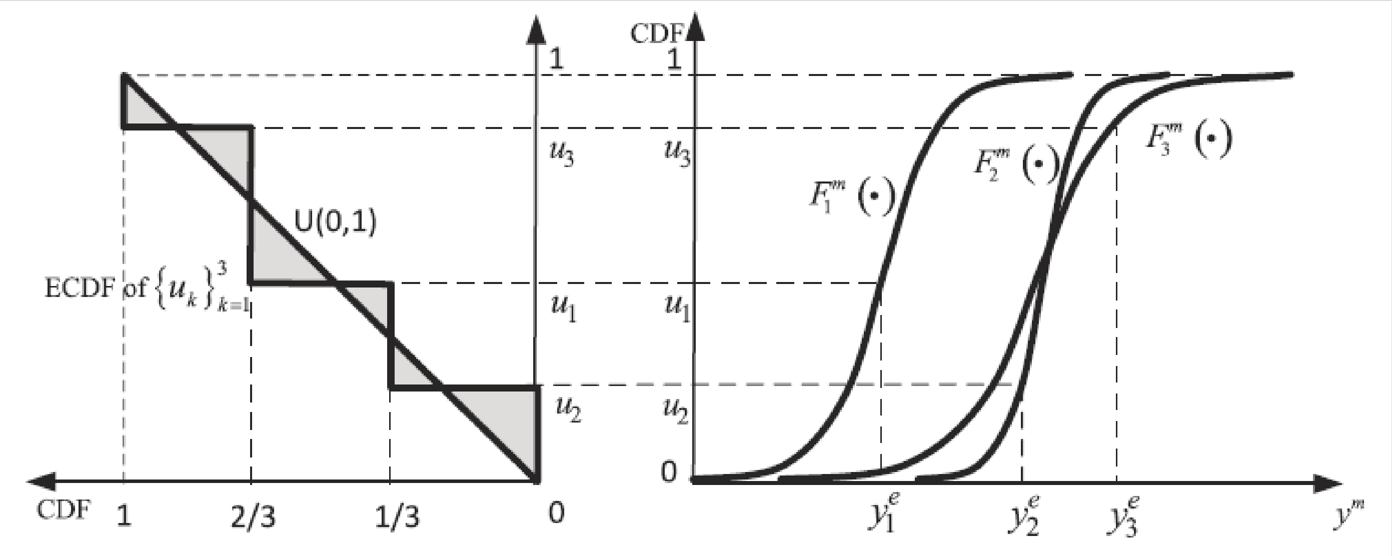
Validation Metrics

Root-mean-square error (RMSE)

- $$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}}$$

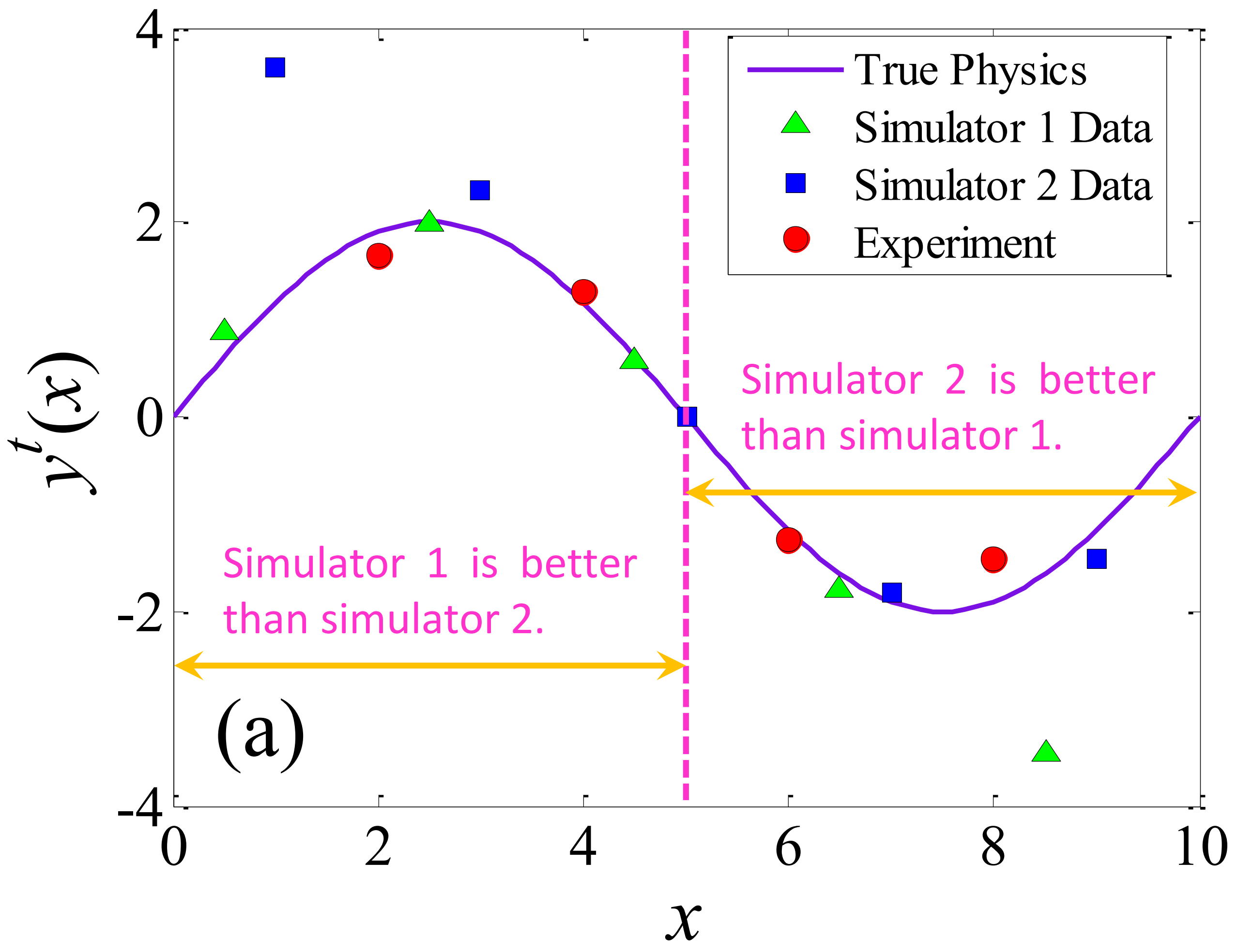
U-pooling

- $$u_i = F_{\mathbf{x}_i}^{m}(y^e(\mathbf{x}_i))$$



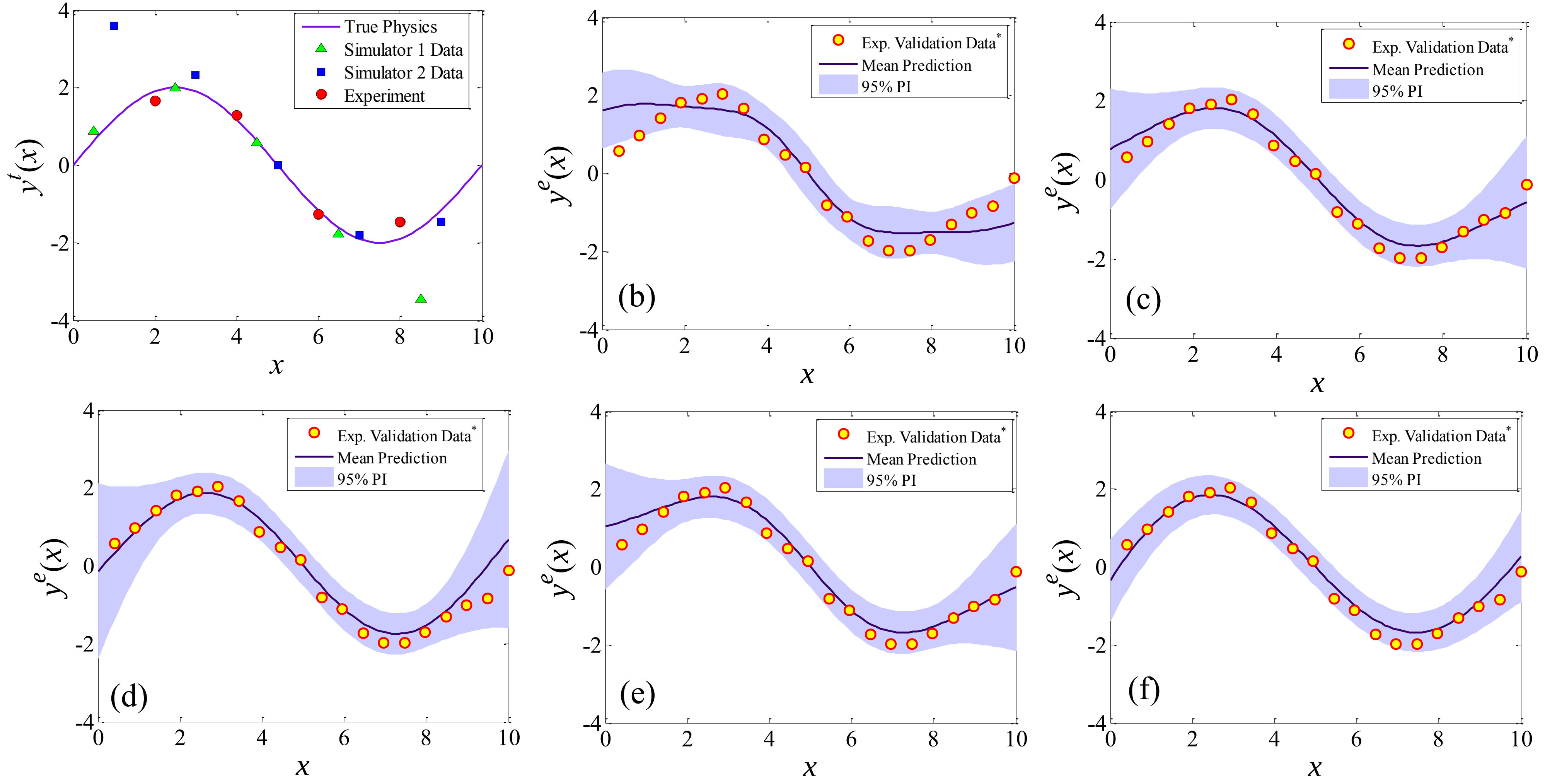
Ferson, S., W.L. Oberkampf, and L. Ginzburg, Model validation and predictive capability for the thermal challenge problem. Computer Methods in Applied Mechanics and Engineering, 2008. 197(29): p. 2408-2430.

Example 2: Range-Dependent Model Fidelity



- The fidelity levels of both simulator 1 and 2 change over the design space
- 5 samples from each simulator, 4 observations from experiment

Example 2: Range-Dependent Model Fidelity



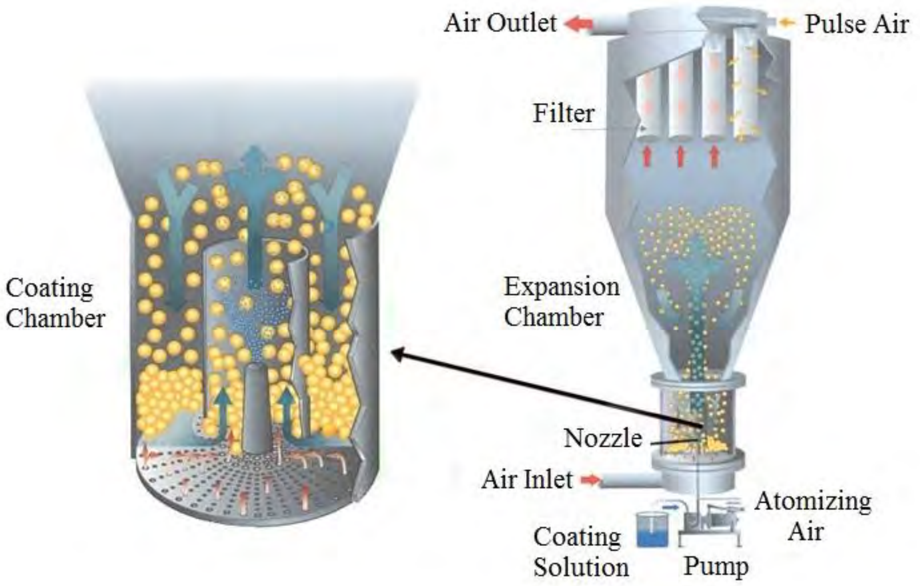
	Approach 1 with 0.01<ω^δ<50	Approach 2	Approach 3	Approach 1 with 0.01<ω^δ<10	Approach 1 with 0.01<ω^δ<5
RMSE	0.5692	0.3329	0.3542	0.3598	0.2996
u-pooling	0.0797	0.0952	0.0966	0.1035	0.0823

Example 3: Fluidized-Bed Processes

- Used in the food industry to tune the effect of functional ingredients and additives.
- Important thermo-dynamic response: steady-state outlet air temperature.
- First studied by Dewettinck et al., 1999; employed by Reese et al., 2004; Qian et al., 2008.

- V_f : Fluid velocity of the fluidization air
- T_a : Temperature of the air from the pump
- R_f : Flow rate of the coating solution
- P_a : Pressure of atomization air
- T_r : Room temperature
- H_r : Room humidity

Input Variables



$Y^m{}_1$: Least accurate model because of its neglecting both heat losses and inlet airflow

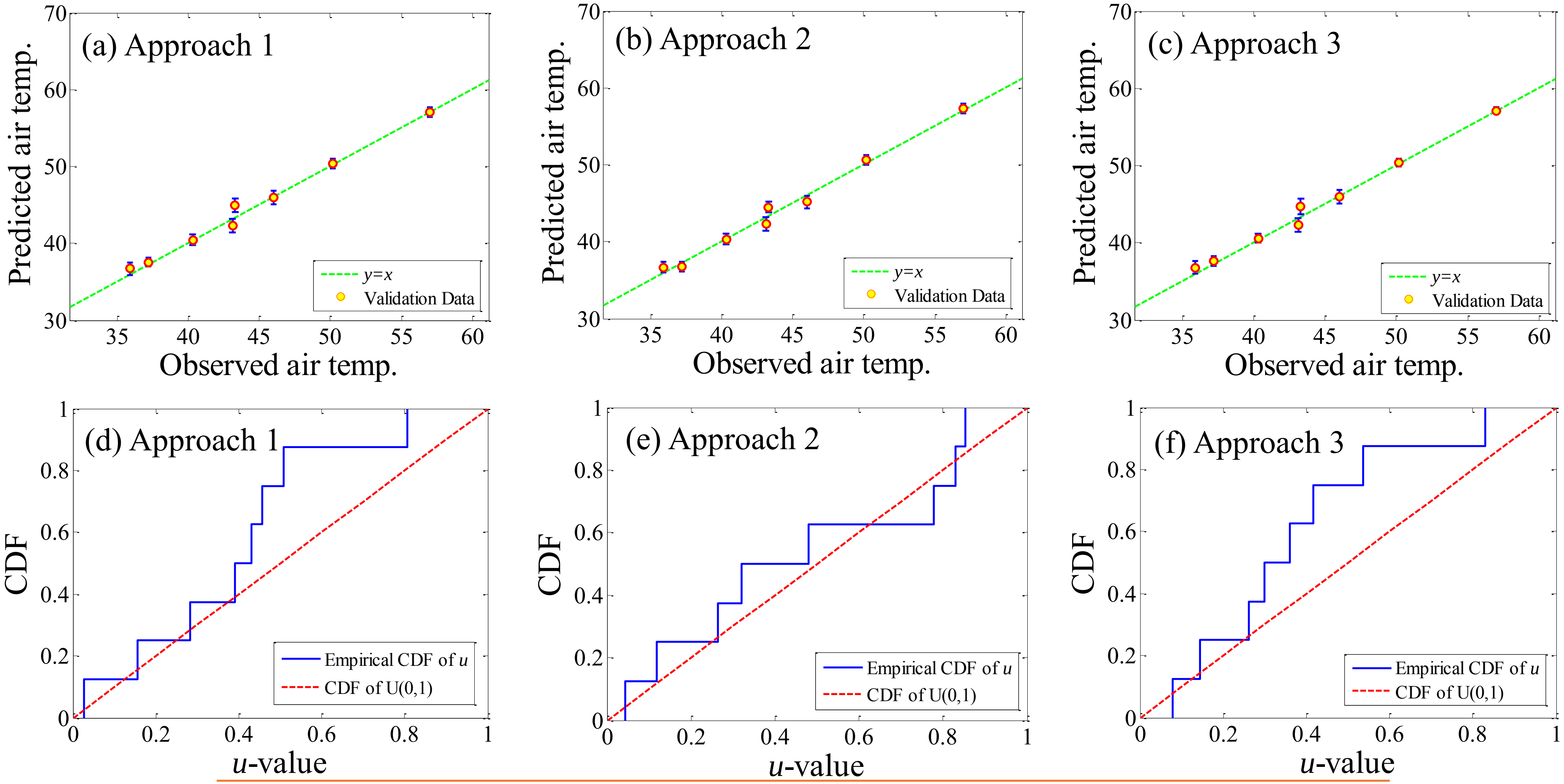
$Y^m{}_2$: Intermediately accurate model taking those heat losses in the process

Y^e : Most accurate experiment test

Hierarchical Model Resources

Example 3: Fluidized-Bed Processes (Results)

Model Fusion



	Approach 1	Approach 2	Approach 3	Qian and Wu's approach
RMSE	0.7402	0.6884	0.6925	/
u-pooling	0.1210	0.0706	0.1410	/
SRMSE	0.0177	0.0163	0.0169	0.020

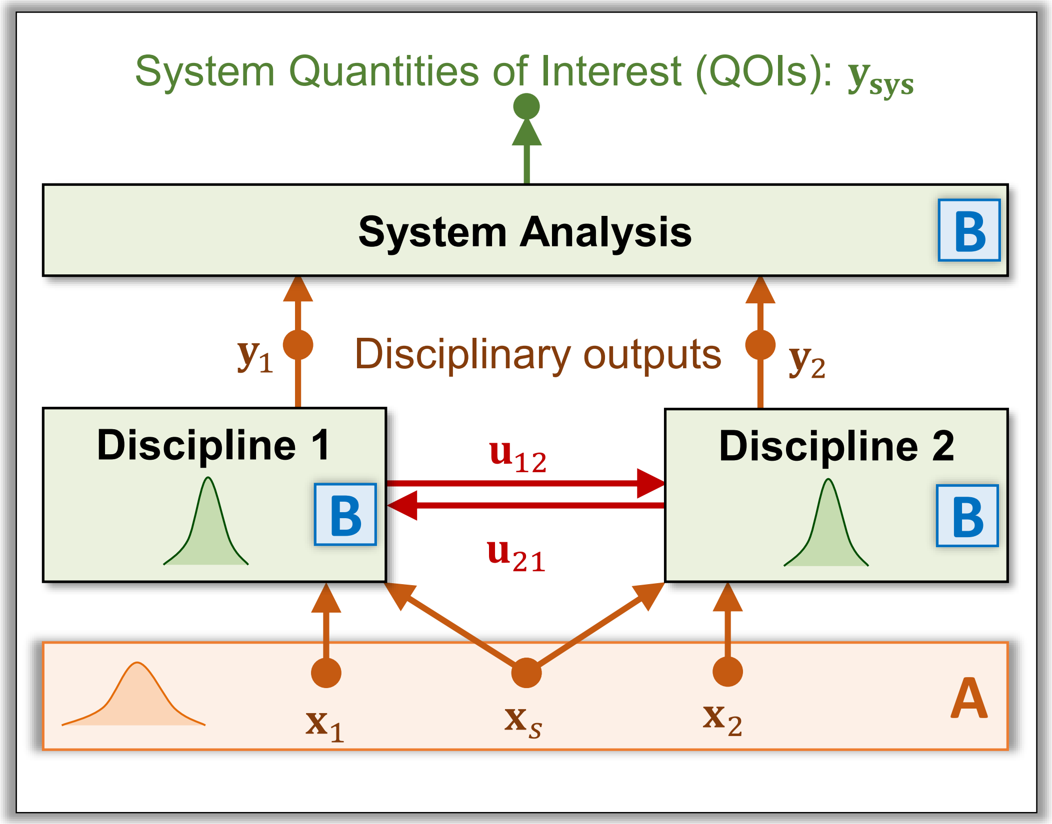
Topic 2

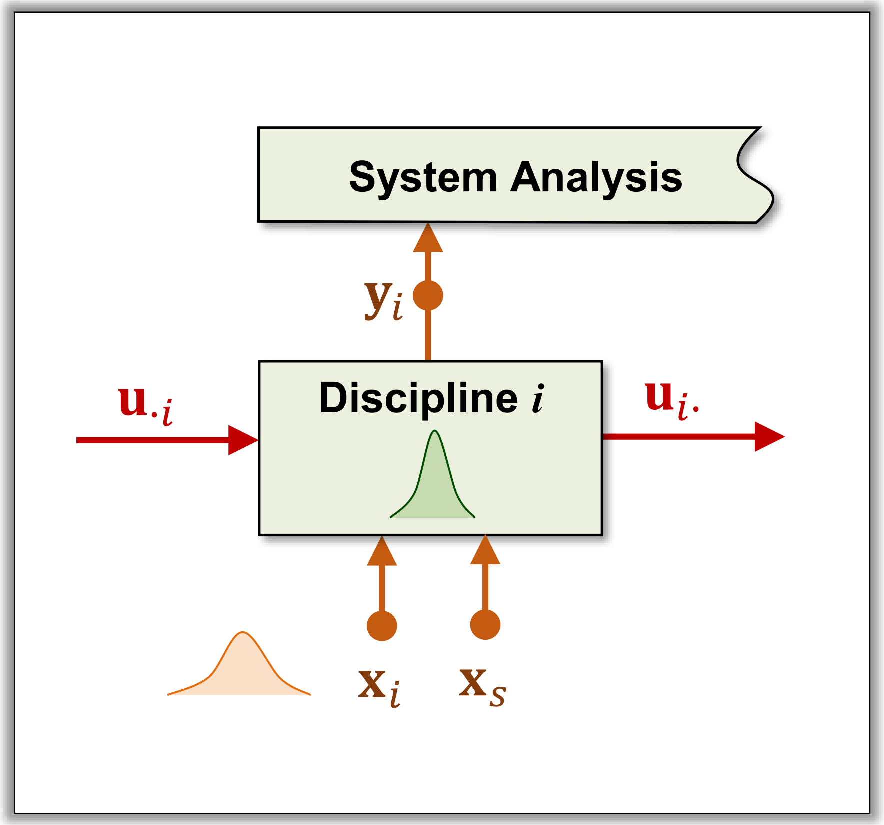
Managing Coupling and Information Complexity in MDO

Jiang, Z., German, B., and Chen, W., **"Multidisciplinary Statistical Sensitivity Analysis Considering both Aleatory and Epistemic Uncertainties"**, *AIAA Journal*, doi: 10.2514/1.J054464, 2015.

Jiang, Z., Li., W., Apley, D., and Chen, W., "**A Spatial-Random-Process Based Multidisciplinary System Uncertainty Propagation Approach with Model Uncertainty**", *Journal of Mechanical Design*, 2015.

A Multidisciplinary System



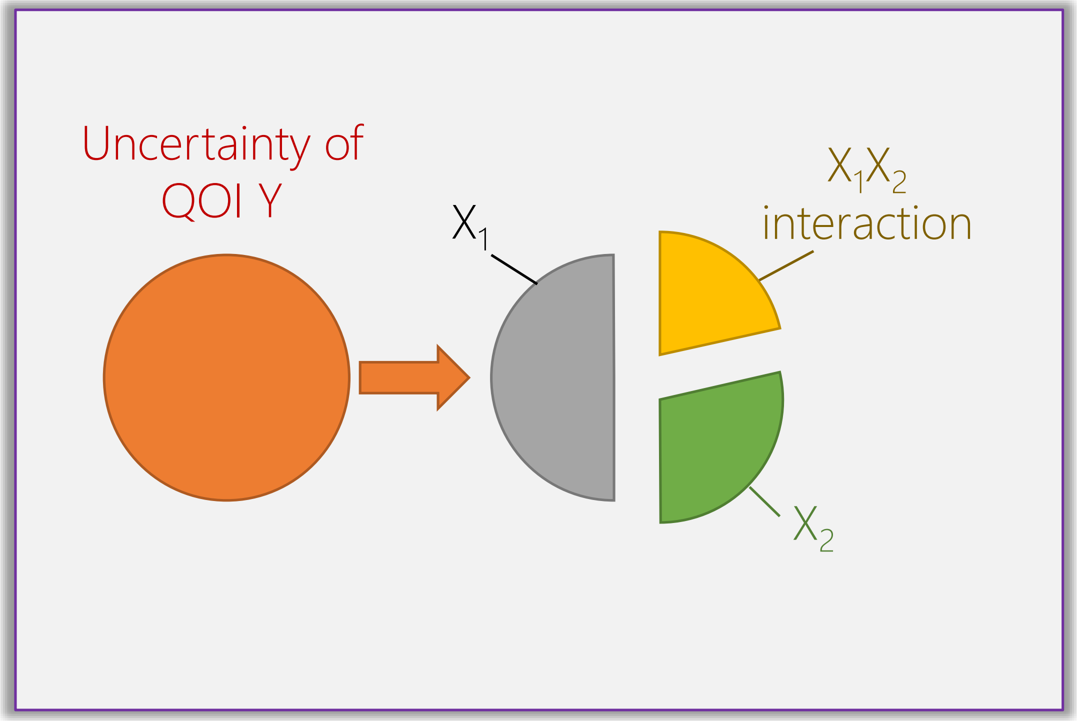


A Aleatory Uncertainty B Epistemic Model Uncertainty

Z is used to stand both disciplinary output y_i and linking variables u_i.

Multidisciplinary Statistical Sensitivity Analysis (MSSA)

VARIANCE-BASED SENSITIVITY INDICES



Impact of Aleatory Uncertainty

- $$\mathrm{MSI}(X_i) = \frac{\mathrm{Var}_{X_i}\left(\mathrm{E}_{\mathbf{Z},\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right)}{\mathrm{Var}(Y)}$$
- $$\mathrm{TSI}(X_i) = 1 - \frac{\mathrm{Var}_{\mathbf{Z},\mathbf{X}_{\sim i}}\left(\mathrm{E}_{X_i}\left(Y \mid \mathbf{Z}, \mathbf{X}_{\sim i}\right)\right)}{\mathrm{Var}(Y)}$$

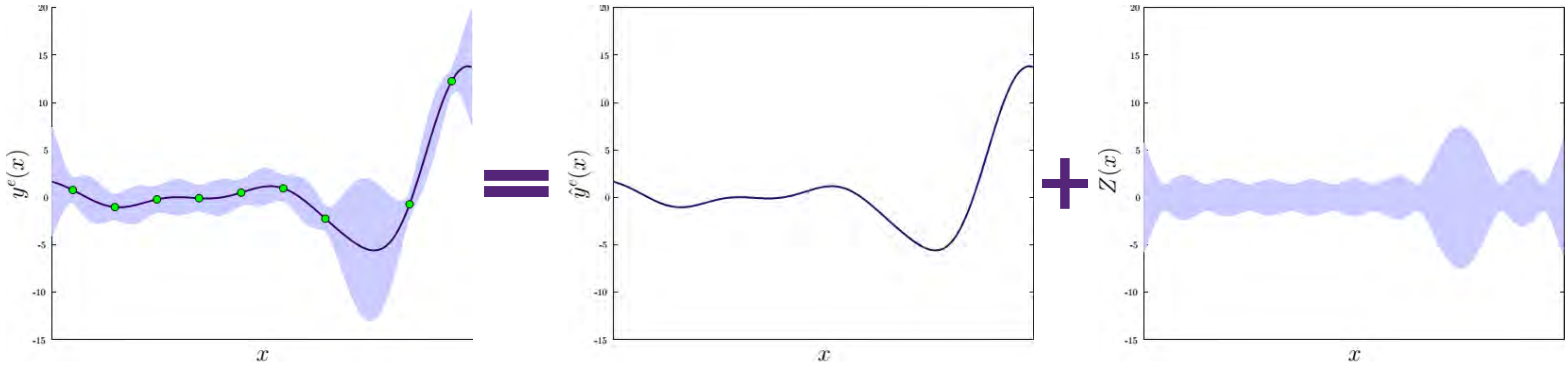
Impact of Epistemic Model Uncertainty

- $$\mathrm{MSI}(Z_k) = \frac{\mathrm{Var}_{Z_k}\left(\mathrm{E}_{\mathbf{Z}_{\sim k},\mathbf{X}}\left(Y \mid Z_k\right)\right)}{\mathrm{Var}(Y)}$$
- $$\mathrm{TSI}(Z_k) = 1 - \frac{\mathrm{Var}_{\mathbf{Z}_{\sim k},\mathbf{X}}\left(\mathrm{E}_{Z_k}\left(Y \mid \mathbf{Z}_{\sim k}, \mathbf{X}\right)\right)}{\mathrm{Var}(Y)}$$

Challenges in SSA of model uncertainty

- Traditional Sobol's method considers stochastic inputs as scalar variables
- Z are stochastic functional responses over model inputs.
- Nested situation where model uncertainty (Z) is a function of aleatory uncertainty (X)

Separating Model Uncertainty in Disciplinary SRP



Updated model (prediction mean)

Experiment ← $y^e(\mathbf{x}) = \hat{y}^e(\mathbf{x}) + Z(\mathbf{x})$ → Quantified uncertainty (zero-mean random process)

DISCIPLINARY UNCERTAINTY QUANTIFICATION

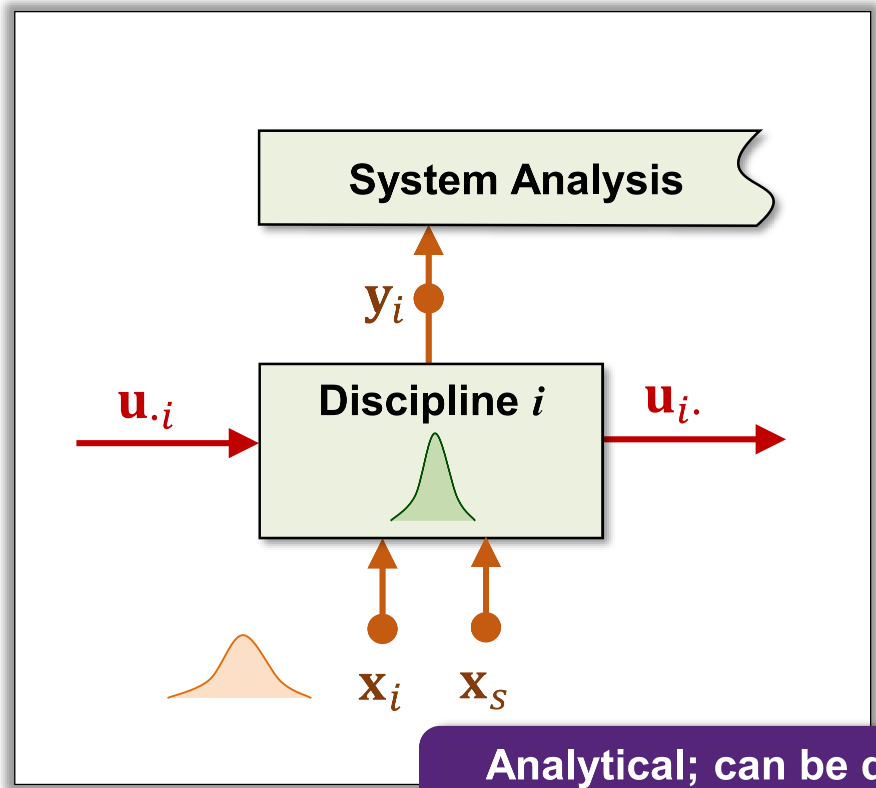
$$\mathbf{u}_{i\cdot}^{e}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e}) = \hat{\mathbf{u}}_{i\cdot}^{e}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e}) + \mathbf{Z}_{ui\cdot}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e})$$

$$\mathbf{y}_{i}^{e}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e}) = \hat{\mathbf{y}}_{i}^{e}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e}) + \mathbf{Z}_{yi}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^{e})$$

TO AVOID NESTED SIMULATIONS IN SSA

- **Analytically derived multidisciplinary uncertainty propagation (MUA)**

SRP-Based Multidisciplinary Uncertainty Analysis (MUA) Method



DISCIPLINARY UNCERTAINTY QUANTIFICATION

$$\mathbf{u}_{i\cdot}^e(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)=\hat{\mathbf{u}}_{i\cdot}^e(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)+\mathbf{Z}_{ui\cdot}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)$$

$$\mathbf{y}_{i}^e(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)=\hat{\mathbf{y}}_{i}^e(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)+\mathbf{Z}_{yi}(\mathbf{x}_i,\mathbf{x}_s,\mathbf{u}_{\cdot i}^e)$$

Evaluation of means of linking variables and disciplinary outputs

↓

Evaluation of (co)variance of linking variables u

↓

Evaluation of (co)variance of disciplinary outputs y

↓

Evaluation of mean and (co)variance of system QOIs

Analytical; can be derived from the structure of SRP

A MATRIX FORM

$$\mathbf{A}(\mathbf{u}^e-\boldsymbol{\mu}_u)\approx\mathbf{B}(\mathbf{X}-\boldsymbol{\mu}_X)+\mathbf{Z}_u,\quad \mathbf{y}^e-\boldsymbol{\mu}_y\approx\left(\mathbf{E}\mathbf{A}^{-1}\mathbf{B}+\mathbf{F}\right)(\mathbf{X}-\boldsymbol{\mu}_X)+\mathbf{E}\mathbf{A}^{-1}\mathbf{Z}_u+\mathbf{Z}_y$$

$$\boldsymbol{\mu}_{ui\cdot}\approx\hat{\mathbf{u}}_{i\cdot}^e(\boldsymbol{\mu}_{xi},\boldsymbol{\mu}_{xs},\boldsymbol{\mu}_{u\cdot i}),\qquad \boldsymbol{\mu}_{yi}\approx\hat{\mathbf{y}}_{i}^e(\boldsymbol{\mu}_{xi},\boldsymbol{\mu}_{xs},\boldsymbol{\mu}_{u\cdot i}),$$

$$\boldsymbol{\Sigma}_u\approx(\mathbf{A}^{-1}\mathbf{B})\boldsymbol{\Sigma}_X(\mathbf{A}^{-1}\mathbf{B})^T+(\mathbf{A}^{-1})\boldsymbol{\Sigma}_{Zu}(\mathbf{A}^{-1})^T.\qquad \boldsymbol{\Sigma}_y\approx\left(\mathbf{E}\mathbf{A}^{-1}\mathbf{B}+\mathbf{F}\right)\boldsymbol{\Sigma}_X\left(\mathbf{E}\mathbf{A}^{-1}\mathbf{B}+\mathbf{F}\right)^T+\left(\mathbf{E}\mathbf{A}^{-1}\right)\boldsymbol{\Sigma}_{Zu}\left(\mathbf{E}\mathbf{A}^{-1}\right)^T+\boldsymbol{\Sigma}_{Zy}.$$

Case Study: An Aircraft Design Problem

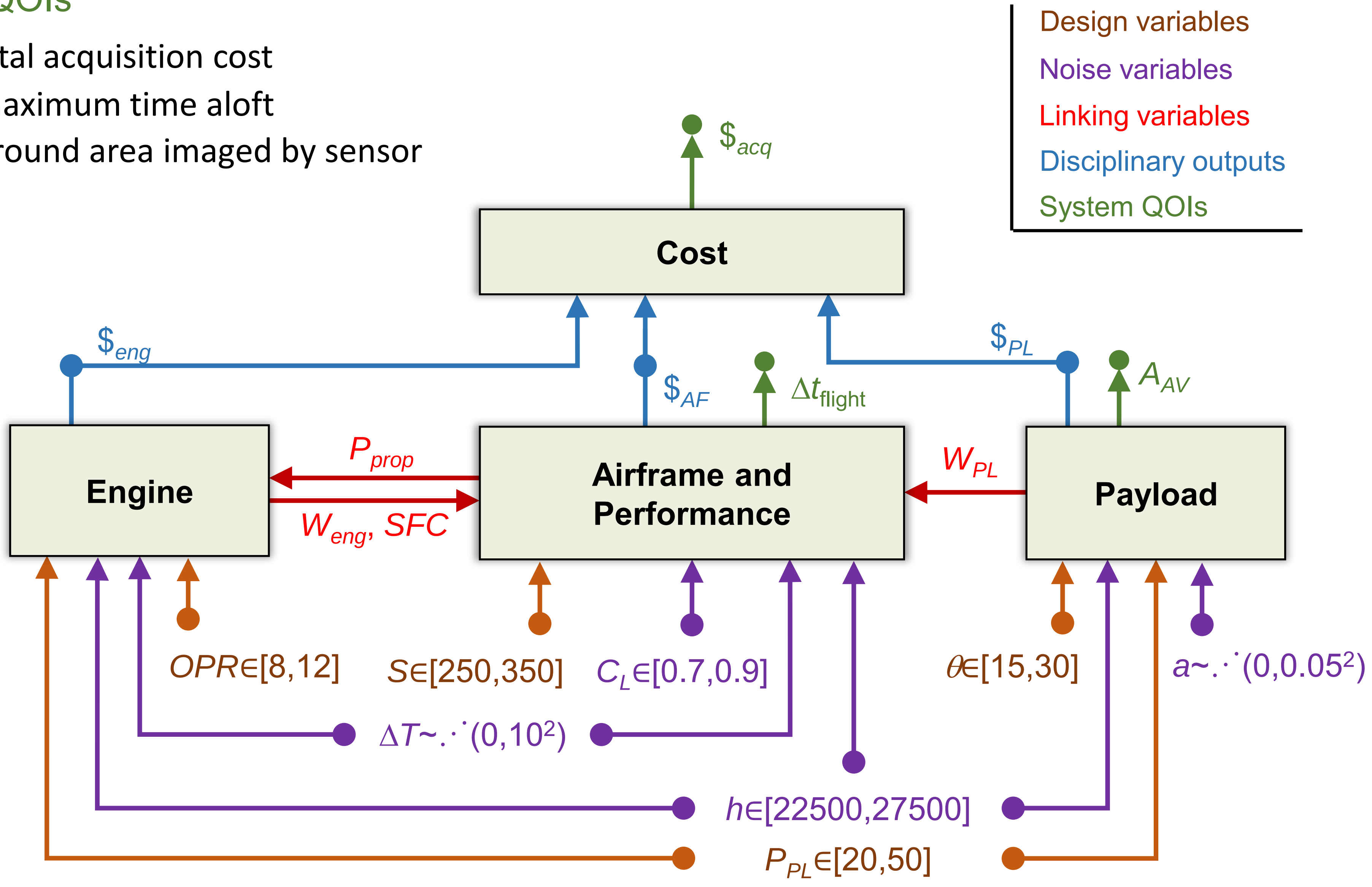
Multidisciplinary UP & SSA

System QOIs

$\$_{acq}$ -total acquisition cost

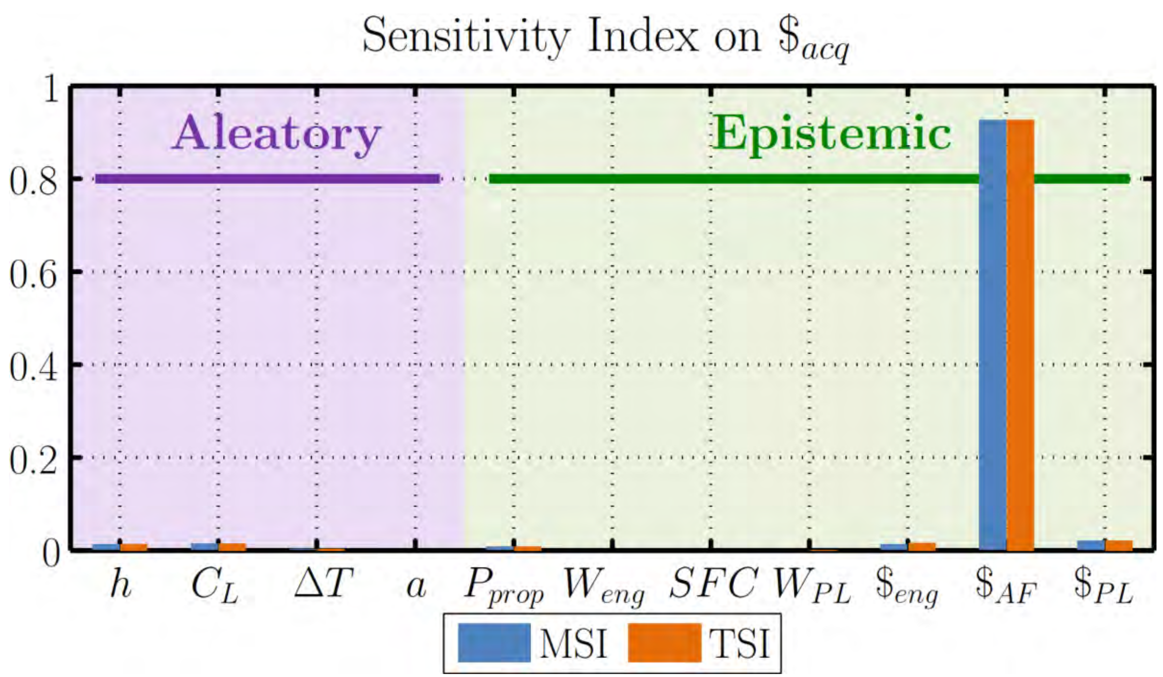
Δt_{flight} -maximum time aloft

A_{AV} -Ground area imaged by sensor

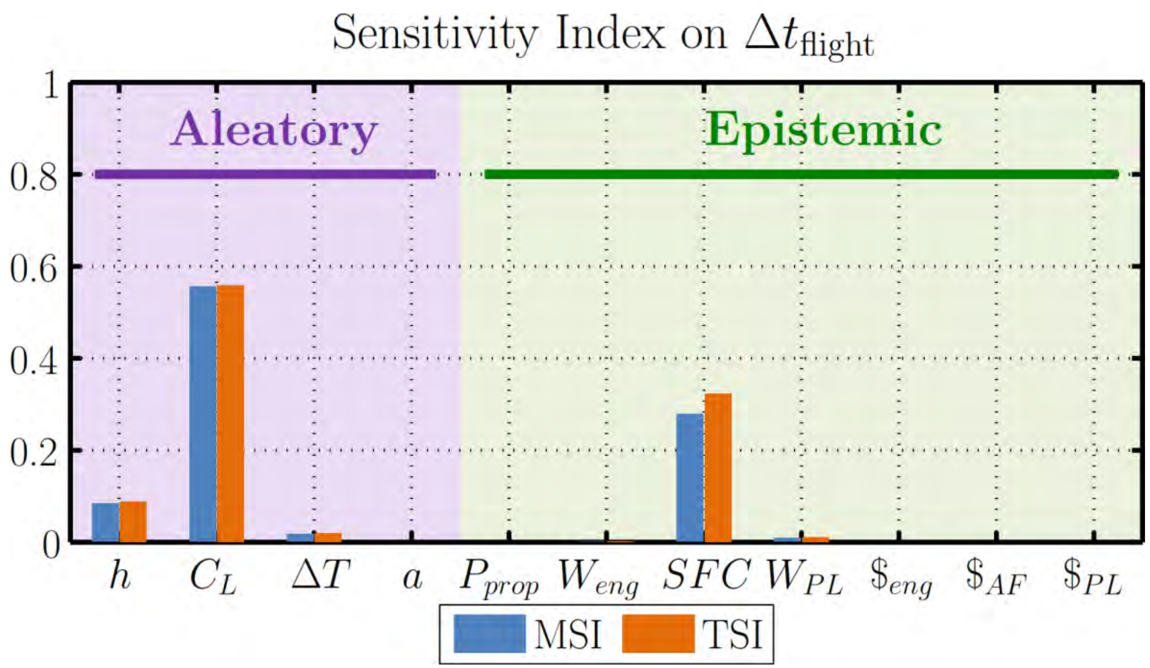


Sensitivity Analysis for both Aleatory and Epistemic Uncertainties

Aleatory Uncertainty: 6~7%



Epistemic Uncertainty: 5%



Topic 3
Resource Allocation for Reduction of Epistemic Uncertainty in Multidisciplinary Design

Jiang, Z., Chen, S., Apley, D., and Chen, W., "**Resource Allocation for Reduction of Epistemic Uncertainty in Simulation-based Multidisciplinary Design**", *ASME 2015 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference,* IDETC2015-47302, August 2-4, Boston, MA, 2015.

Introduction

OBJECTIVE

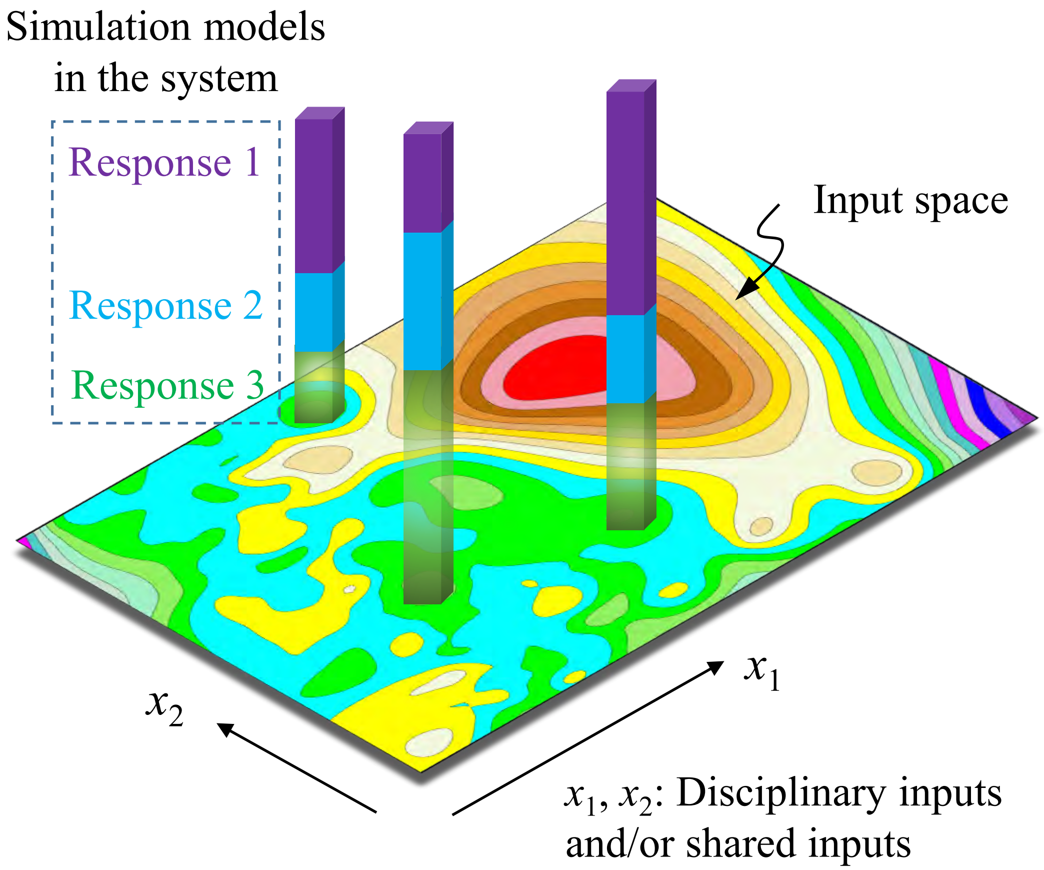
- To improve the ***global*** modeling capability of a multidisciplinary system

  Such that the epistemic uncertainty of system QOIs is acceptable over the input space.

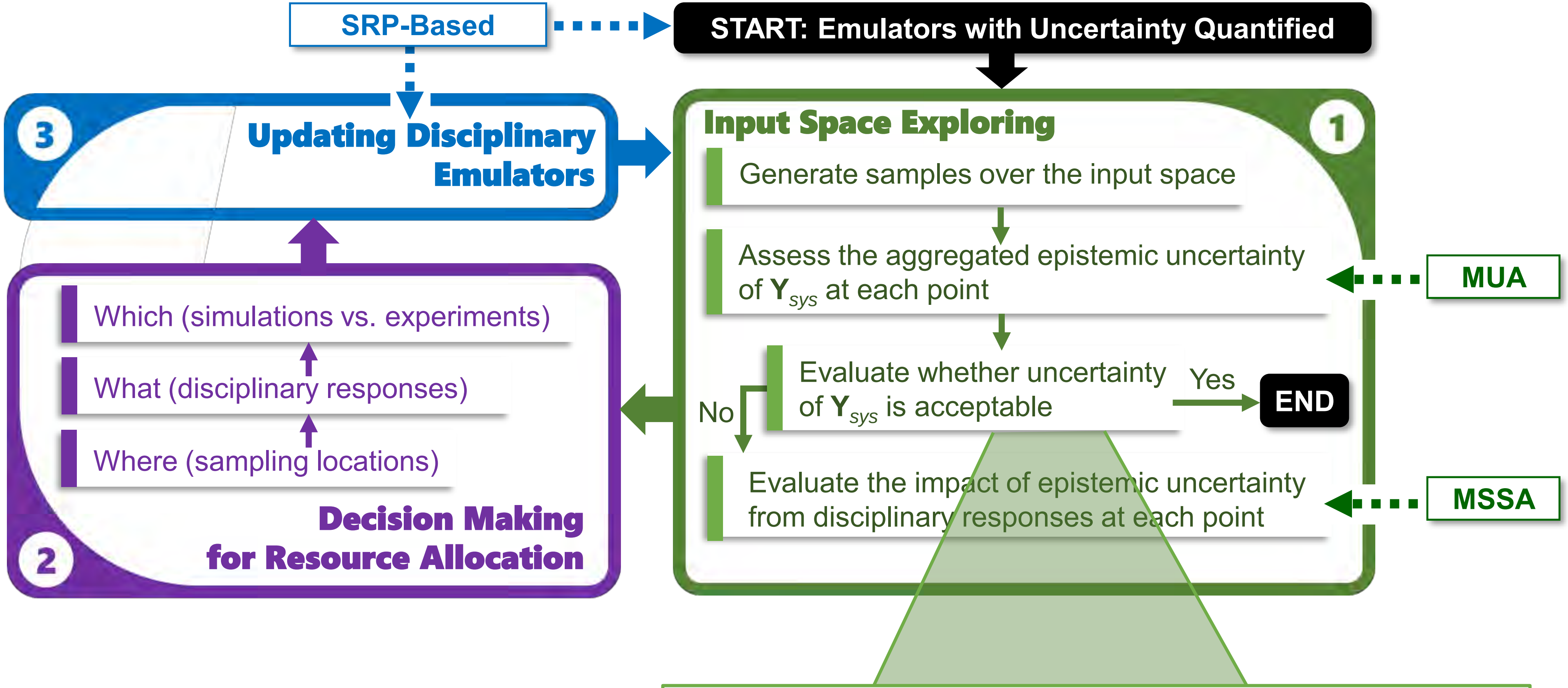
Resources: Experiments and/or simulations

RESEARCH QUESTIONS

- **Where** in the input space of a multidisciplinary system shall we allocate more resources?
- To **what** disciplinary response(s) shall we allocate more resources?
- **Which** type of resource shall we allocate, experiments or simulations?
-



A Sequential Resource Allocation Strategy

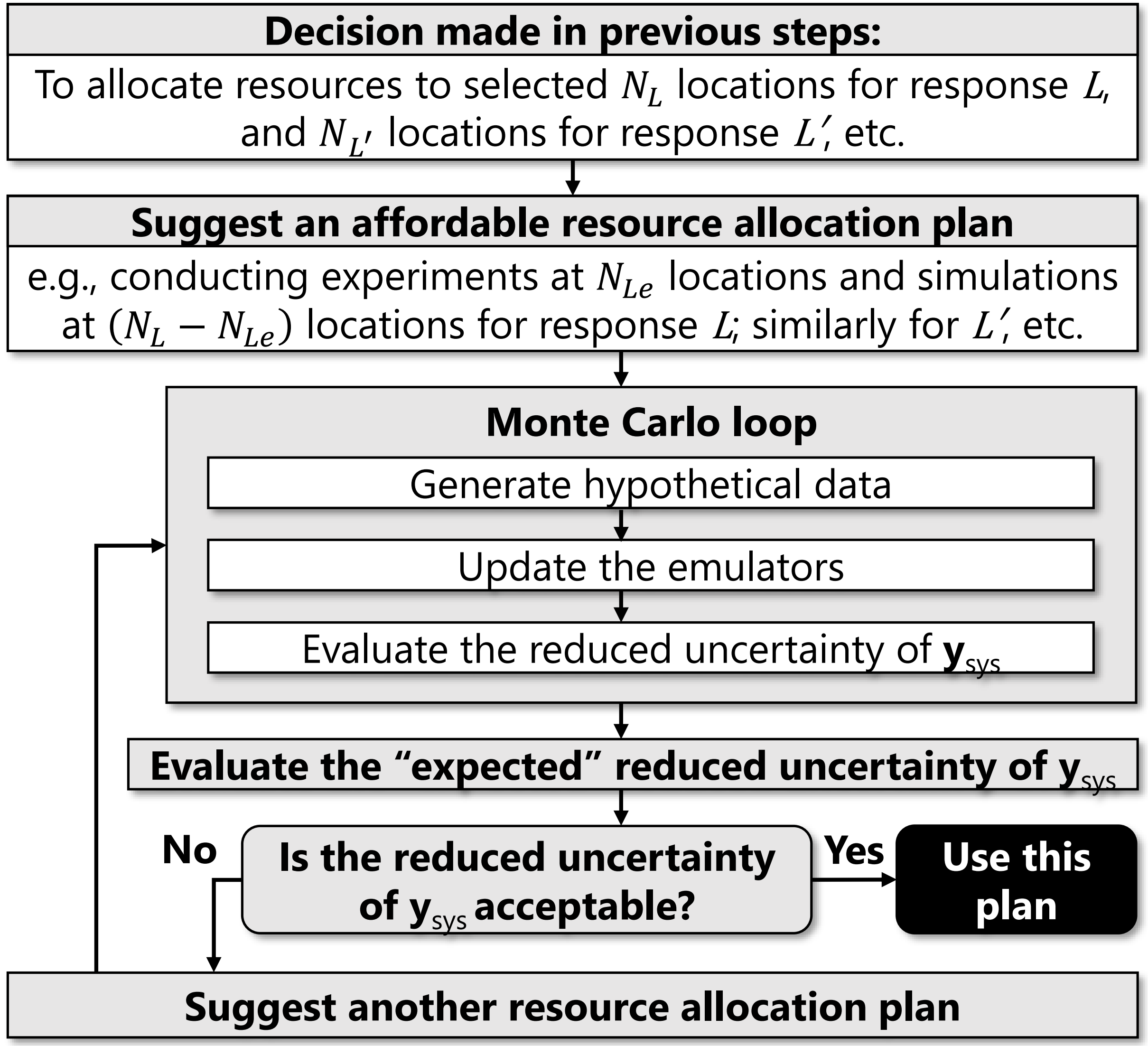


$$\gamma(\mathbf{x}_{\text{ind}}, \mathbf{x}_s) \triangleq \frac{\sqrt{\text{Var}\left[\mathbf{Y}_{\text{sys}}(\mathbf{x}_{\text{ind}}, \mathbf{x}_s)\right]}}{\iint \left\| \mathbf{Y}_{\text{sys}}(\mathbf{x}_{\text{ind}}, \mathbf{x}_s) \right\| d\mathbf{x}_{\text{ind}} d\mathbf{x}_s \Big/ \iint d\mathbf{x}_{\text{ind}} d\mathbf{x}_s} \le \alpha\%, \quad \text{for } \forall \mathbf{x}_{\text{ind}}, \mathbf{x}_s$$

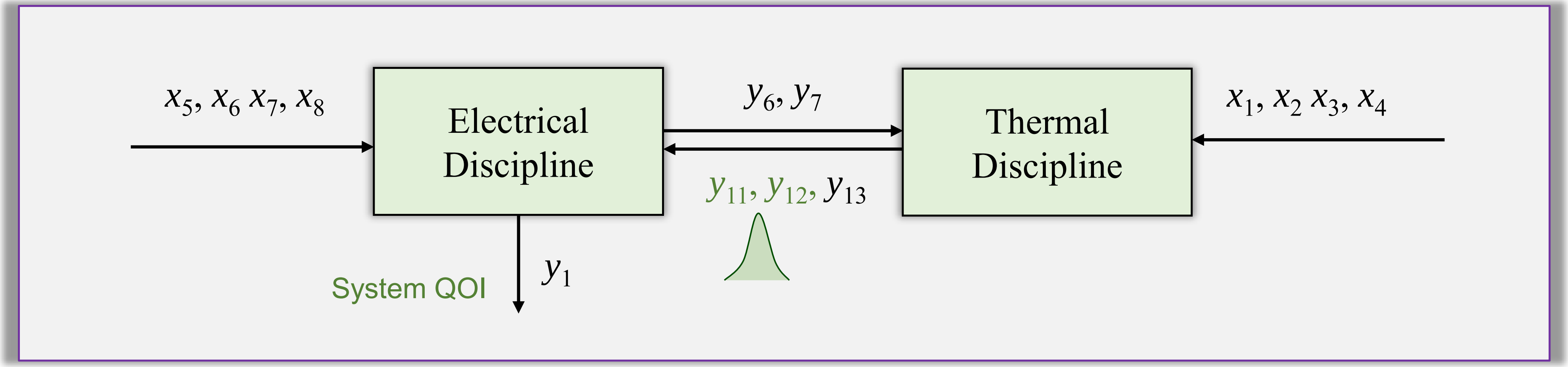
- SRP: Spatial-Random-Process
- MUA: Multidisciplinary Uncertainty Analysis
- MSSA: Multidisciplinary Statistical Sensitivity Analysis

Which (simulations vs. experiments): A Preposterior Analysis

AFTER SELECTING LOCATIONS AND RESPONSES…



Case Study: Electronic Packaging



- **http://www.eng.buffalo.edu/Research/MODEL/mdo.test.orig/class2prob3.html**

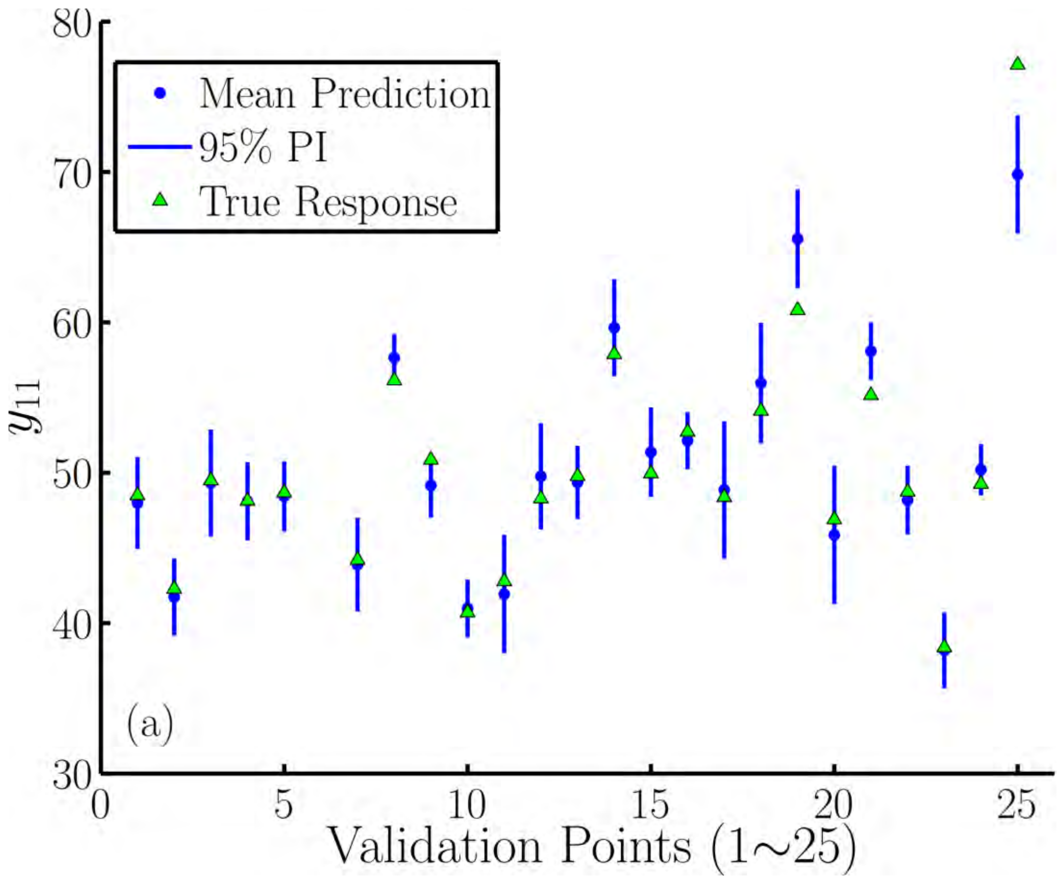
x_1	Heat sink width (m)	y_1	Negative of watt density ($watts/m^3$)
x_2	Heat sink length (m)	y_4	Current in resistor #1 ($amps$)
x_3	Fin length (m)	y_5	Current in resistor #2 ($amps$)
x_4	Fin width (m)	y_6	Power dissipation in resistor #1 ($watts$)
x_5	Nominal resistance #1 at temperature 20 ºC (Ω)	y_7	Power dissipation in resistor #2 ($watts$)
x_6	Temperature coefficient of electrical resistance #1 (ºK^{-1})	y_{11}	Component temperature of resistor #1 (ºC)
x_7	Nominal resistance #2 at temperature 20 ºC (Ω)	y_{12}	Component temperature of resistor #2 (ºC)
x_8	Temperature coefficient of electrical resistance #2 (ºK^{-1})	y_{13}	Heat sink volume (m^3)

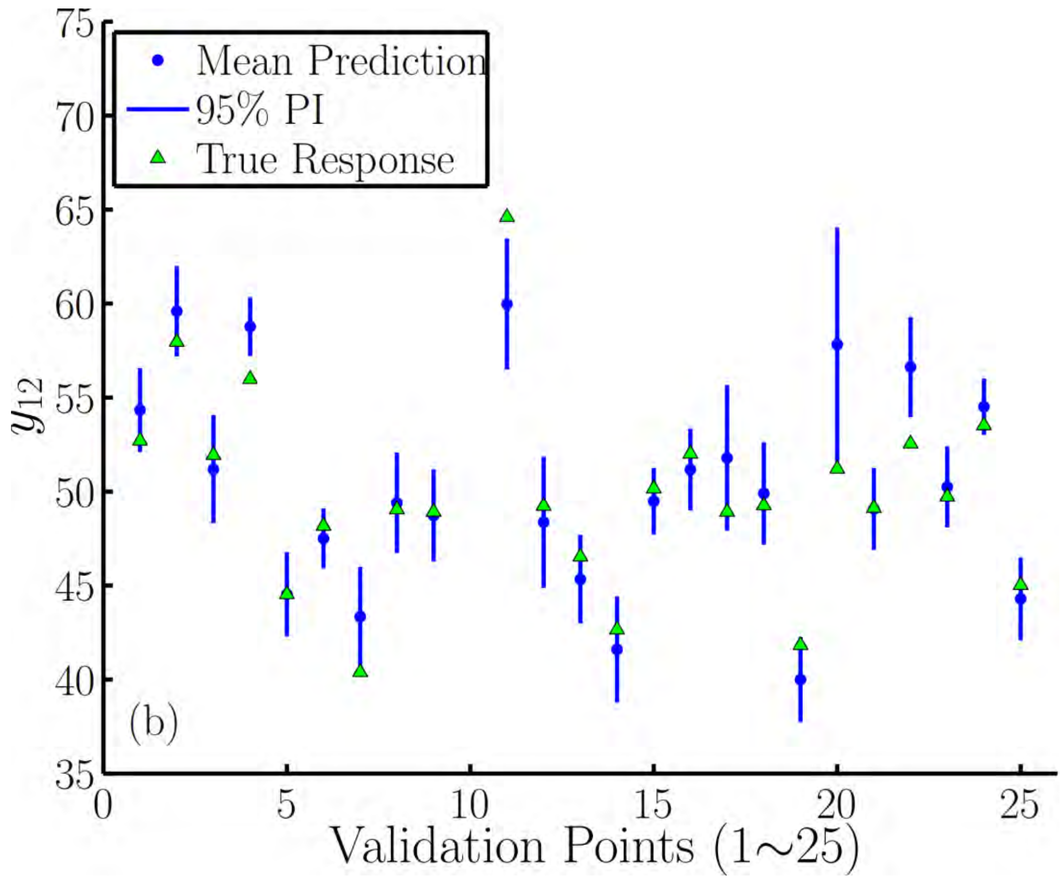
Uncertainty Quantification

Resource Allocation

1ST ITERATION

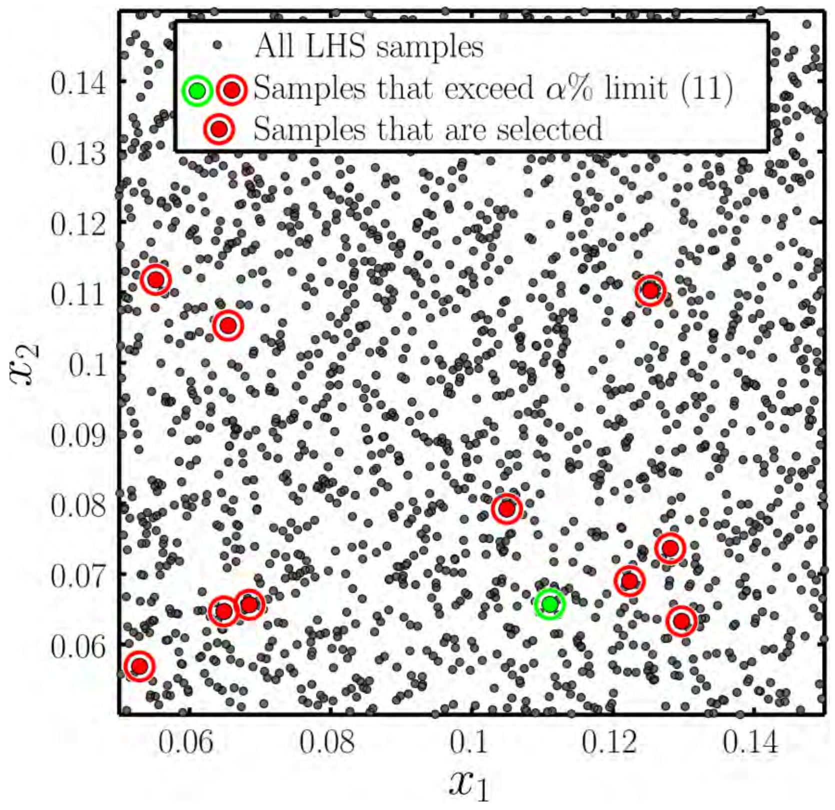
- Model UQ: 40 experiments + 40 simulations

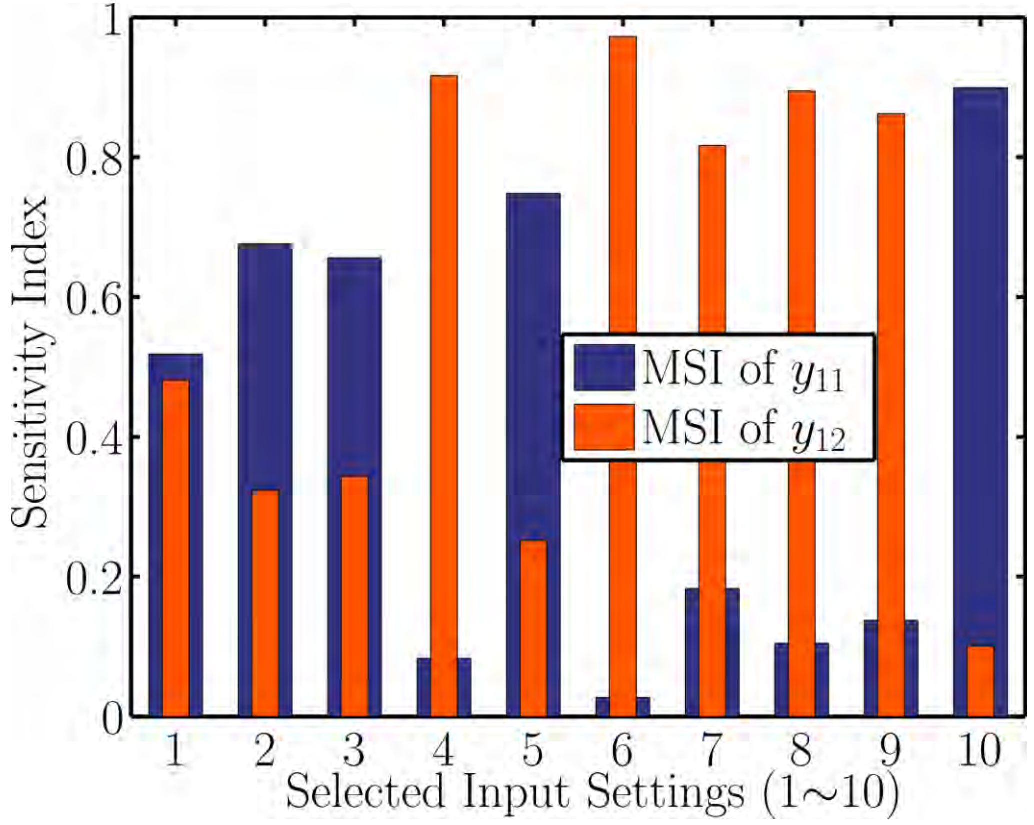




1ST ITERATION

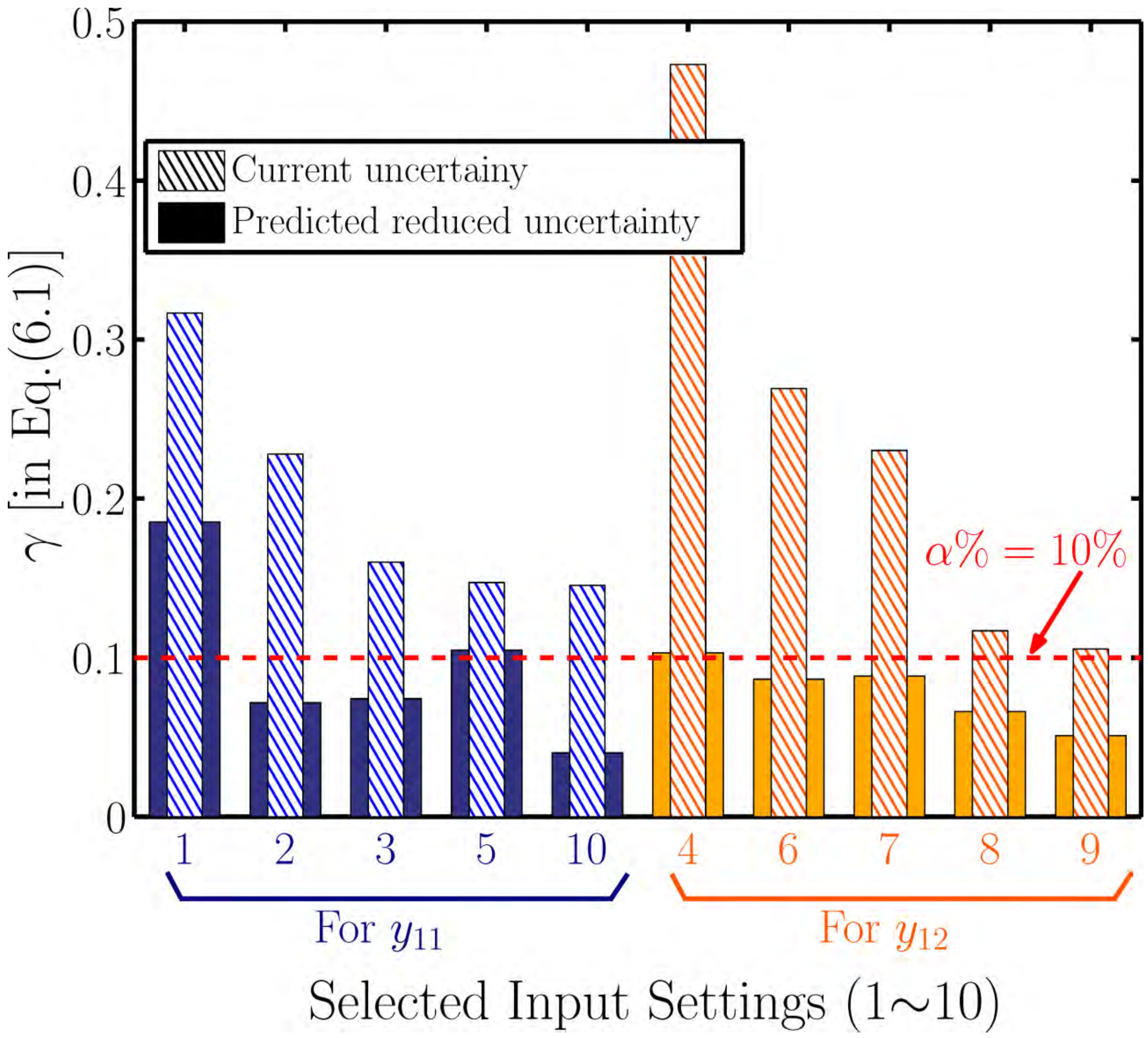
- Selection of input settings (from 2,000 samples) and responses





α=10%

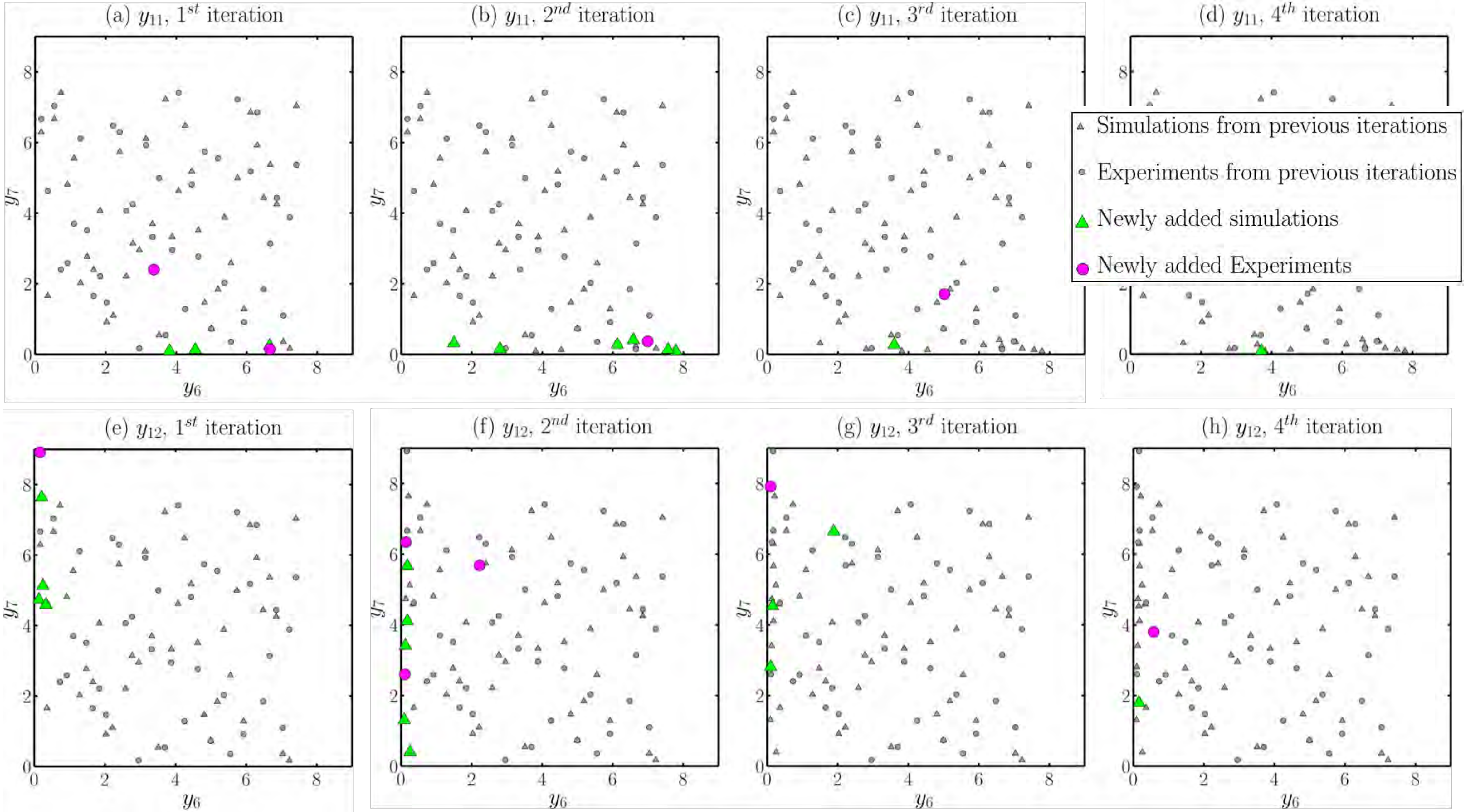
Preposterior Analysis to Decide the Type of Resources to Allocate



DECISION (1ST ITERATION)

(1) Allocate simulations of y_{11} to points #2, 3, 10;
(2) Allocate simulations of y_{12} to points #6~9;
(3) Allocate experiments of y_{11} to points #1, 5;
(4) Allocate experiment of y_{12} to point #4.

Subsequent Four Iterations (24 simulations + 10 experiments)



Summary

MODEL FUSION

- Approaches can handle both hierarchical and non-hierarchical rankings of fidelity
- Multiple approaches work equally well with reasonable assumptions

MULTIDISCIPLINARY UNCERTAINTY PROPAGATION AND SENSITIVITY ANALYSIS

- Considers both aleatory and epistemic uncertainties
- Utilizes the structure of SRP emulators, which allows for analytical derivation
- Decomposed disciplinary analyses, provide useful information for resource allocation

RESOURCE ALLOCATION FOR REDUCTION OF EPISTEMIC UNCERTAINTY

- Breaks a complex decision making problem into a sequential process
- Considers not only physical experiments but also simulations

Thank You!