Introduction to Uncertainty Quantification

James Warner and Patrick Leser
Durability, Damage Tolerance, and Reliability Branch
NASA Langley Research Center

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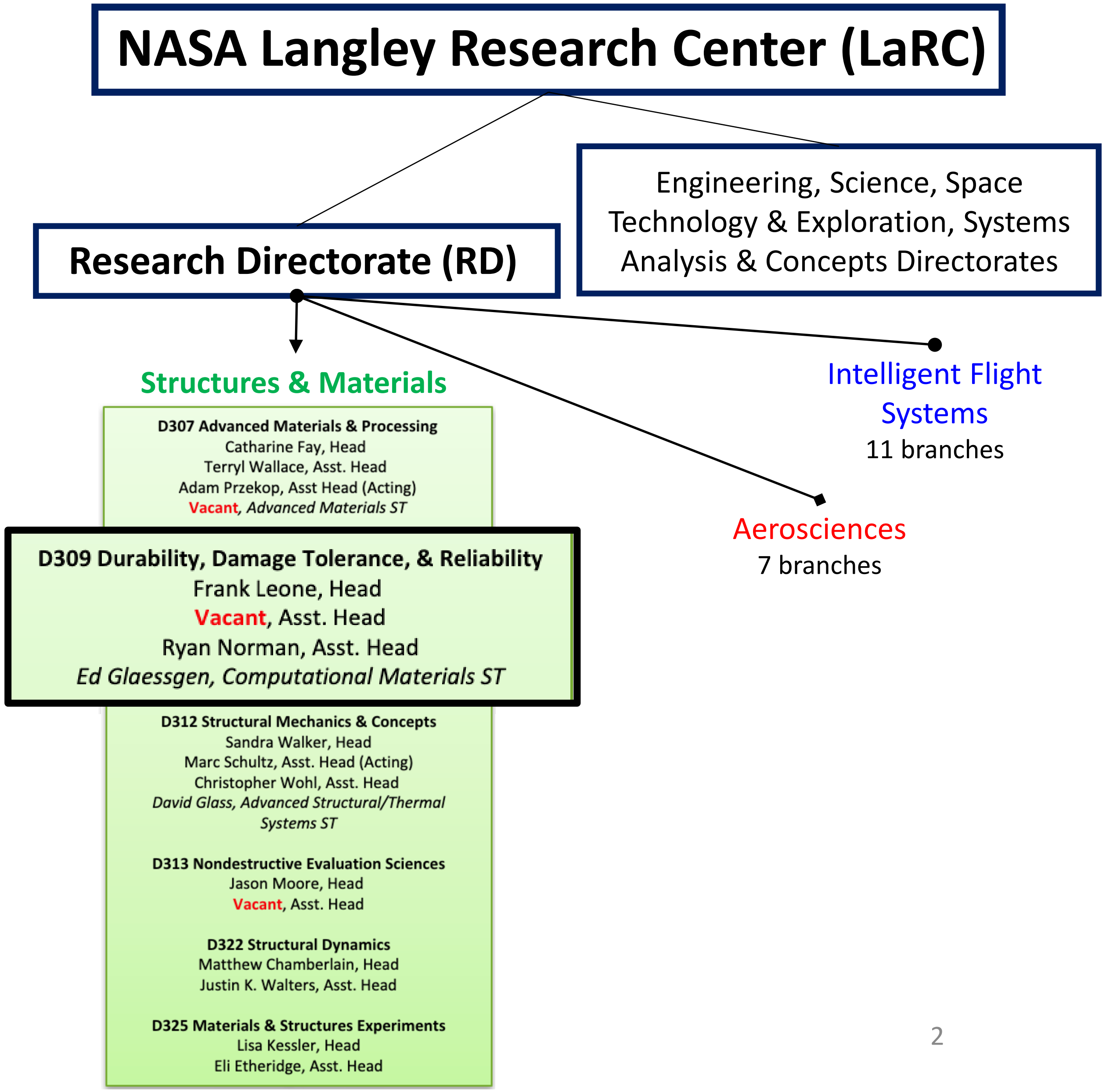
Introducing Ourselves

- James Warner (LaRC, D309)
  - **B.S.** Mechanical Engineering Binghamton University (2008)
  - **PhD** Civil & Environmental Engineering Cornell University (2014)
  - Computational Scientist @ LaRC (2014 – Present)
- Patrick Leser (LaRC, D309)
  - **B.S.** Aerospace Engineering N.C. State (2012)
  - **PhD** Aerospace Engineering N.C. State (2017)
  - Materials Research Engineer @ LaRC (2014 – Present)



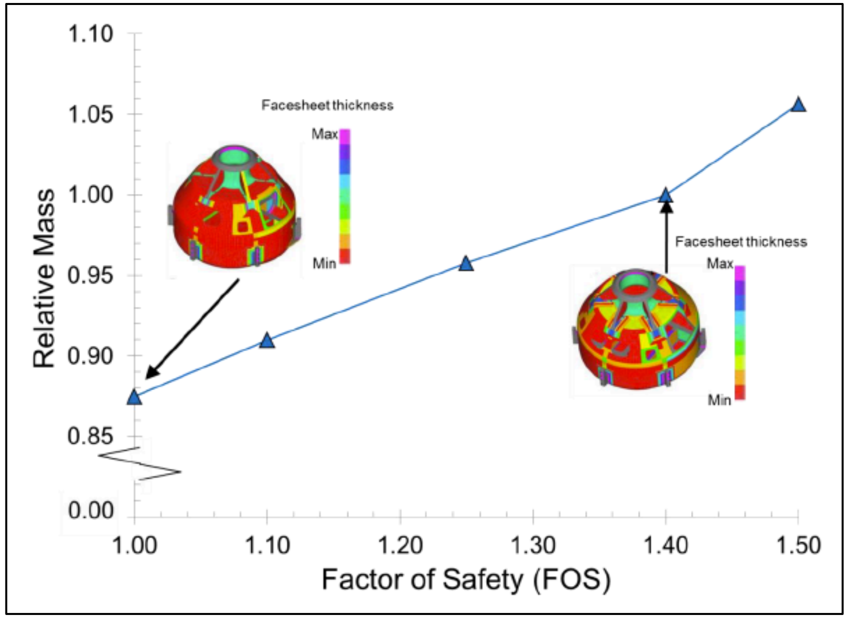
Outline

- Motivation & Background
- Uncertainty Quantification (UQ) Concepts
- Example
- Challenges and Best Practices
- NASA UQ Community of Practice
- Summary

Motivating Example: Reliability-Based Design

Probabilistic Design Case Study – Composite Crew Module

- Demonstrated significant mass savings (~12.5%) were possible at the expense of reduced (but quantified) reliability using probabilistic methods
- Showed a factor of safety of 1.4 resulted in extremely small failure probability (1 in ~10M)
- Highlighted the importance of UQ as a discipline + practical challenges



Scotti, et al. Probabilistic Design Case Study – Composite Crew Module. NESC-RP-10-00611. 2010.

What is Uncertainty Quantification (UQ)?

"All models are wrong,
but some are useful"

George E.P. Box

So how wrong might our models be?
(When) are they useful from an engineering perspective?
And how confident are we in their predictions?

UQ provides a framework for answering these questions and making our models useful.

What is Uncertainty Quantification (UQ)?

"

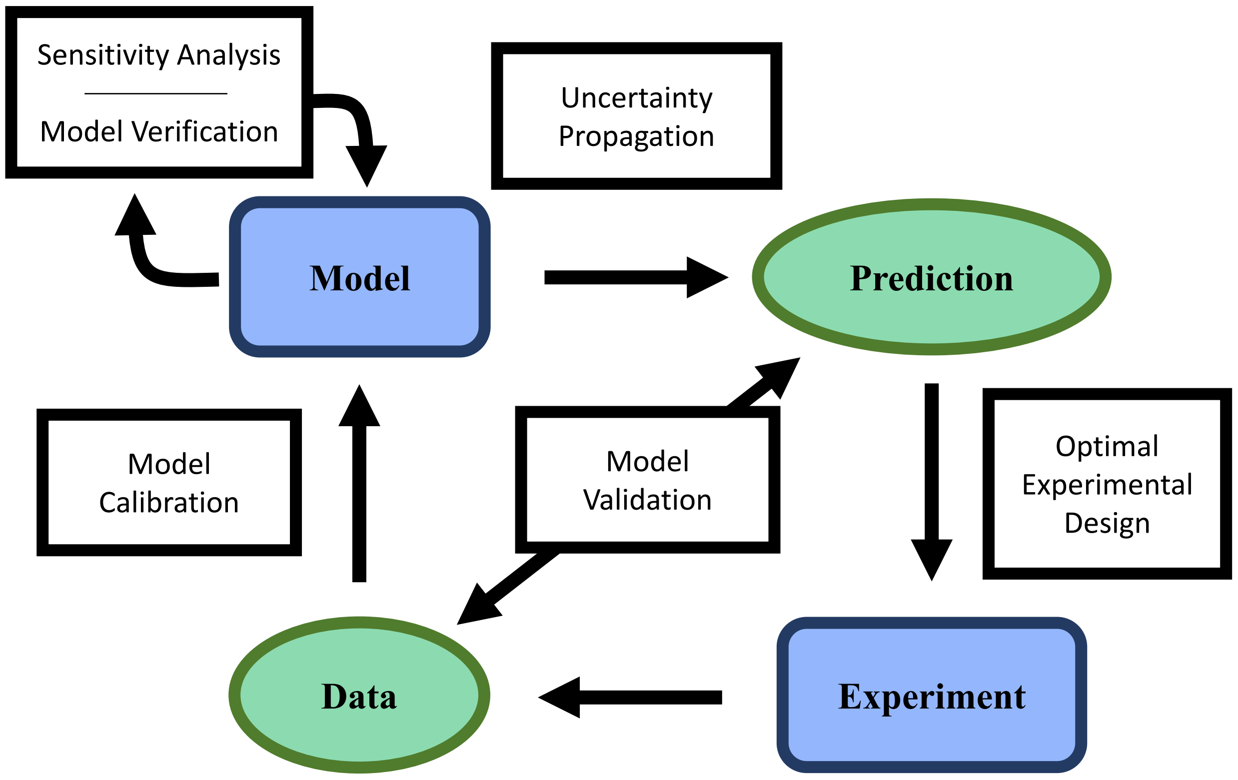
…the science of identifying, quantifying, and reducing uncertainties associated with models, numerical algorithms, experiments and predicted outcomes…

RALPH SMITH

North Carolina State University

Smith, Ralph C. *Uncertainty quantification: theory, implementation, and applications*. Society for Industrial and Applied Mathematics, 2024.

- Naturally incorporates experimental data and models
- Typically iterative; data/experiments updated over time



UQ Workflow for Models and Experiments

Quick Review of Terminology

- Random Variable, $\boldsymbol{X}$
  - Variable with unknown true value

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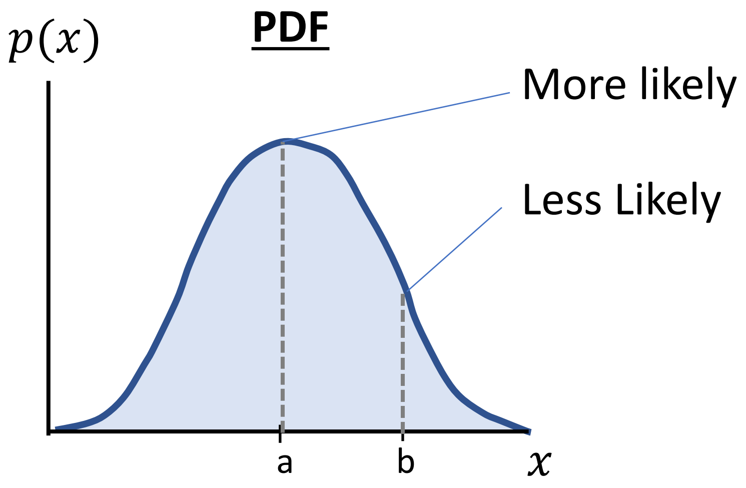
- Probability Density Function (PDF), $p(x)$
  - Function describing the <u>relative</u> likelihood that $\boldsymbol{X}$ takes a specific value, x



Quick Review of Terminology

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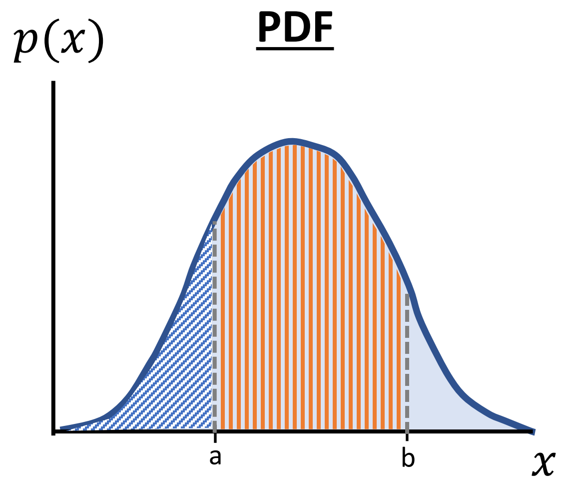
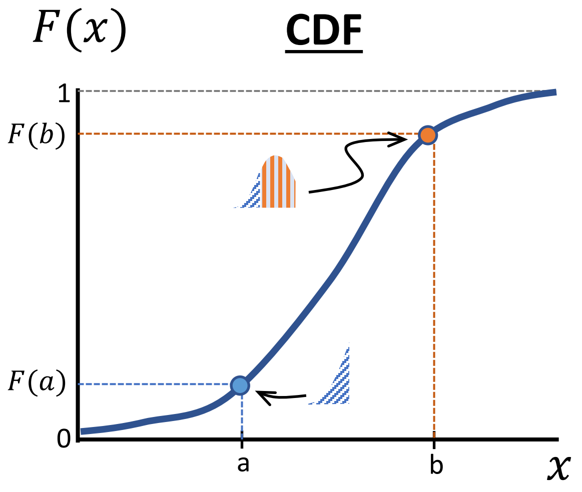
- Probability Density Function (PDF), $p(x)$
  - Function describing the <u>relative</u> likelihood that $\boldsymbol{X}$ takes a specific value, x
- Cumulative Distribution Function (CDF), $F(x)$
  - <u>Probability</u> that $\boldsymbol{X}$ takes a value *less than or equal to* x
  - CDF = integral of the PDF from $-\infty$ to x
  - Can obtain other probabilities by integrating the PDF; e.g., $P(a \leq X \leq b)$





Types of Uncertainty

- **Deterministic:** Quantity that is “known precisely (or with negligibly small* uncertainty)” [1]
- **Aleatory:** “Also known as statistical, stochastic, or *irreducible uncertainty*… that in principle cannot be reduced by additional physical or experimental knowledge.” [2]
- **Epistemic:** *Reducible uncertainty* that is “due to simplifying model assumptions, missing physics, or basic lack of knowledge.” [2]

1. Roy, Christopher J., and William L. Oberkampf. "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing." *Computer methods in applied mechanics and engineering* 200.25-28 (2011): 2131-2144.
2. Smith, Ralph C. *Uncertainty quantification: theory, implementation, and applications*. Society for Industrial and Applied Mathematics, 2013.

* “Negligibly small” is based on precise measurement and/or sensitivity analysis

Treatment of Uncertainties by Type

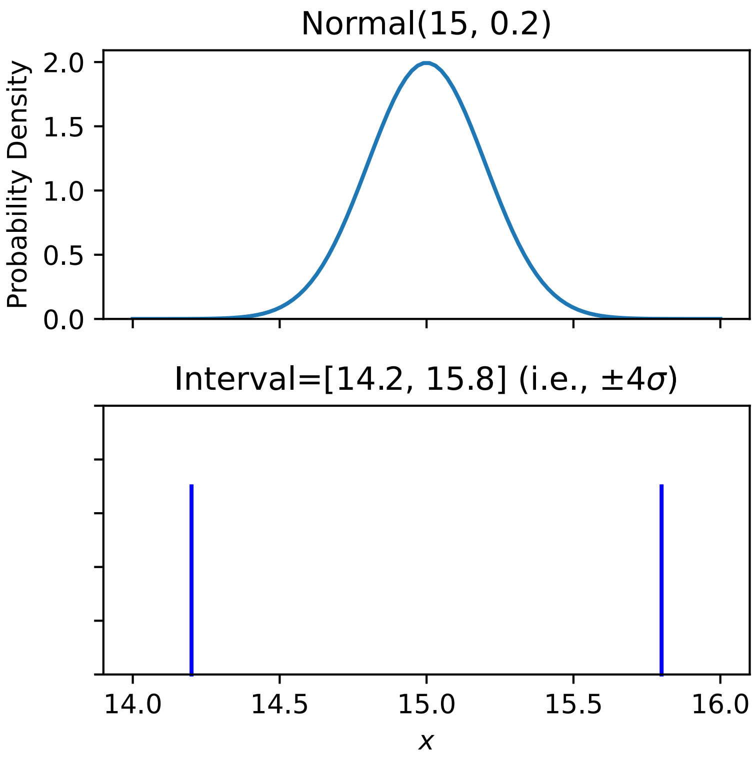
- Aleatory uncertainties are generally characterized using a *probability density function* (PDF).
- Two popular approaches for characterizing epistemic uncertainties are:

Approach	Goal
1. Probabilistic (Bayesian)	Probabilistic quantification of engineering beliefs
2. Interval / p-box	Conservative bounds on probabilistic estimates

- Treatment of uncertainties is up to the analyst and the “right” choice depends on the application and goals of the analysis.

How to Classify Uncertainties (1/2)

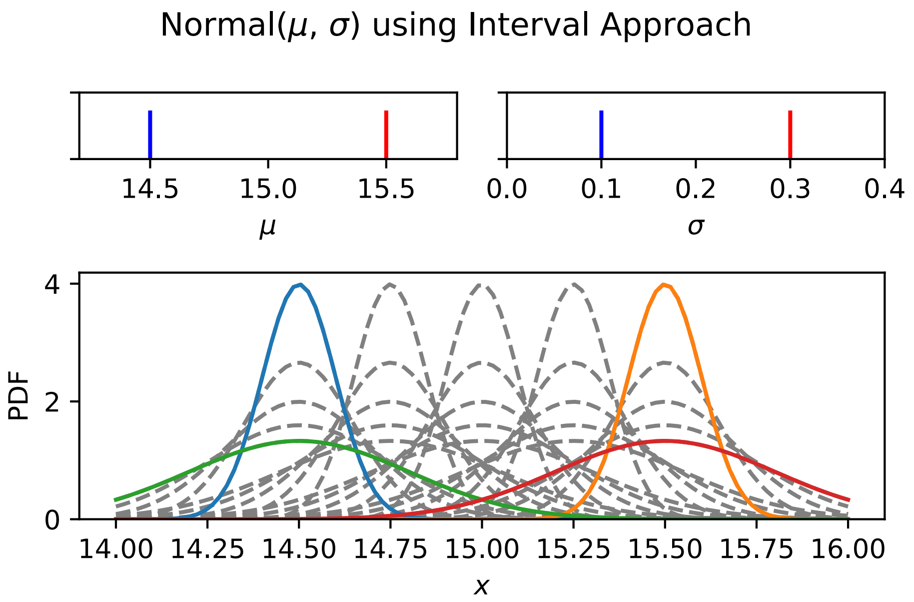
- A common distinction between aleatory and epistemic uncertainty is whether the quantity has a measurable frequency of occurrence or is a single occurrence [1, 2]
- Aleatory (irreducible)
  - Example: lengths of future beams produced by a given manufacturing process
  - Characterized by a probability density function (PDF) with fixed parameters
- Epistemic (reducible with more information)
  - Example: length of beam that has been manufactured
  - Characterized by either an interval **or** a PDF representing a *degree of belief* (fundamentally distinct from aleatory)
- What if we measure the beam after manufacturing?

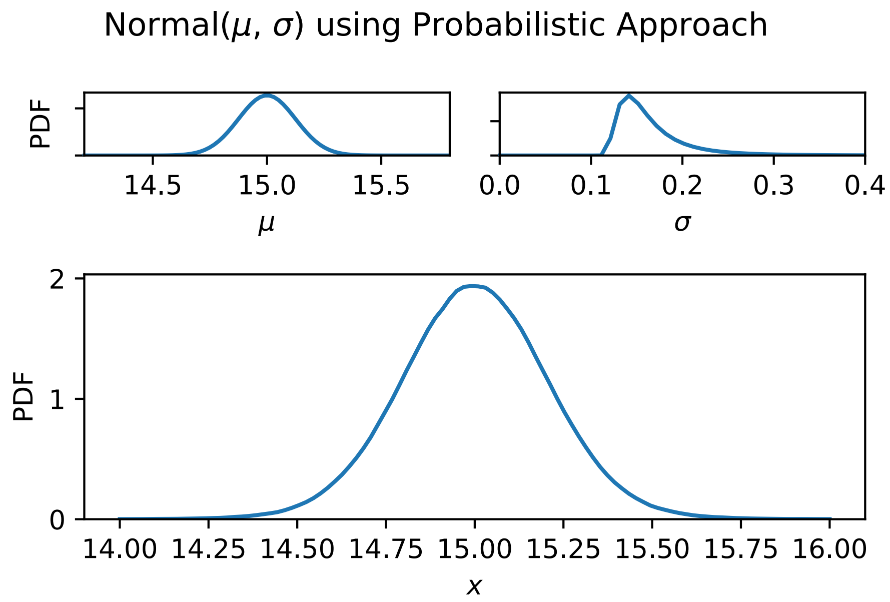


1. Roy, Christopher J., and William L. Oberkampf. "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing." *Computer methods in applied mechanics and engineering* 200.25-28 (2011): 2131-2144.
2. Fox, Craig R., and Gülden Ülkümen. "Distinguishing two dimensions of uncertainty." in Essays in Judgment and Decision Making, Brun, W., Kirkebøen, G. and Montgomery, H., eds. Oslo: Universitetsforlaget (2011).

How to Classify Uncertainties (2/2)

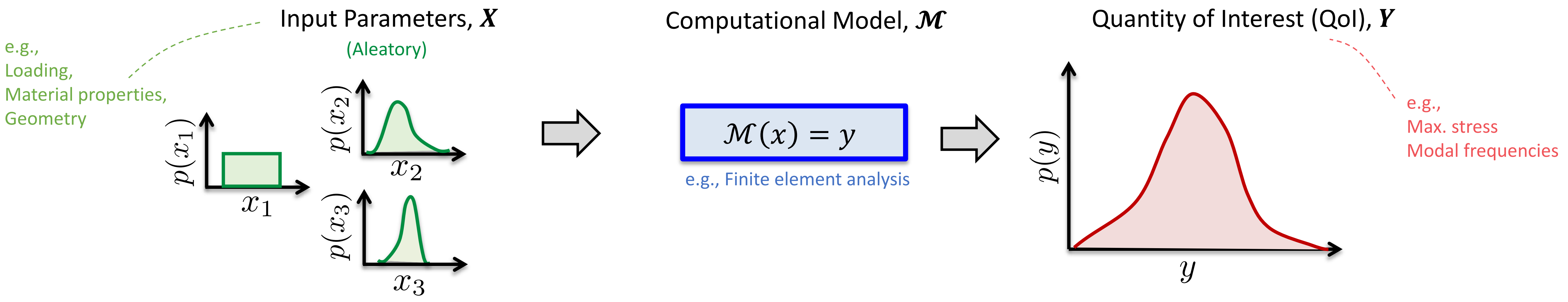
- The line between types is blurred when a variable is considered *aleatory* but there is uncertainty in its distributional form.
- This occurs, for example, if an inadequate number of observations are available.
- Mixed uncertainty (irreducible but uncertain)
  - Example: lengths of future beams produced by a novel manufacturing process
  - Characterized by a PDF with unknown parameters that are assigned an uncertainty measure





How to Propagate Uncertainties (1/4)

- ***Uncertainty propagation*** methods make *probabilistic* predictions using *deterministic* computational models



- Given PDFs for uncertain input parameters, $p(x)$, and a governing computational model, $\mathcal{M}$, of a system/structure, estimate the _______ of/for the QoI:
  - **PDF:** $p(y)$
  - Expected value (i.e., the mean), standard deviation of the QoI: $\mathbb{E}[Y], \mathrm{Std}[Y]$
  - 95% prediction intervals: y_L, y_U such that $P(y_L \leq Y \leq y_U) = 0.95$
  - Probability of exceeding a critical value: $P(Y \geq y^{crit})$

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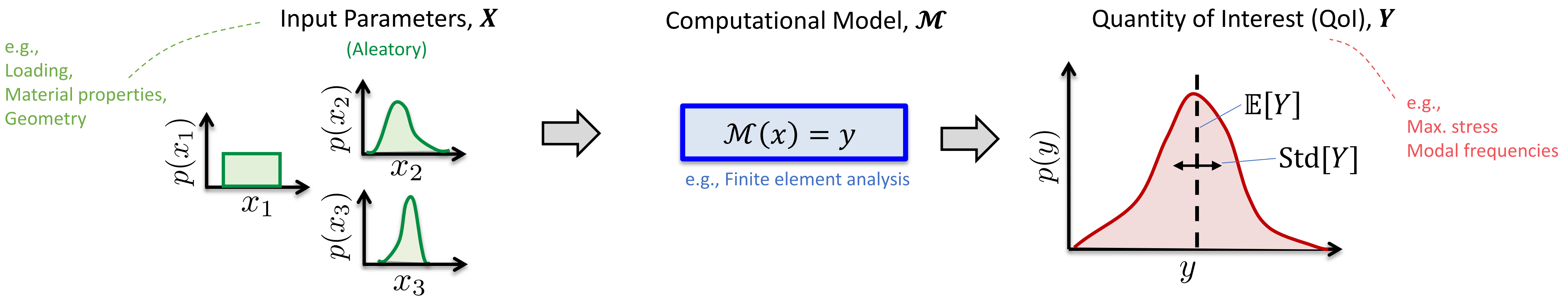

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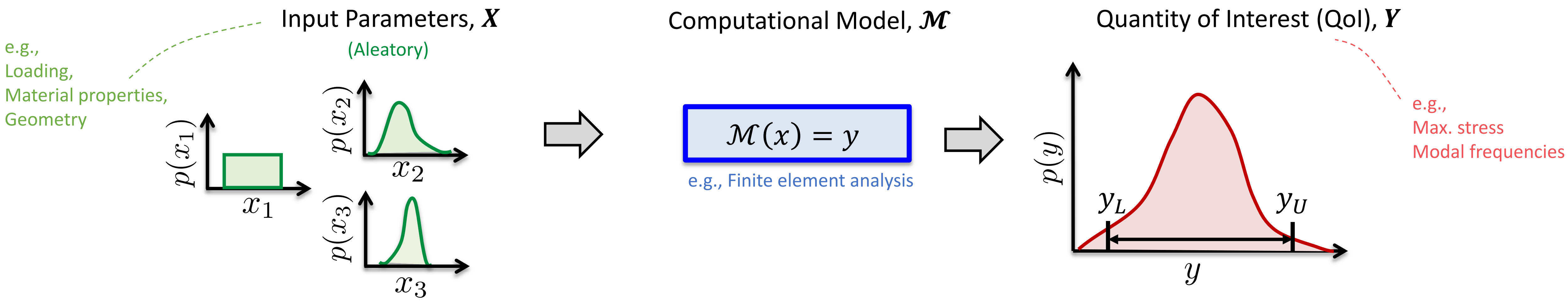

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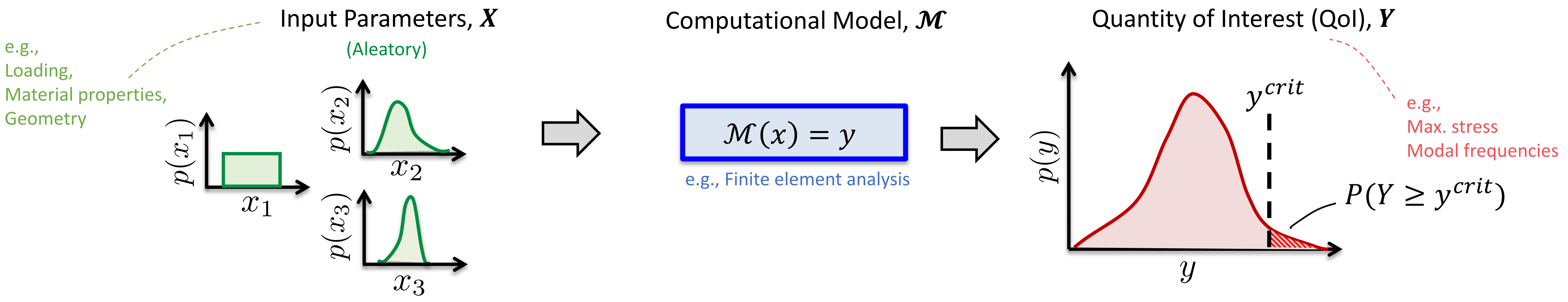

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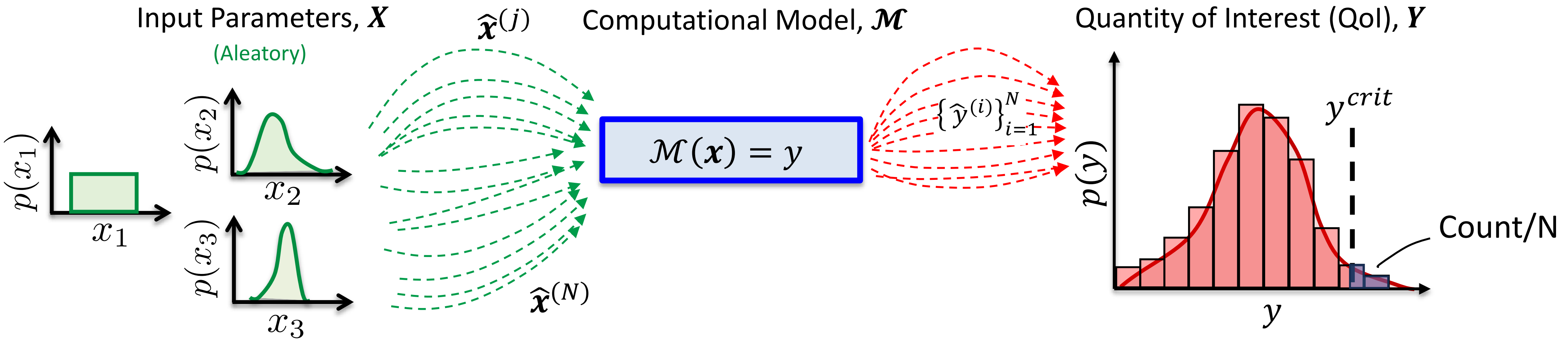
How to Propagate Uncertainties (2/4)

- ***Monte Carlo simulation*** is a general-purpose and conceptually-simple uncertainty propagation method



1. For j $= 1, \dots, N$ samples:
   - I. Generate random sample of input parameters: $\widehat{\boldsymbol{x}}^{(j)} \sim p(x)$
   - II. Evaluate model and store output: $\widehat{y}^{(j)} = \mathcal{M}(\widehat{\boldsymbol{x}}^{(j)})$
2. Postprocess the output samples, $\{\widehat{y}^{(j)}\}_{j=1}^{N}$, to estimate statistics of QoI:
   - $p(y)$ (use histogram or kernel density estimate)
   - $\mathbb{E}[Y] \approx \frac{1}{N}\sum_{i=1}^{N} y^{(i)}$ (expected value ≈ sample average)
   - $P\left(Y \geq y^{crit}\right) \approx \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}(y^{i} \geq y^{crit})$ (failure probability ≈ proportion of samples that failed)

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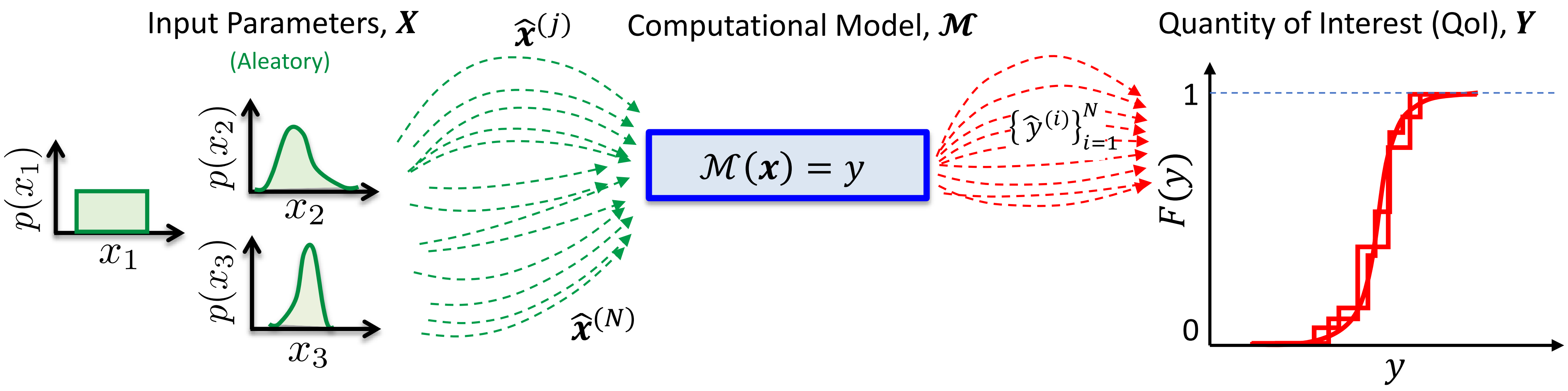

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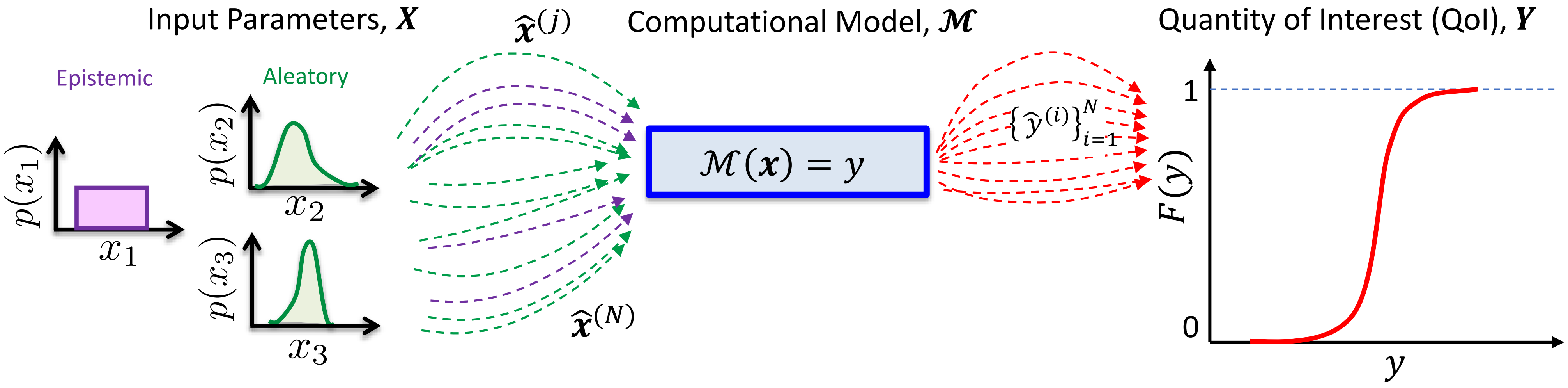
2. Build $\hat{F}(y)$, the empirical CDF given samples $\{\hat{y}^{(j)}\}_{j=1}^{N}$
   - $\hat{F}(y) = \frac{1}{N}\sum_{j=1}^{N} 1(\hat{y}^{(j)} \leq y)$ (Smoother as N increases)

How to Propagate Uncertainties (3/4)

- ***Probabilistic*** treatment of epistemic uncertainty using ***Monte Carlo simulation***



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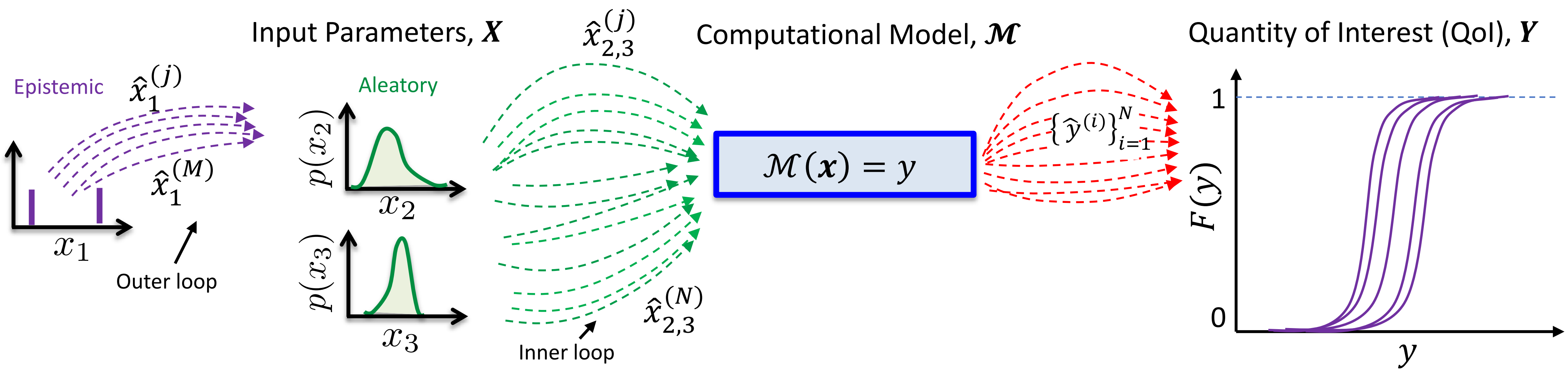
   - $\hat{F}(y) = \frac{1}{N}\sum_{j=1}^{N} 1(\hat{y}^{(j)} \leq y)$

➢ **The probabilistic/Bayesian approach is the same for epistemic and aleatory uncertainties**

How to Propagate Uncertainties (4/4)

- ***Interval*** treatment of epistemic uncertainty using ***double loop Monte Carlo simulation***

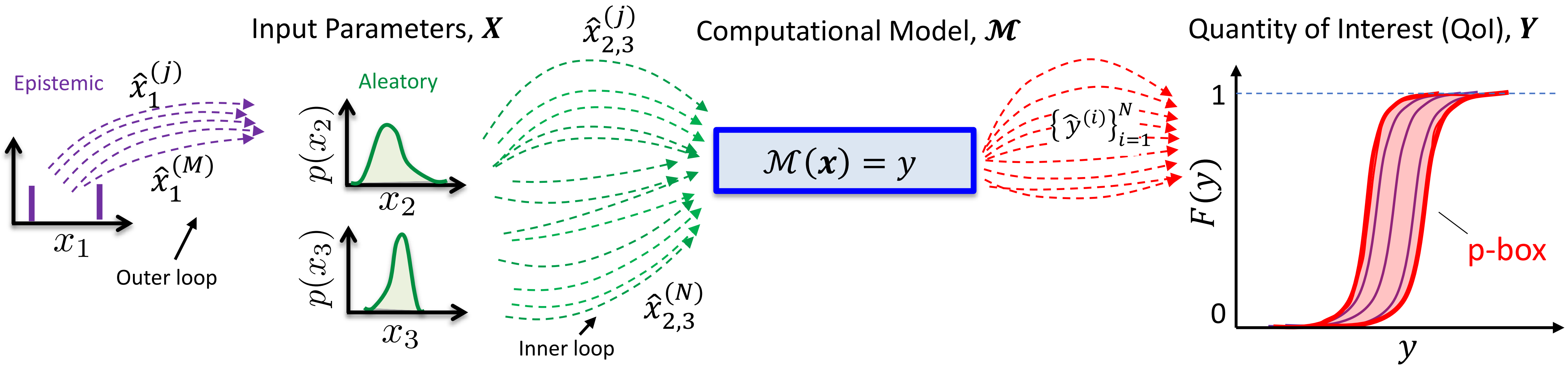


1. For i $= 1, \dots, M$ outer loop samples:
   I. Sample epistemic input parameter $\hat{x}_1^{(i)} \sim\in I_e[x_L, x_U]$
   II. For j $= 1, \dots, N$ samples:
      a) Generate random sample of aleatory input parameters: $\hat{x}_2^{(j)} \sim p(x_2)$, $\hat{x}_3^{(j)} \sim p(x_3)$
      b) Evaluate model and store output: $\hat{y}^{(i,j)} = \mathcal{M}(\hat{x}_1^{(i)}, \hat{x}_2^{(j)}, \hat{x}_3^{(j)})$
   III. Build $\widehat{F}_i(y)$, the empirical CDF given samples $\{\hat{y}^{(i,j)}\}_{j=1}^{N}$

Inner loop is same as before

How to Propagate Uncertainties (4/4)

- ***Interval*** treatment of epistemic uncertainty using ***double loop Monte Carlo simulation***



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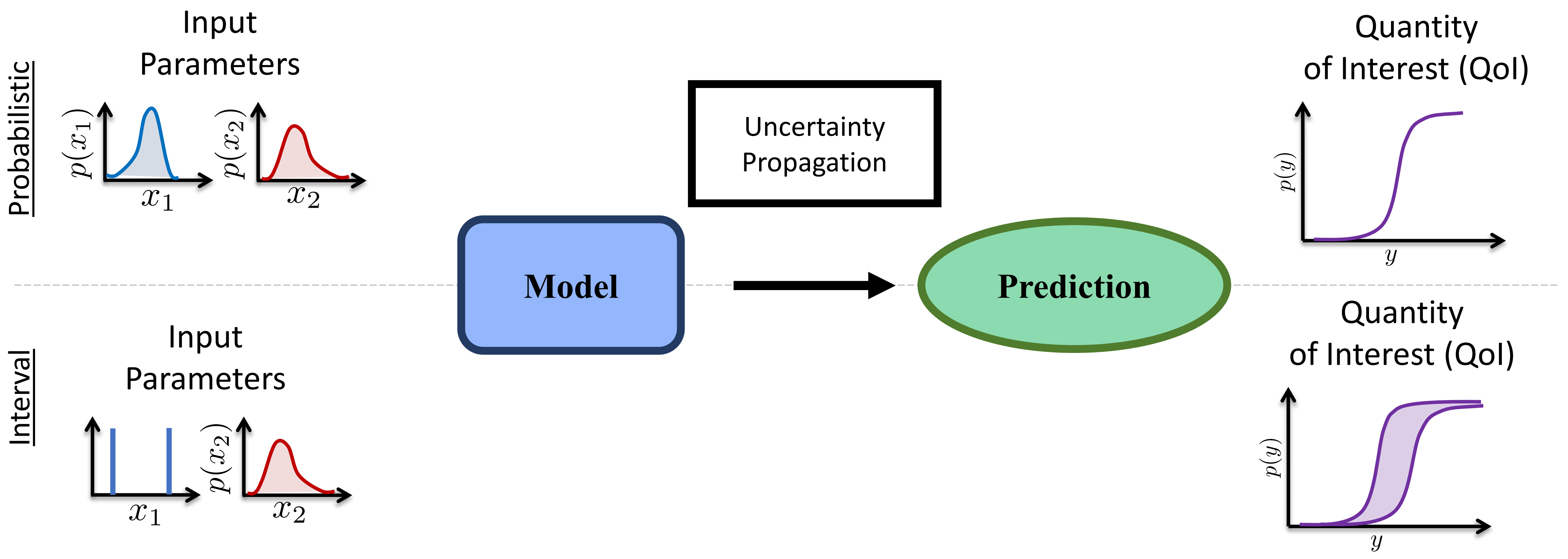
   III. Build $\widehat{F}_i(y)$, the empirical CDF given samples $\{\hat{y}^{(i,j)}\}_{j=1}^{N}$
2. Identify the maximum and minimum extents for all CDFs in the set $\{F_i(Y)\}_{i=1}^{M}$ to define a probability box or "***p-box***"

Components of a UQ Analysis



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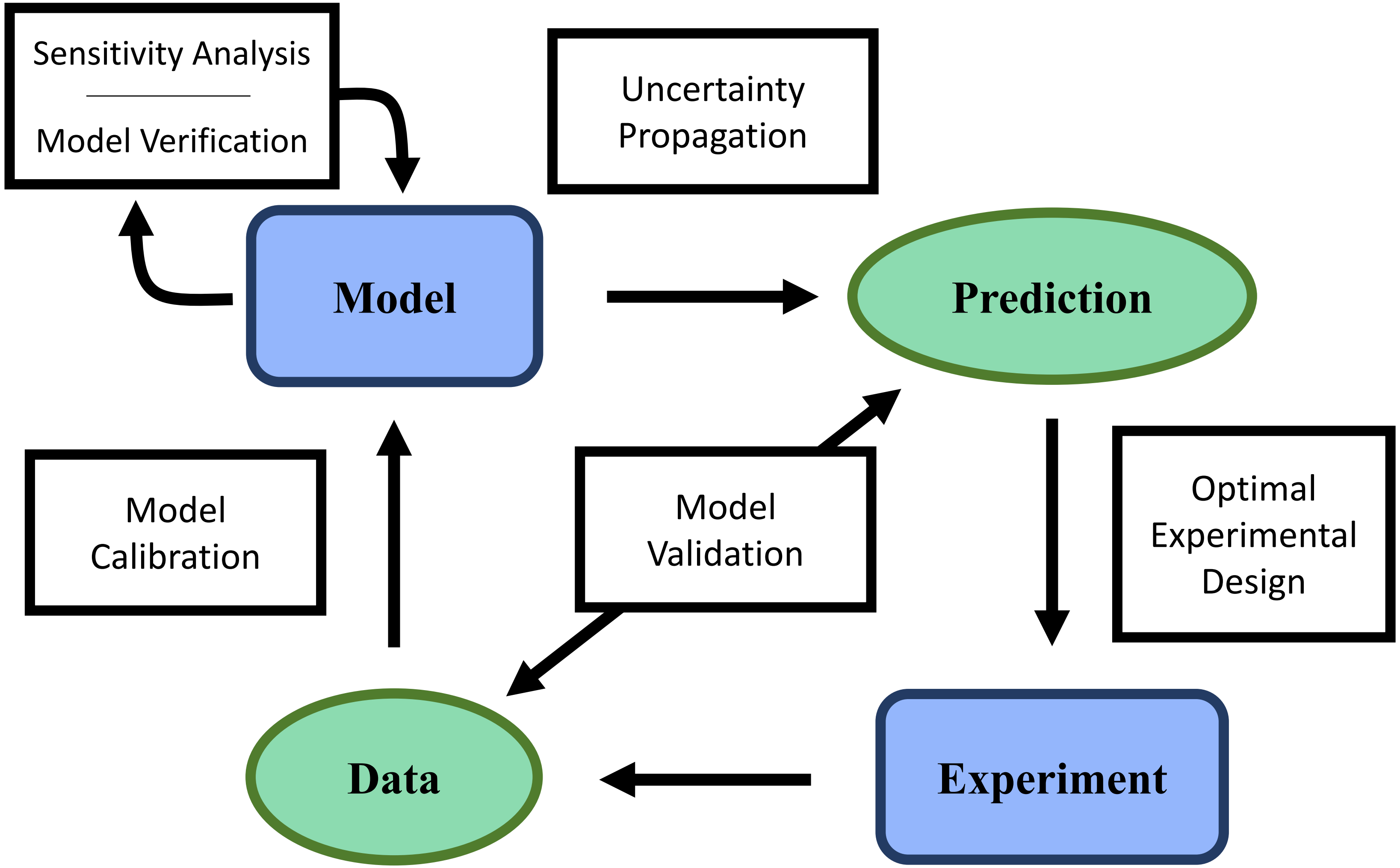

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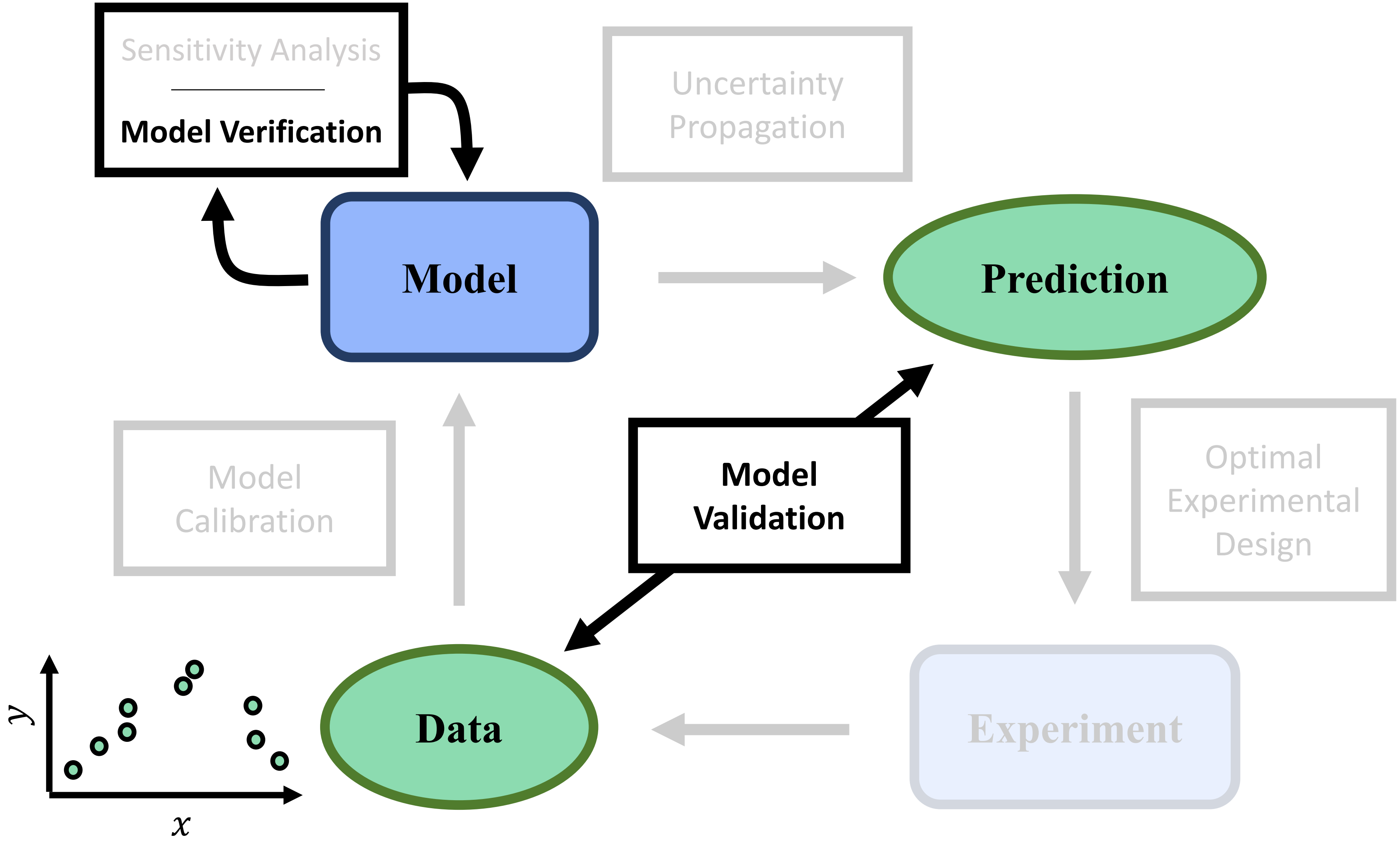


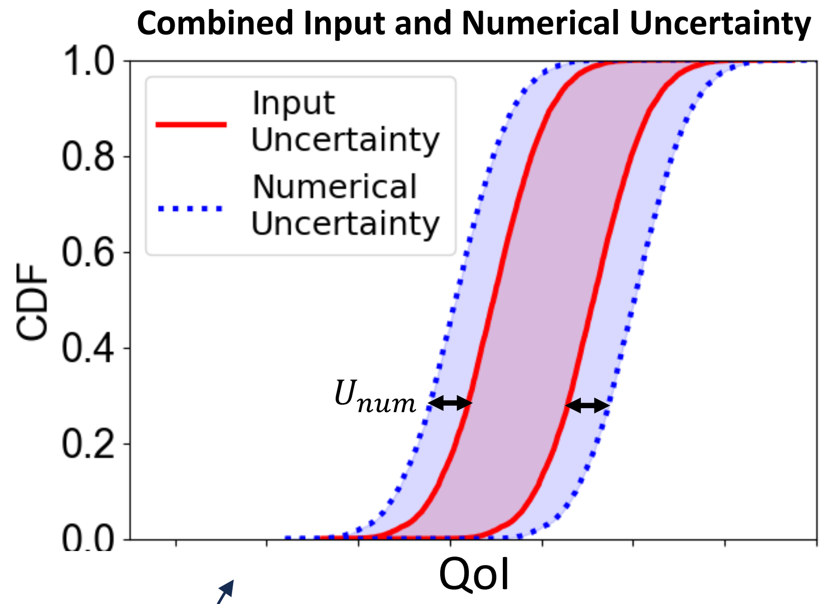
Verification & Validation

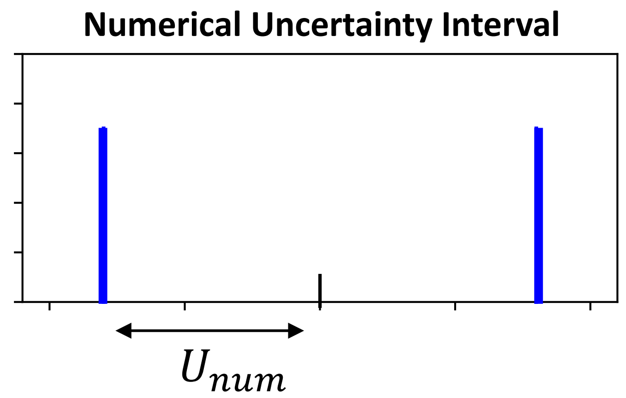
- Verification: The process of determining that a computational model accurately represents the underlying mathematical model and its solution [1].
  - *Are we solving the equations correctly?*
- Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model [1].
  - *Are we solving the correct equations?*
- Verification deals with mathematics while validation deals with physics [2].

1. Schwer, L. E. "Guide for verification and validation in computational solid mechanics. Engineering with Computers. 2007.
2. Roache, P. J. “Verification and validation in computational science and engineering”. Volume 895. Albuquerque, NM. 1998.

Model Verification

- **Goal**: ensure *numerical errors* are negligible relative to other uncertainties *or* quantify them and incorporate in uncertainty propagation
- **Sources of Error:**
  - Discretization (e.g., finite element size), iterative convergence (e.g., number of Monte Carlo samples), round-off error, software bugs
- **Approaches**:
  - Finite element mesh convergence studies
  - Extrapolation to estimate discretization error [1]
  - Software testing, code coverage tools
- Non-negligible numerical errors (U_{num}) are typically treated as epistemic uncertainty

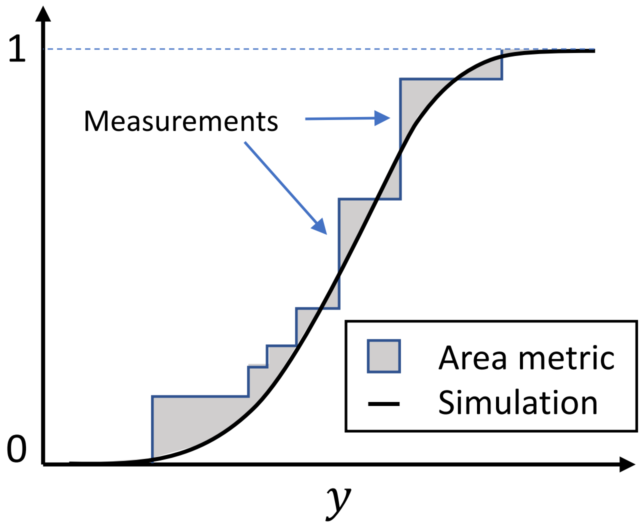




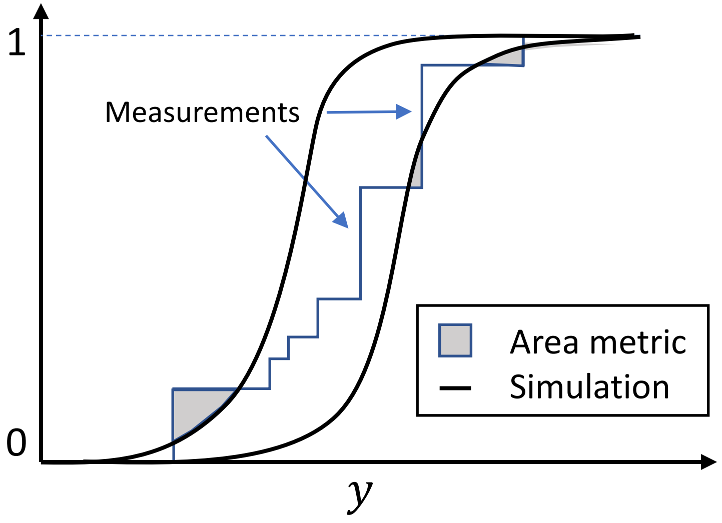
[1] P.J. Roache, Verification and Validation in Computational Science and Engineering, Hermosa Publishers, Albuquerque, New Mexico, 1998.

Model Validation (1/2)

Validation metric based on experiment CDF and simulation **CDF**



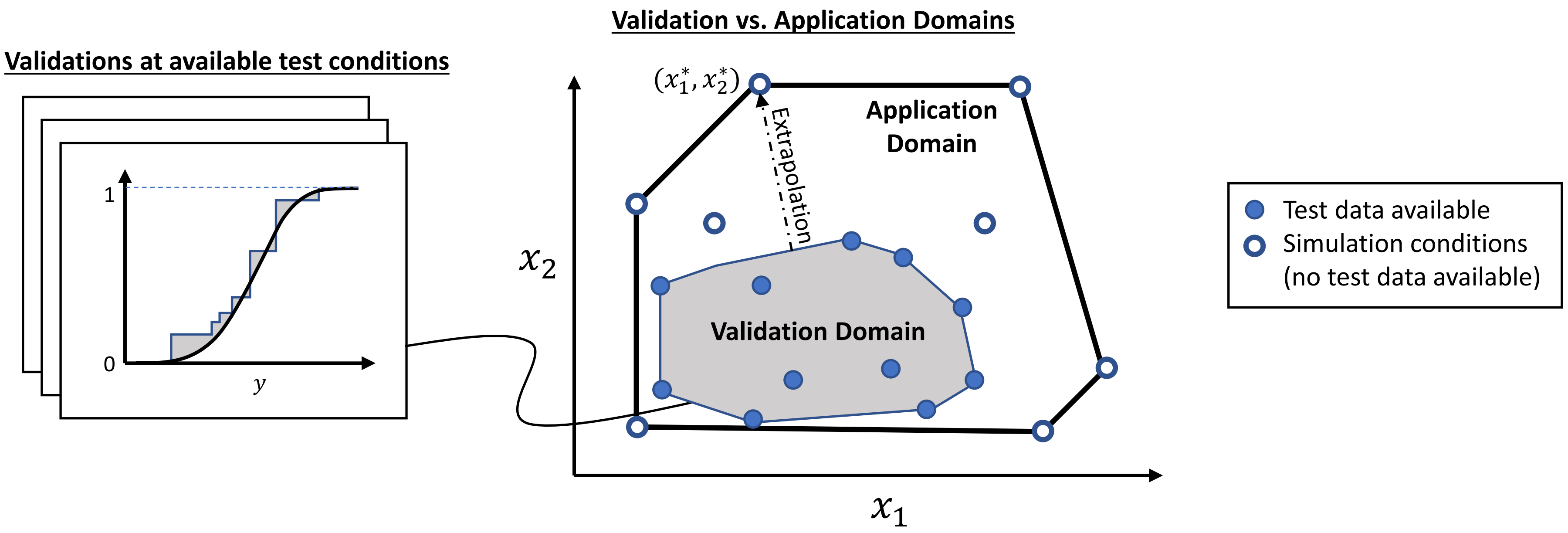
Validation metric based on experiment CDF and simulation **p-box**



➢ VVUQ approach [1]:
- The area of mismatch between simulated and empirical CDFs can serve as an error metric for model validation

1. Roy, Christopher J., and William L. Oberkampf. "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing." *Computer methods in applied mechanics and engineering* 200.25-28 (2011): 2131-2144.

Model Validation (2/2)



- VVUQ approach [1]:
  - The area of mismatch between simulated and empirical CDFs can serve as an error metric for model validation
  - Calculate validation error metric at series of points in validation domain & build regressor to estimate model form uncertainty in application domain
- Requires estimation of CDF (or p-box) for simulation output, which requires UQ

1. Roy, Christopher J., and William L. Oberkampf. "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing." *Computer methods in applied mechanics and engineering* 200.25-28 (2011): 2131-2144.

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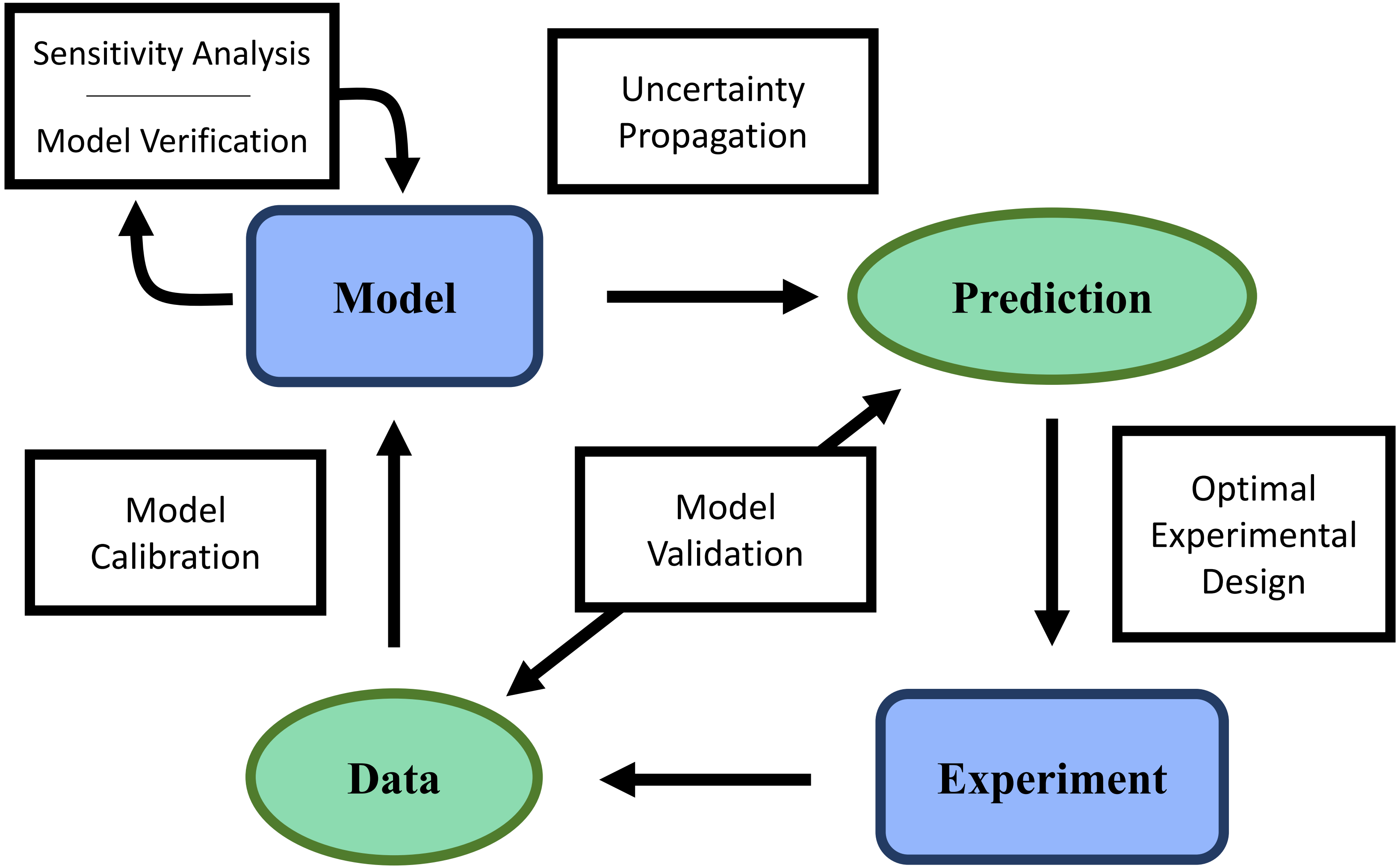

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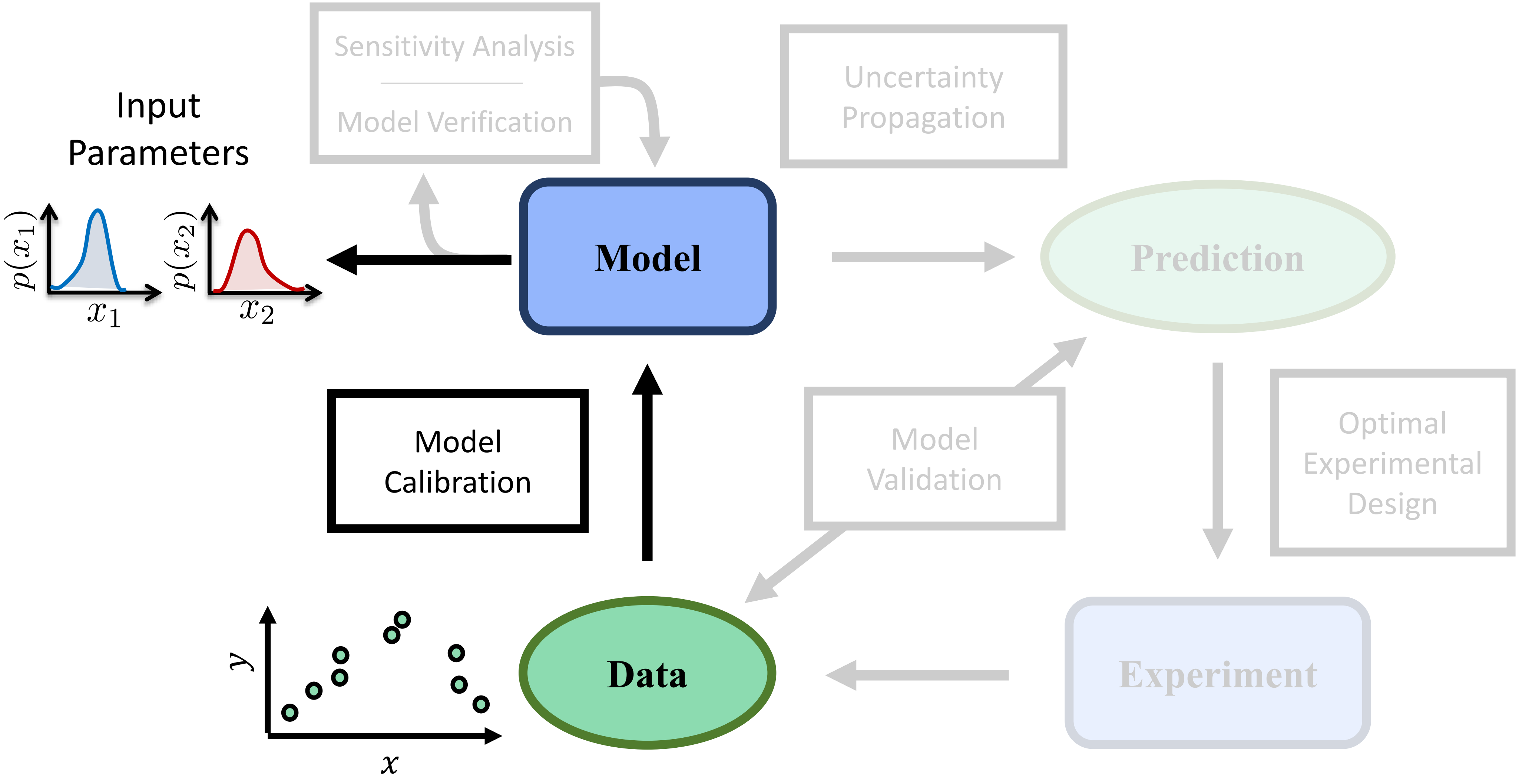
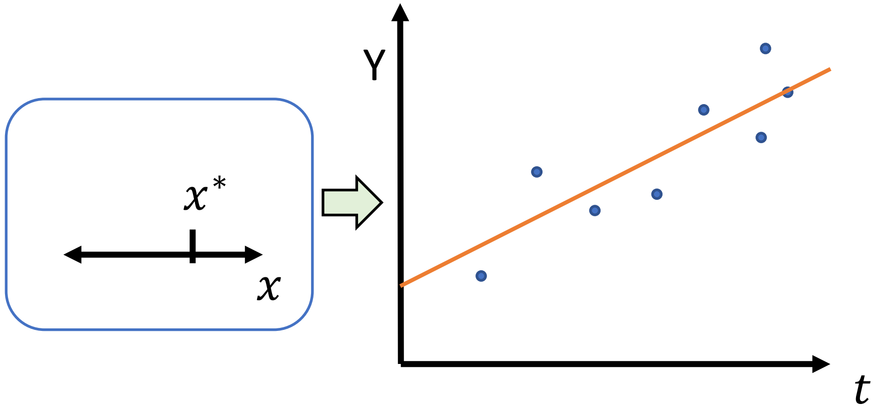


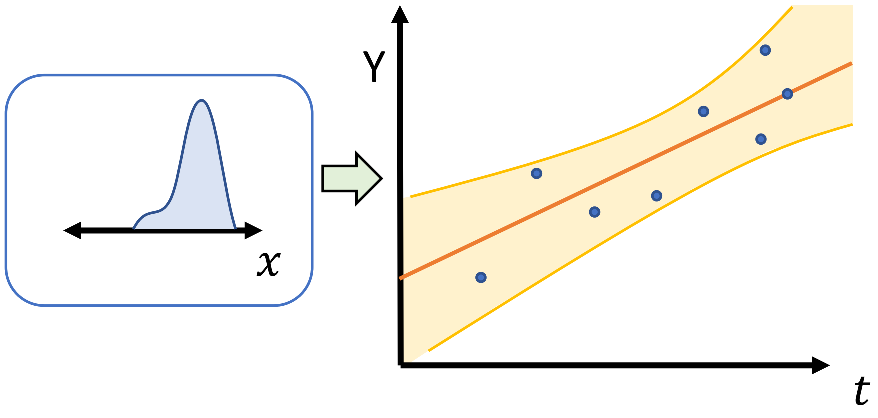
Deterministic vs. Probabilistic Calibration

- Assume:
  - $D = \mathcal{E}(\boldsymbol{x}; \boldsymbol{\epsilon})$ is measurement data from experiment, $\mathcal{E}$, with measurement error/noise, $\boldsymbol{\epsilon}$
  - $Y_{\mathcal{E}} = \mathcal{M}_{\mathcal{E}}(\boldsymbol{x})$ is a computational model that predicts the measured quantity from the experiment

- Deterministic calibration:
  Find deterministic parameters that result in best agreement by minimizing some error metric; e.g., sum of squared error, $SSE = \sum_i (Y_{\mathcal{E},i} - D_i)^2$



- Probabilistic calibration:
  Find a PDF, $p(x|D)$, assigning probability density to all potential values of the parameters based on the observed data and accounting for noise $\boldsymbol{\epsilon}$

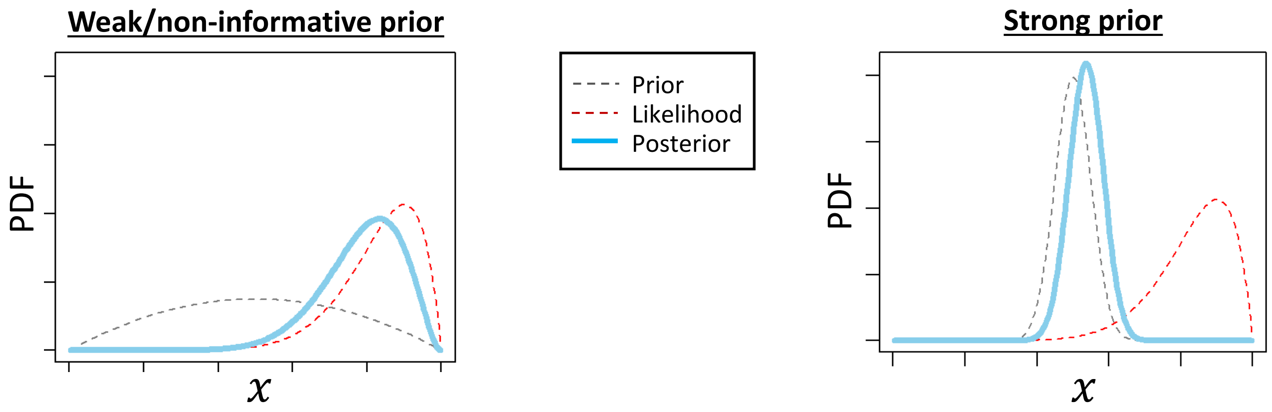


Probabilistic Calibration

"Find a PDF, $p(x|D)$, assigning probability density to all potential values of the parameters based on the observed data and accounting for noise $\boldsymbol{\epsilon}$"

How does this work in practice?

- Formulate such that $p(x|D)$ is high when error, $||Y_{\mathcal{E}} - D||$, is low and vice versa
  - Typically implemented as a *Bayesian inference* problem
  - Starts with an initial guess for uncertainty (*prior distribution*) then updates it using the measurement data (using a *likelihood function*) to acquire a *posterior distribution*.

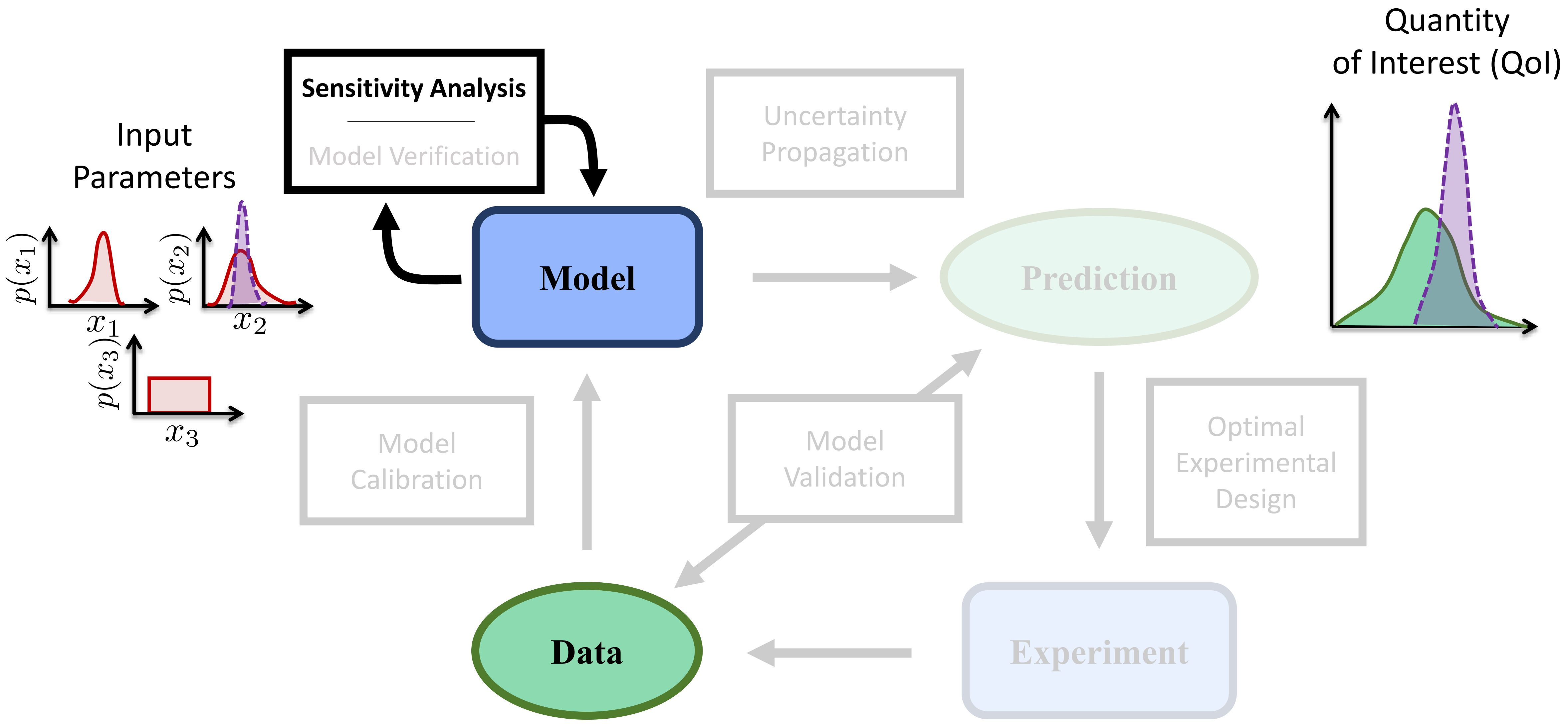


✓ The calibrated PDF $p(x|D)$ naturally includes estimates of *correlations*

✓ Less data = more uncertainty; more data = less uncertainty

✓ Variety of well-established methods exist for performing probabilistic calibration

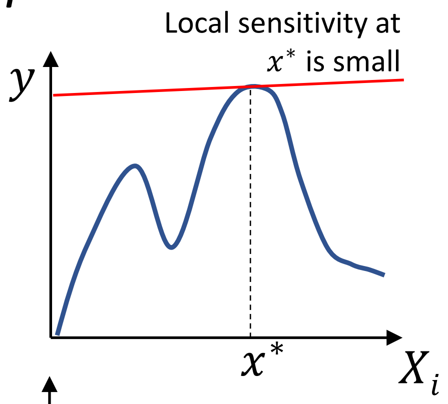
Components of a UQ Analysis

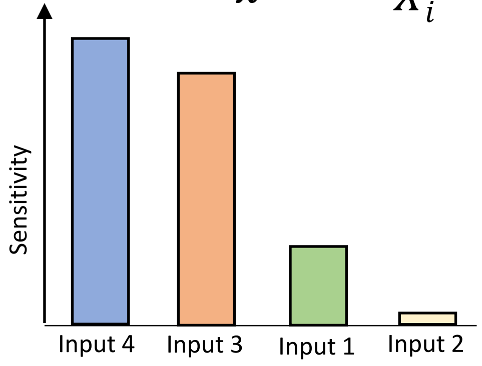


Sensitivity Analysis

*How uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input**

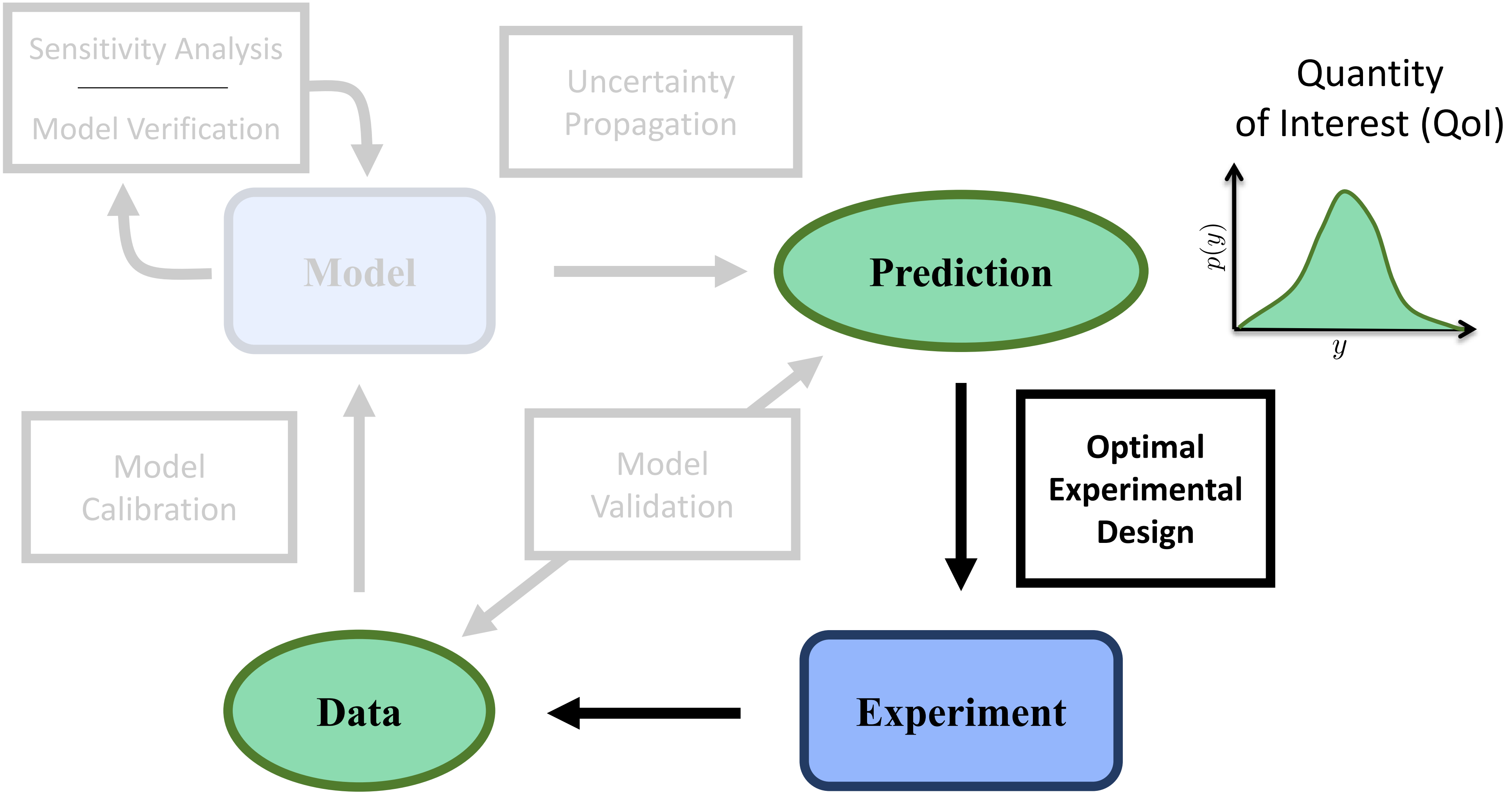
- Local sensitivity analysis – based on derivatives, $\frac{\partial Y}{\partial X_i}|_{X=x^*}$
  - Computationally efficient
  - Does not consider input uncertainty, global model non-linearity
- Global sensitivity analysis
  - More computationally expensive
  - Holistically assesses effect of uncertainty & model behavior
  - Used to reduce dimensionality or inform additional experiments





*Global sensitivity analysis. The primer. Andrea Saltelli. 2007.

Components of a UQ Analysis

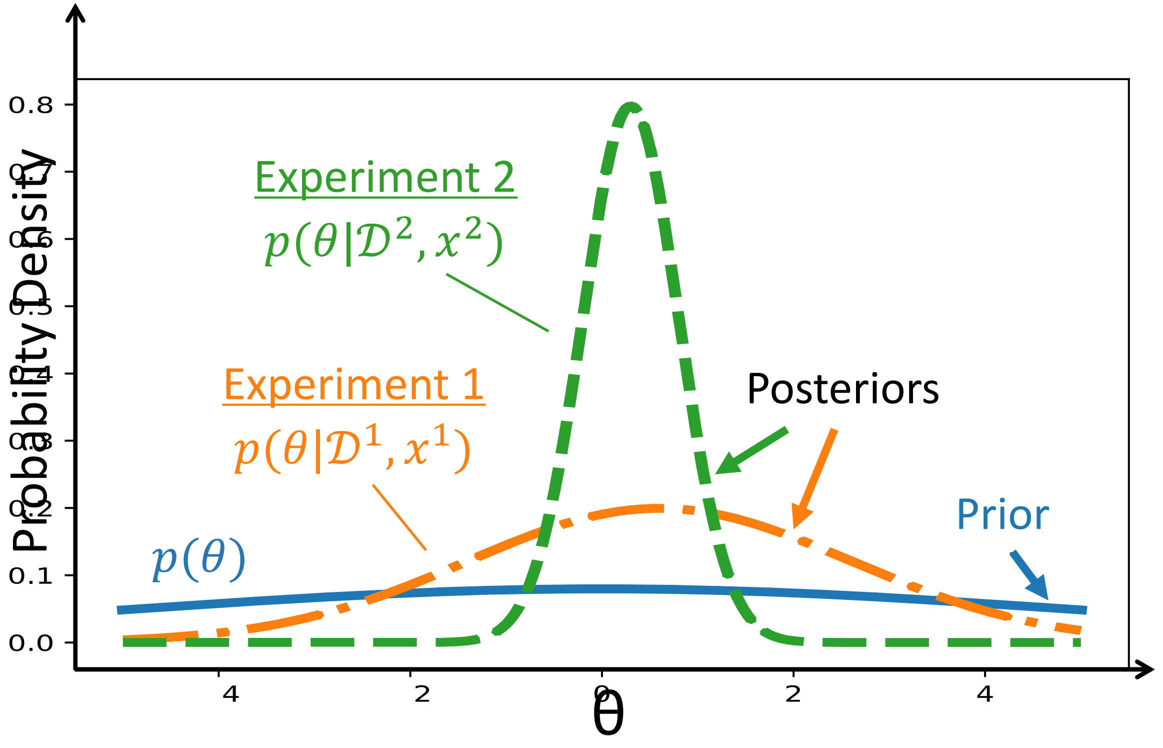


Optimal Experimental Design (OED)

Determining the most effective tests to run under resource constraints

- Select an experimental design that maximizes a statistical criteria depending on the testing goals
- Potential use cases
  - Uncertainty propagation: maximizing precision of probabilistic model predictions
  - Model validation: discriminating between multiple candidate models
  - Model calibration: minimizing uncertainty in unknown model parameters

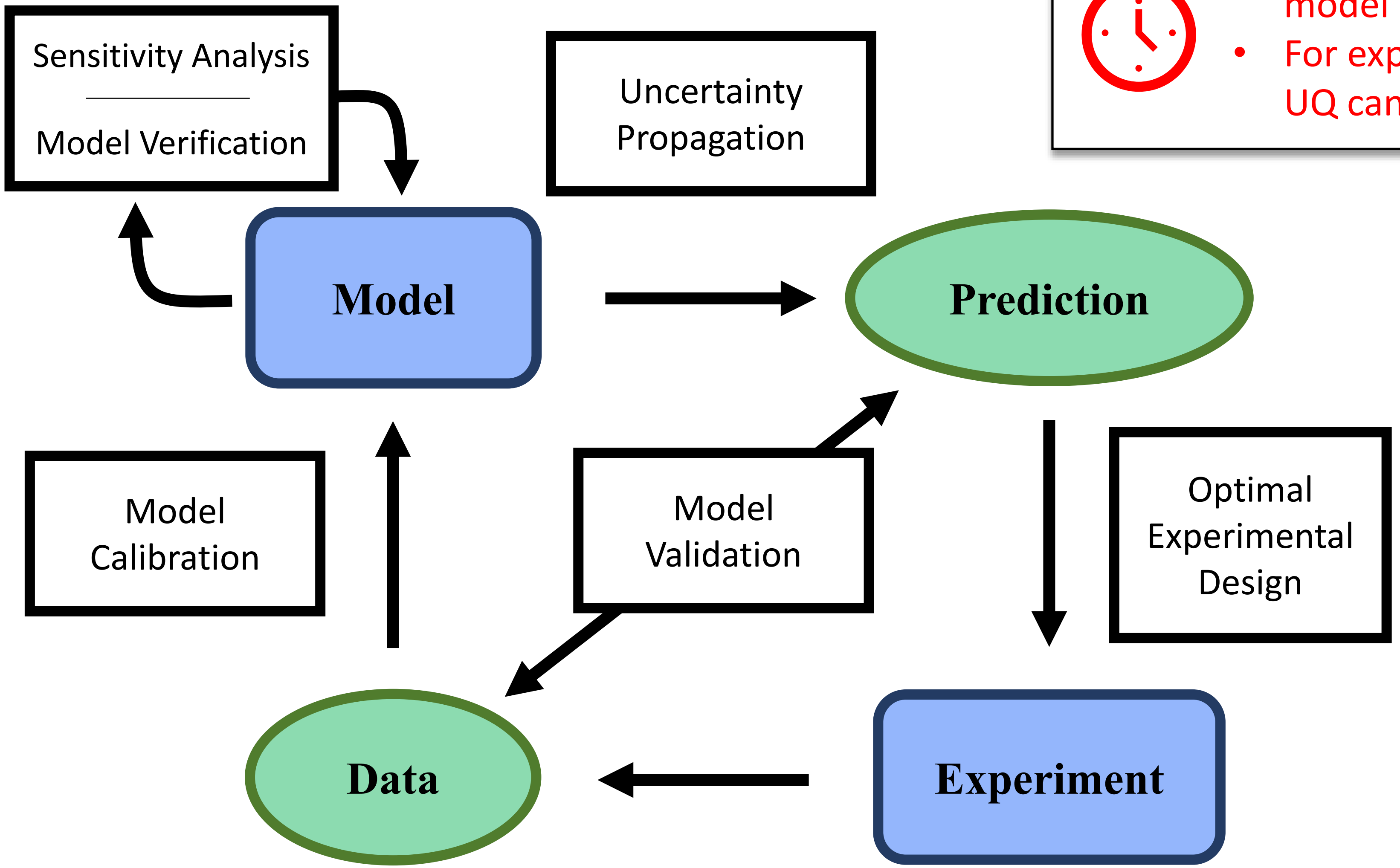
Notional OED for Model Calibration



➢ Experiment 2 is more effective than experiment 1

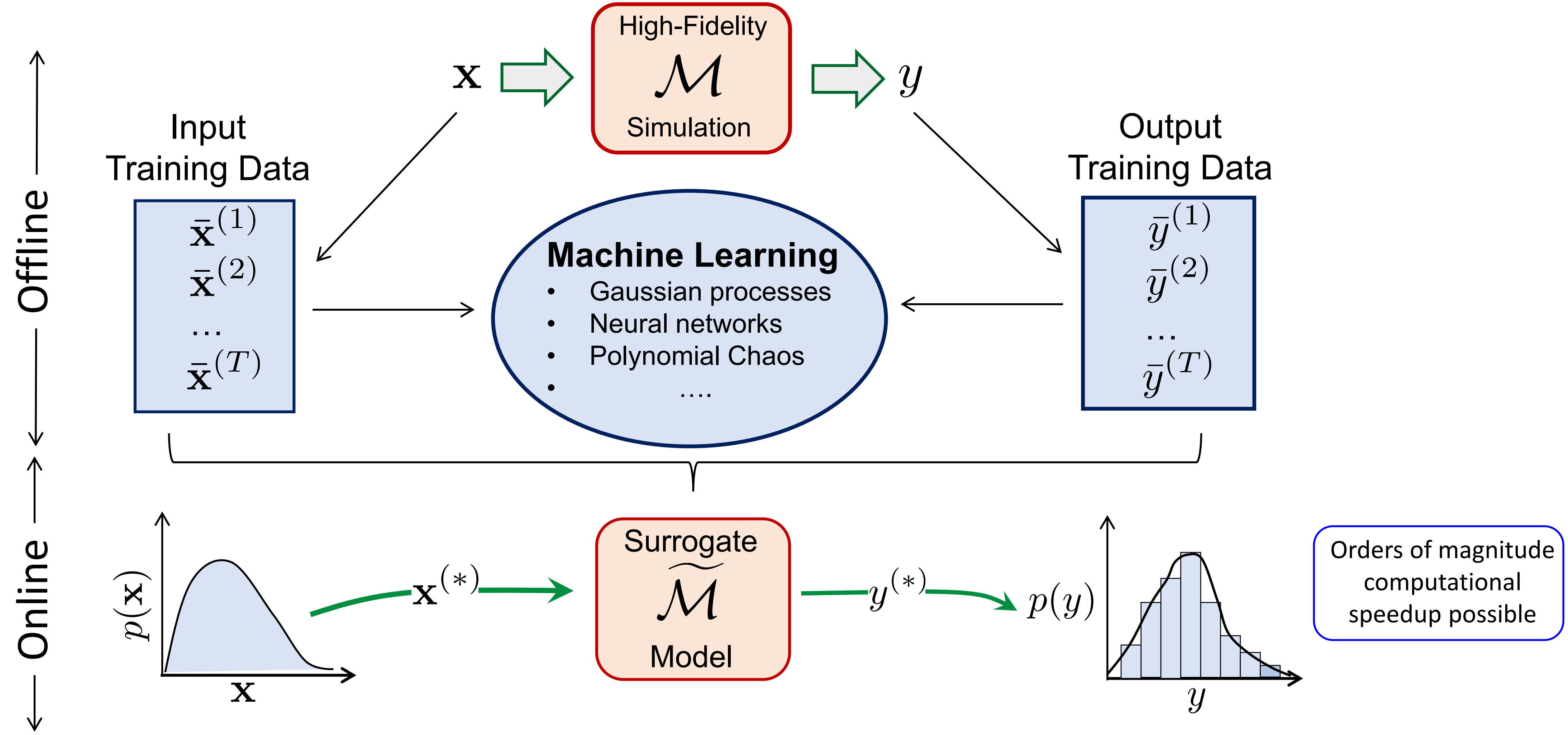
Components of a UQ Analysis

- UQ can require $\gg 10^3$ model evaluations
- For expensive models, UQ can be intractable



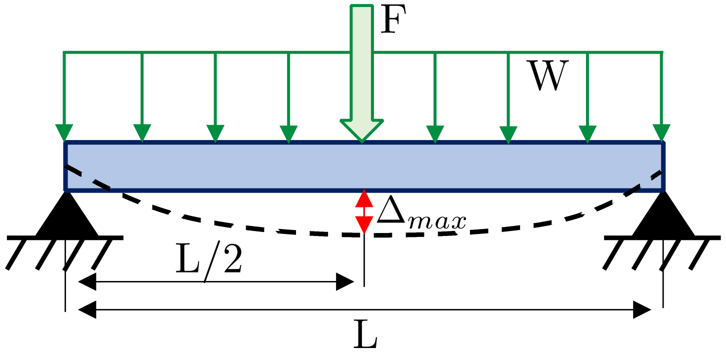
Surrogate Modeling for Computational Speedup

Overcoming computational burden when the model is expensive



➢ **Note**: Both the high-fidelity and surrogate model must be validated.

Example: Beam with Uncertain Loading/Geometry



EI = fixed/known
= 1.33 x 10^7 lb·in^2

- Assumptions:
  - Stiffness and moment of inertia are known with negligibly small uncertainty
  - Precise estimates for PDFs of loads (F, W) and manufactured beam length (L) are available based on measurement data
  - Beam fails when $\Delta_{max} > 0.52in$
- "Computational model":
  - $\Delta_{max} = M(L, F, W) = \frac{FL^3}{48EI} + \frac{5WL^4}{384EI}$
- Goal:
  - Use Monte Carlo simulation to estimate probability of failure, $P_f \equiv P(\Delta_{max}$>0.52in)
  - Demonstrate results for different treatments of epistemic uncertainty

Case 1: Reliability of a Future Beam Design

Input Parameter Uncertainty

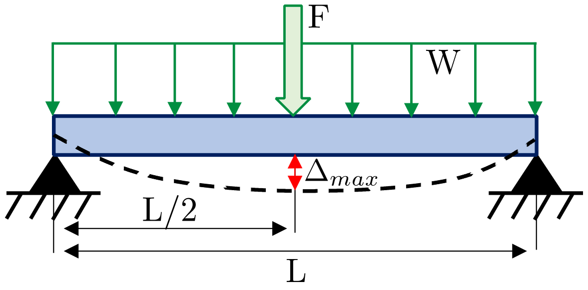
Beam length – aleatory

$L \sim \mathrm{N}(\mu_L = 36, \sigma_L = 0.25)\ in$

Loads – aleatory:

$F \sim \mathrm{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

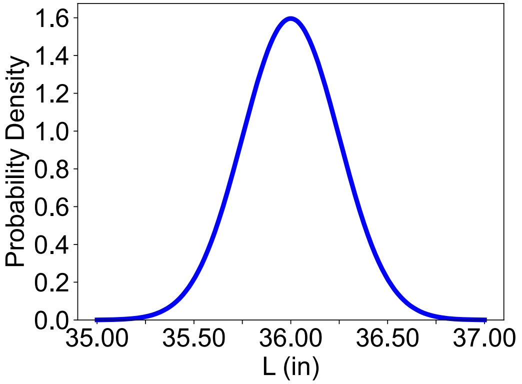
$W \sim \mathrm{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



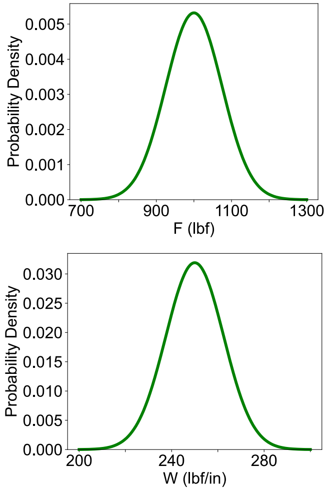
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Approach**: standard Monte Carlo simulation with 10000 random samples

Beam Length PDF



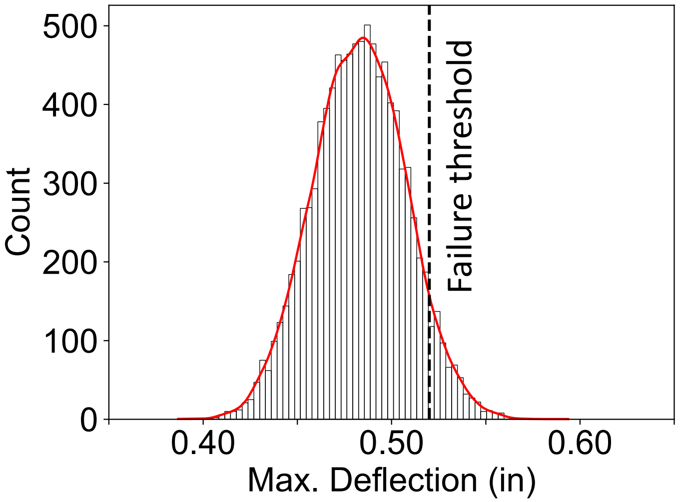
Load PDFs



Computational Model

$$\Delta_{max} = M(L, F, W)$$

Max. Deflection Histogram



➢ Probabilistic and interval approaches are the same (no epistemic uncertainties)

Case 1: Reliability of a Future Beam Design

Input Parameter Uncertainty

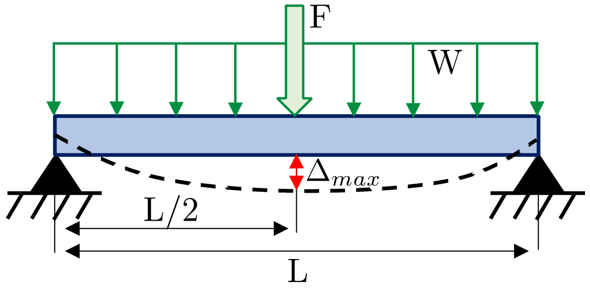
<u>Beam length – aleatory</u>

$L \sim N(\mu_L = 36, \sigma_L = 0.25)\ in$

<u>Loads – aleatory:</u>

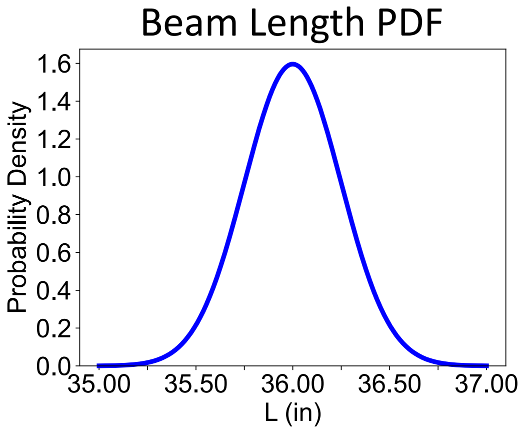
$F \sim N(\mu_F = 1000, \sigma_F = 75)\ lbf$

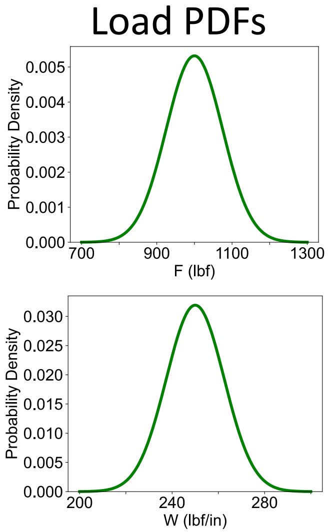
$W \sim N(\mu_W = 250, \sigma_W = 12.5)\ lbf$



EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Approach**: standard Monte Carlo simulation with 10000 random samples



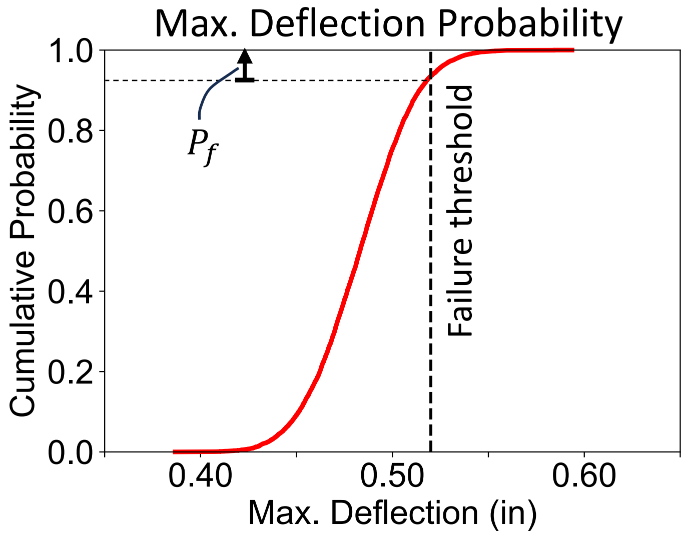


Computational Model

$\Delta_{max} = M(L, F, W)$

Probability of Failure Estimate

$P_f \approx 7.0\%$



➢ Probabilistic and interval approaches are the same (no epistemic uncertainties)

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

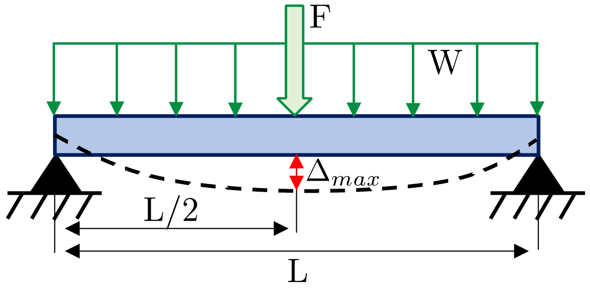
<u>Beam length – **epistemic**</u>

$L \sim \mathrm{N}(\mu_L = 36, \sigma_L = 0.25)\ in$

<u>Loads – aleatory:</u>

$F \sim \mathrm{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

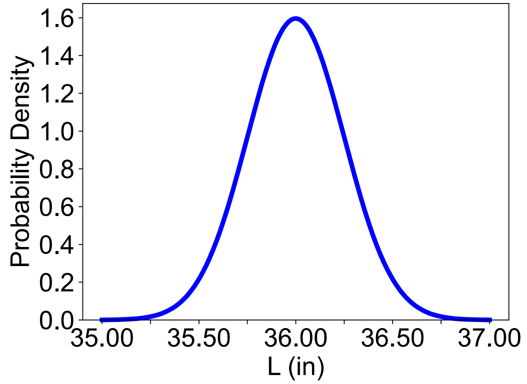
$W \sim \mathrm{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



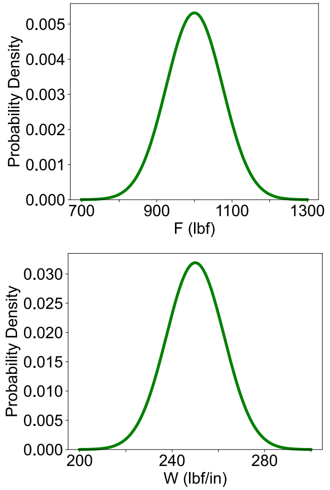
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Probabilistic approach**: Monte Carlo simulation with 10000 random samples

Beam Length PDF



Load PDFs

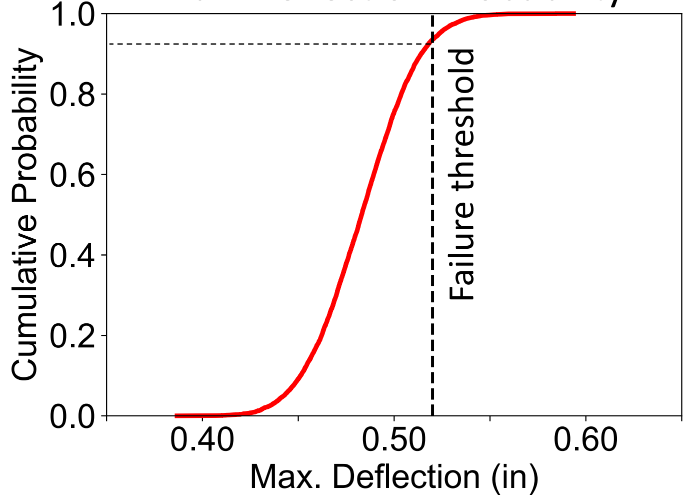


Computational Model

$$\Delta_{max} = M(L, F, W)$$

Probability of Failure Estimate
$P_f \approx 7.0\%$

Max. Deflection Probability



➢ Probabilistic approach remains the same for case 2; Beam length PDF represents our degree of belief in the true length based on manufacturing data

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

<u>Beam length – **epistemic**</u>

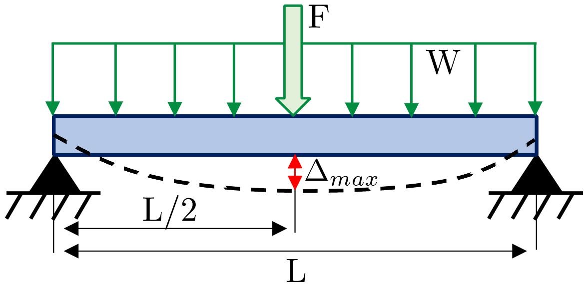
$L \sim \text{Interval}[35.25, 36.75]in$

(**Assumption**: μ_L +/- 3 σ_L)

<u>Loads – aleatory:</u>

$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

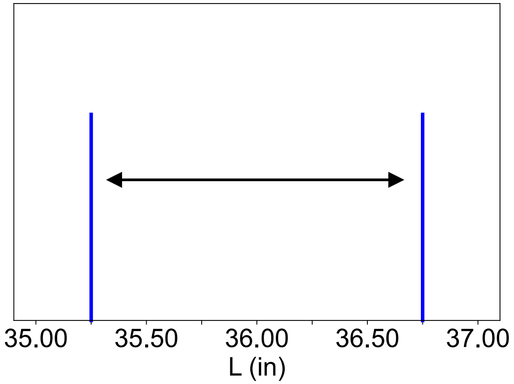
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



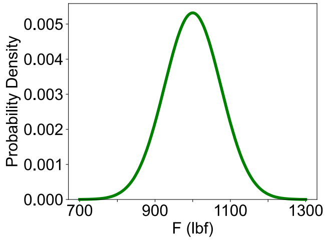
EI = fixed/known
= 1.33 x 10^7 lb·in^2

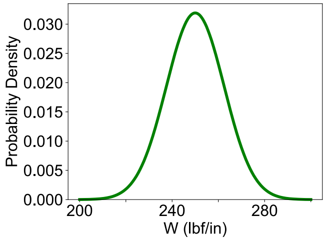
- **Interval approach**: Double loop Monte Carlo simulation with 100 outer loop samples and 10000 inner loop samples

Beam Length Interval



Load PDFs





Computational Model

$$\Delta_{max} = M(L, F, W)$$

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

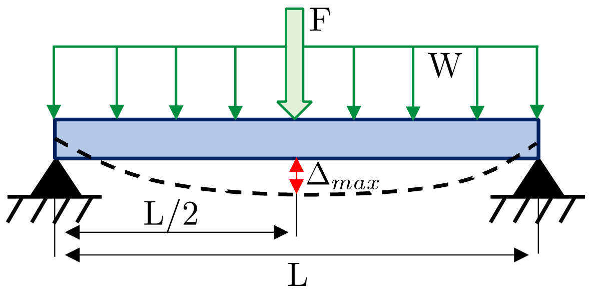
<u>Beam length – **epistemic**</u>

$L \sim \text{Interval}[35.25, 36.75]in$

<u>Loads – aleatory:</u>

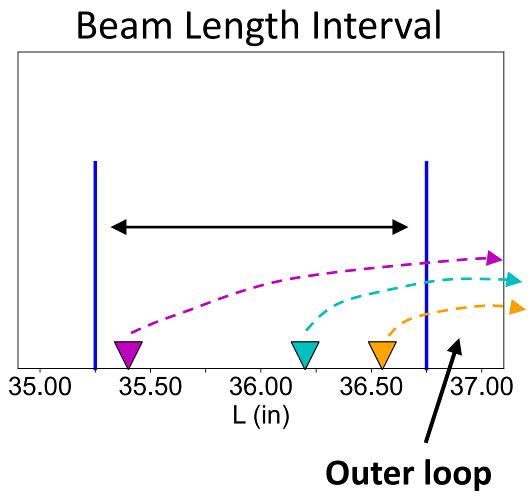
$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

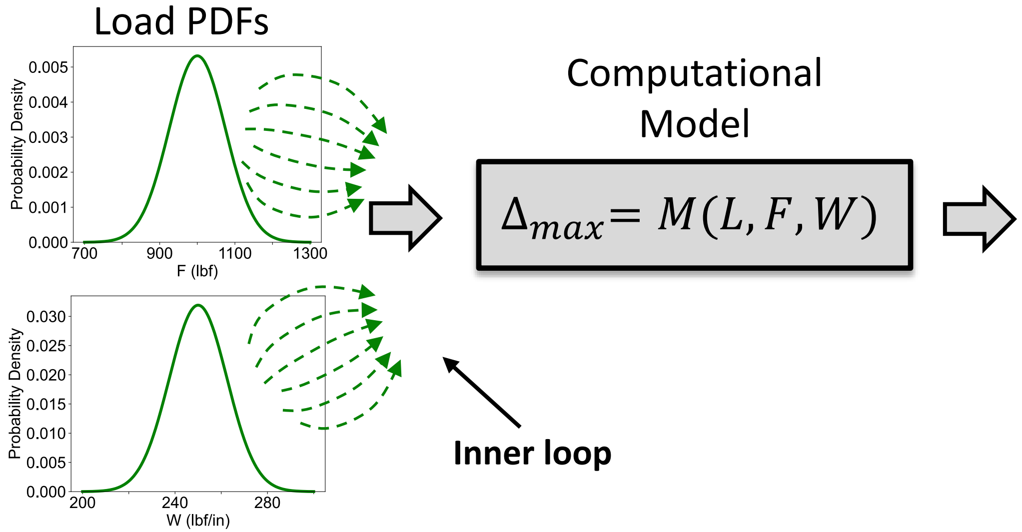
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$

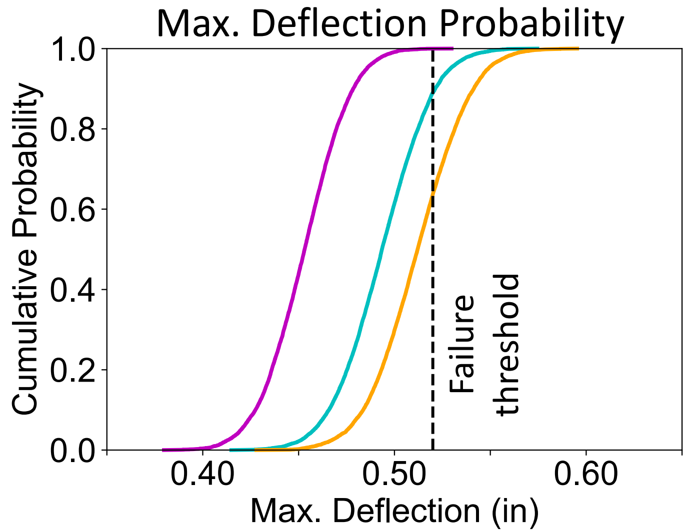


EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Interval approach**: Double loop Monte Carlo simulation with 100 outer loop samples and 10000 inner loop samples







Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

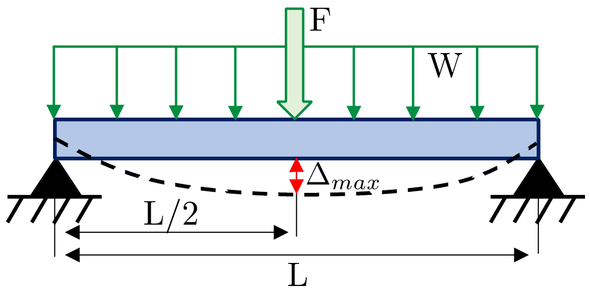
Beam length – **epistemic**

$L \sim \text{Interval}[35.25, 36.75]\,in$

Loads – aleatory:

$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

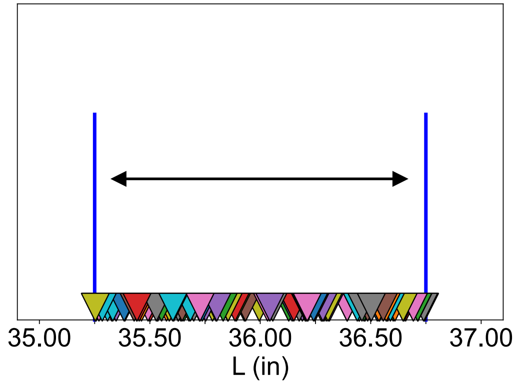
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



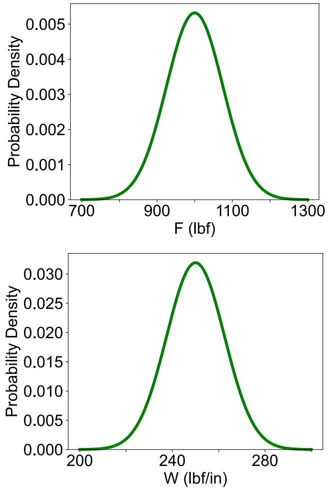
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Interval approach**: Double loop Monte Carlo simulation with 100 outer loop samples and 10000 inner loop samples

Beam Length Interval



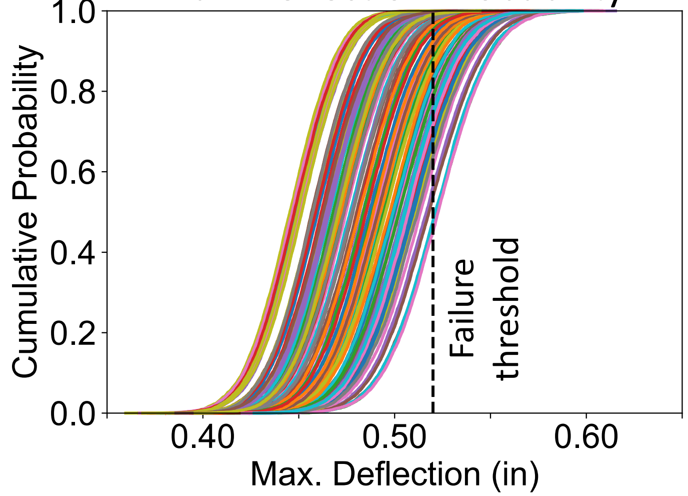
Load PDFs



Computational Model

$$\Delta_{max} = M(L, F, W)$$

Max. Deflection Probability



Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

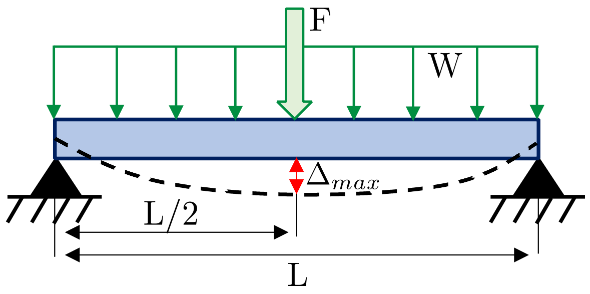
<u>Beam length – **epistemic**</u>

$L \sim \text{Interval}[35.25, 36.75] in$

<u>Loads – aleatory:</u>

$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

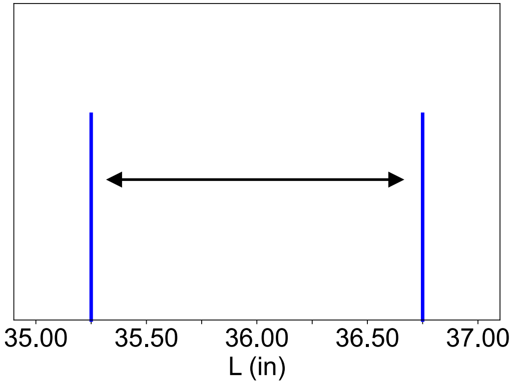
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



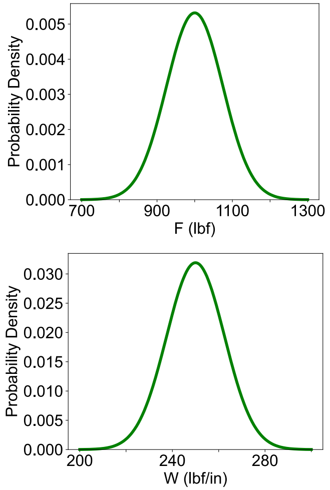
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- **Interval approach**: Double loop Monte Carlo simulation with 100 outer loop samples and 10000 inner loop samples

Beam Length Interval



Load PDFs



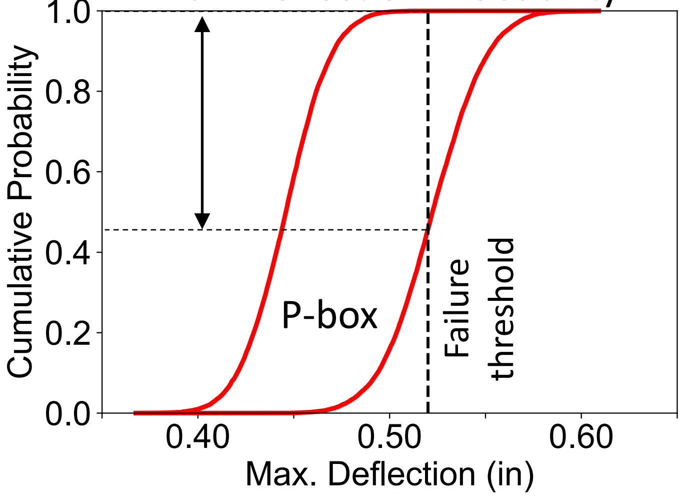
Computational Model

$\Delta_{max} = M(L, F, W)$

Probability of Failure Estimate

$P_f \approx [0.0, 54.3]\%$

Max. Deflection Probability



➢ Interval approach provides more conservatism: if P_f can be as large as 54.3% in the worst case, then this is the value that will be used for engineering decisions

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

<u>Beam length – **epistemic**</u>

$L \sim \text{Interval}[35.25, 36.75]in$

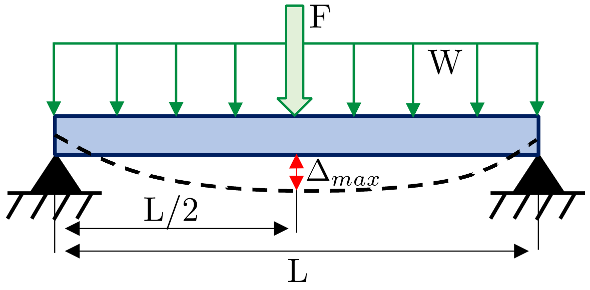
Vs.

$L \sim \text{Uniform}[35.25, 36.75]in$

<u>Loads – aleatory:</u>

$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

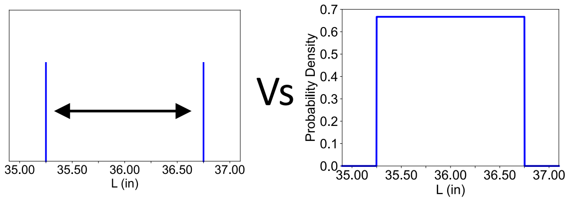
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



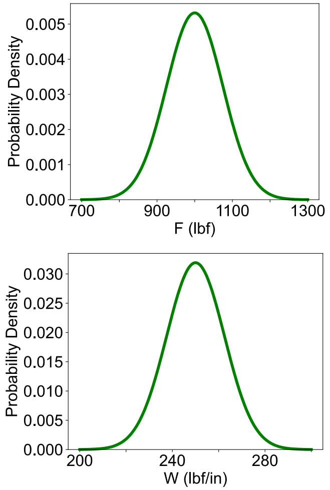
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- Compare interval approach with a probabilistic approach that assumes a uniform PDF on beam length

Beam Length Interval
Vs. Uniform PDF



Load PDFs



Computational
Model

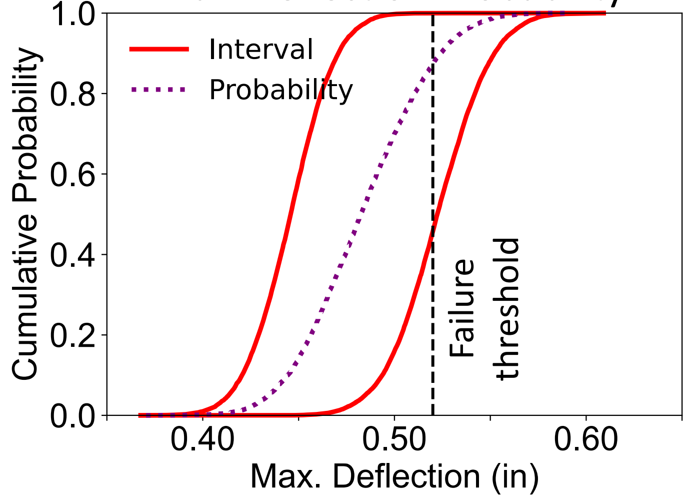
$$\Delta_{max} = M(L, F, W)$$

Probability of Failure Estimates

Interval: $P_f \approx [0.0, 54.3]\%$

Probabilistic: $P_f \approx 12.6\%$

Max. Deflection Probability



➢ Propagating interval ≠ propagating a uniform PDF (but neither answer is right or wrong)

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

<u>Beam length – **epistemic**</u>

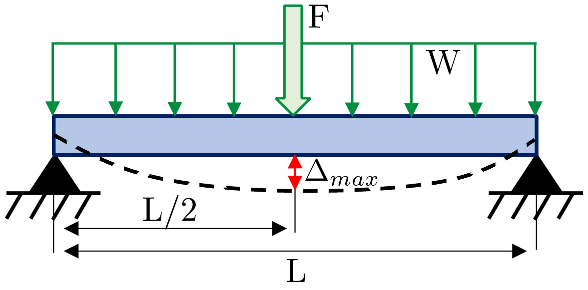
$L \sim \text{Interval}[35.9, 36.1]in$

Measurement: 36” +/- 0.1”

<u>Loads – aleatory:</u>

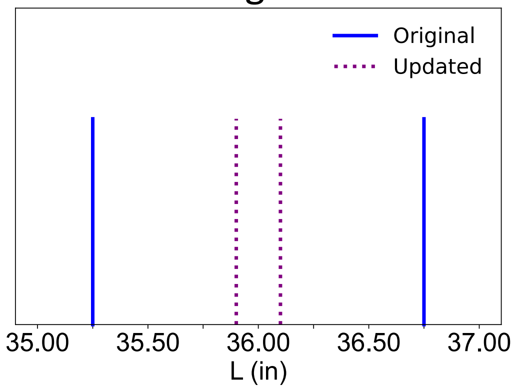
$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

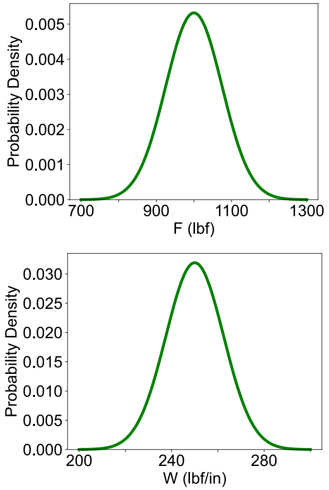
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



EI = fixed/known
= 1.33×10^7 lb·in^2

- Compare results from the original and updated beam length intervals based on new measurement





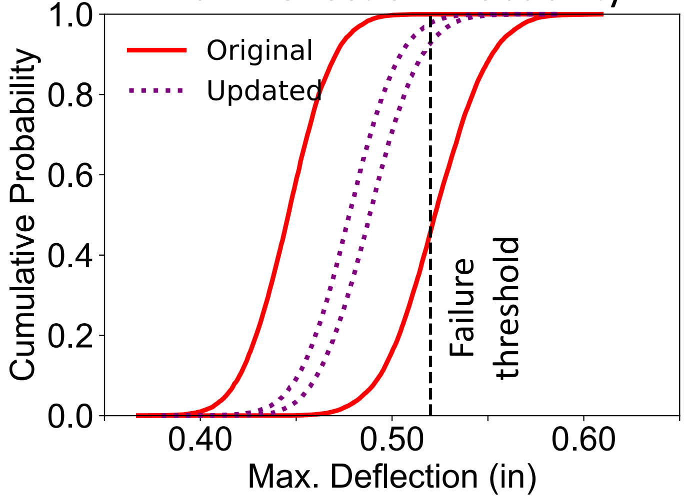
Computational Model

$$\Delta_{max} = M(L, F, W)$$

Probability of Failure Estimates

Original: $P_f \approx [0.0, 54.3]\%$

Updated: $P_f \approx [2.1, 6.8]\%$



➢ P-box width shows reduction in epistemic uncertainty from gaining additional knowledge

Case 2: Reliability of a Single Fabricated Beam

Input Parameter Uncertainty

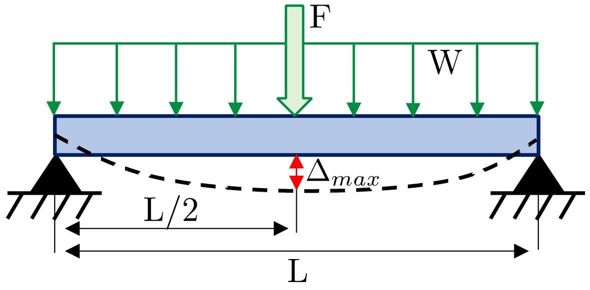
<u>Beam length – **epistemic**</u>

$L \sim \text{Interval}[35.9, 36.1]in$

<u>Loads – aleatory:</u>

$F \sim \text{N}(\mu_F = 1000, \sigma_F = 75)\ lbf$

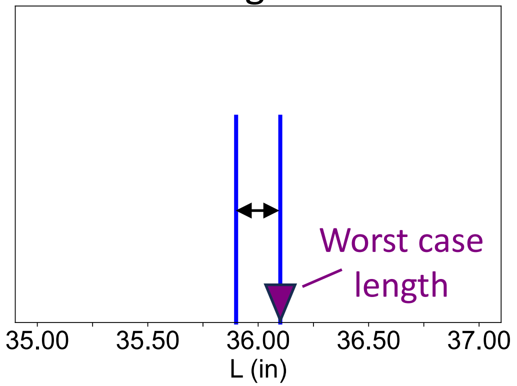
$W \sim \text{N}(\mu_W = 250, \sigma_W = 12.5)\ lbf$



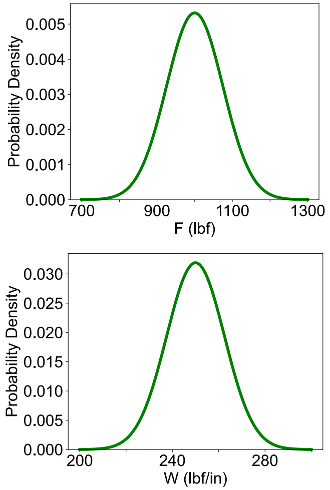
EI = fixed/known
= 1.33 x 10^7 lb·in^2

- Compare interval approach versus standard Monte Carlo approach with fixed, worst-case value for L

Beam Length Interval



Load PDFs



Computational Model

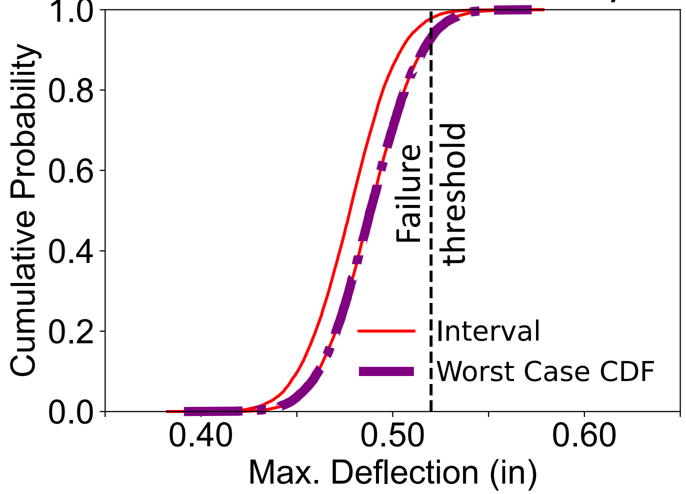
$\Delta_{max} = M(L, F, W)$

Probability of Failure Estimates

Interval: $P_f \approx [2.1, 6.8]\%$

Worst Case: $P_f \approx 6.9\%$

Max. Deflection Probability



➢ If a priori knowledge of worst-case input values is available, the conservative p-box bound can be directly recovered with standard Monte Carlo

Example: Comparison of Approaches

- **Probabilistic approach**
  - Provides a probabilistic quantification of an engineering belief
  - Requires assumptions on distributions
  - Allows for updating distributions based on new/available data, including correlation estimates
  - Can be unconservative
  - Difficult to apply to numerical errors
- **Interval / p-box approach**
  - Provides conservative bounds on probabilistic estimates
  - Requires assumptions on interval bounds
  - Effects of epistemic uncertainty indicated explicitly by p-box
  - Can be overly conservative
  - Can be more computationally intensive

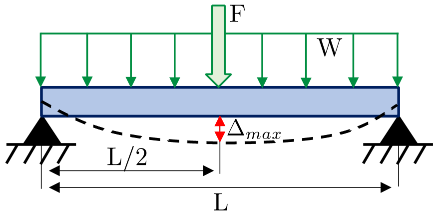
Example: Summary

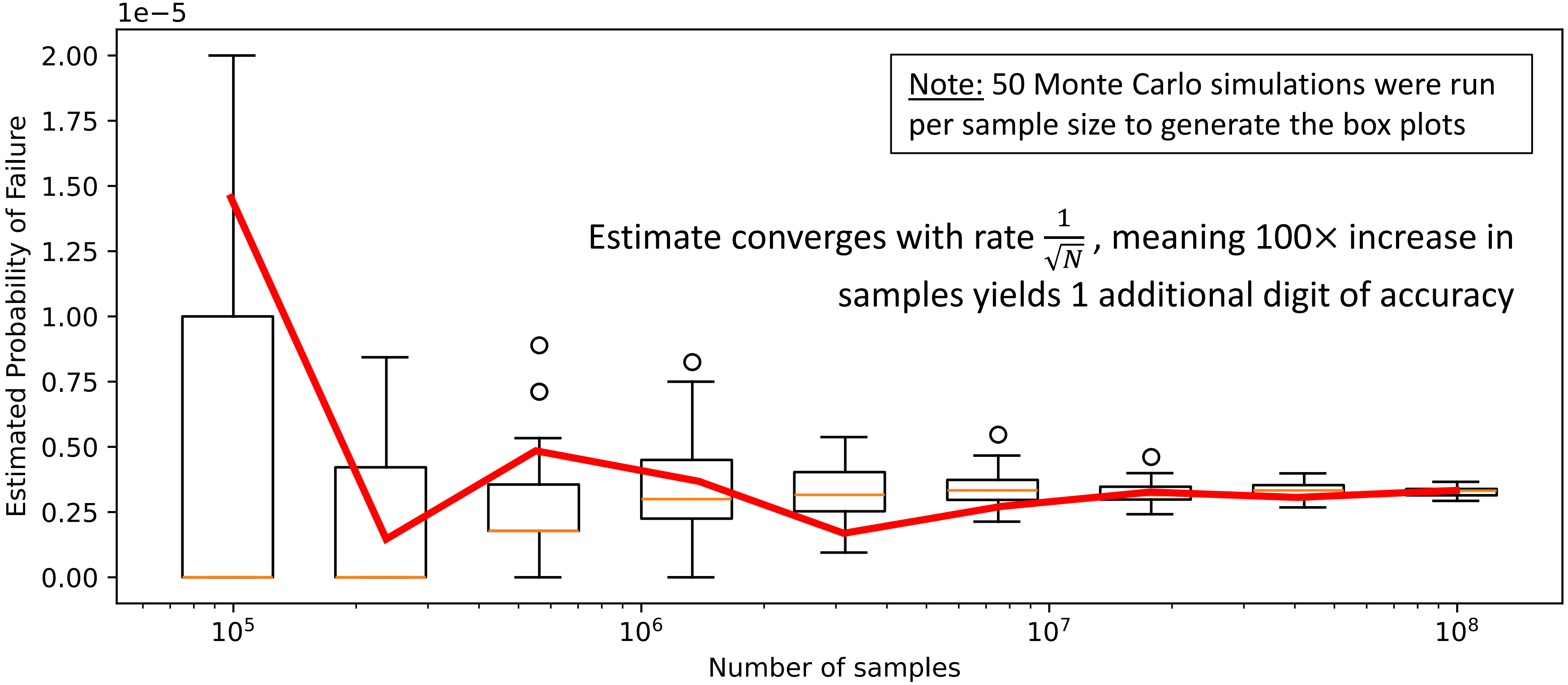
- There are effectively three ways to handle epistemic uncertainty:
  1. Represent as a probability → Use standard Monte Carlo*
  2. Represent as an interval → Use double loop Monte Carlo
  3. Fix at a conservative or worst-case value → Use standard Monte Carlo
- Approach #3 is equivalent to using an interval approach and taking the conservative bound of the p-box solution (but faster)
  - **Note:** this relies on *assumptions* of which input values are conservative
    - Becomes more difficult to specify as the number of inputs and the model complexity increases

Challenges and Best Practices

- **Rigor is key to successfully applying UQ in practice**
  - Probabilistic analyses have significantly increased complexity relative to deterministic analyses
  - Probabilistic results have an *aura of precision* → more responsibility on analyst to be rigorous and potentially modify approach on a case-by-case basis
- Some common pitfalls in practical UQ applications are related to sampling error, model errors, and input errors

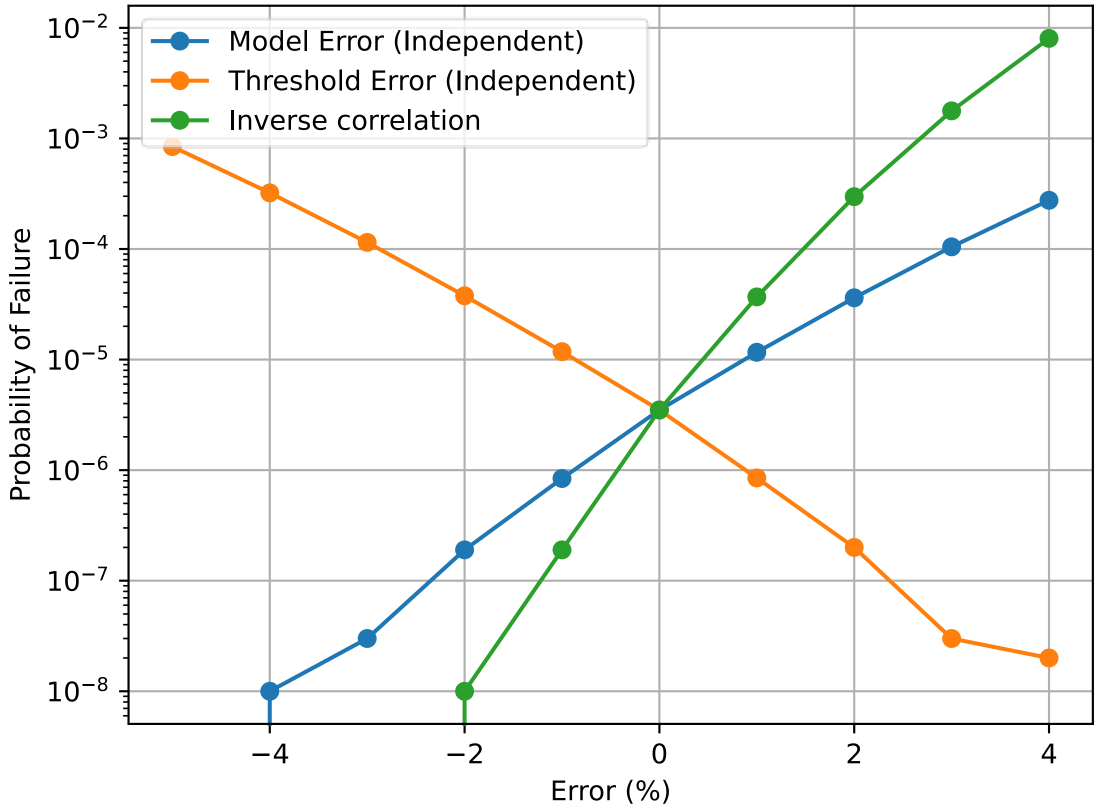
Sampling Error

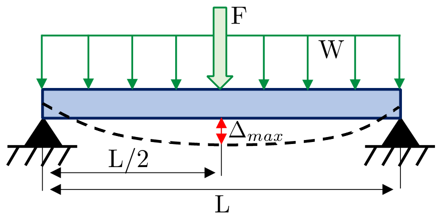




- ➢ Ensure that the number of samples used is appropriate for required accuracy and quantity being estimated.

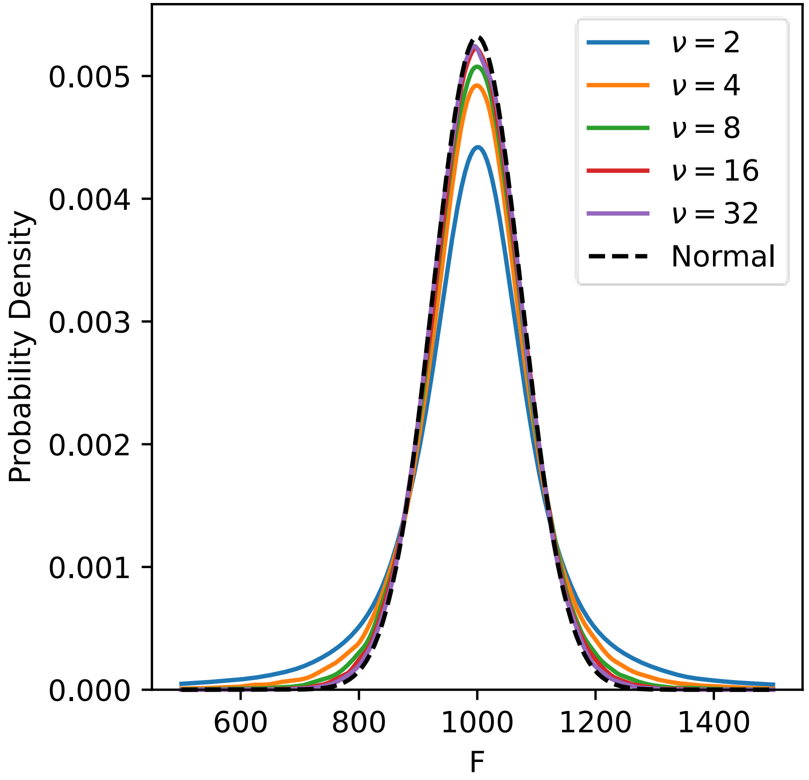
Model Errors

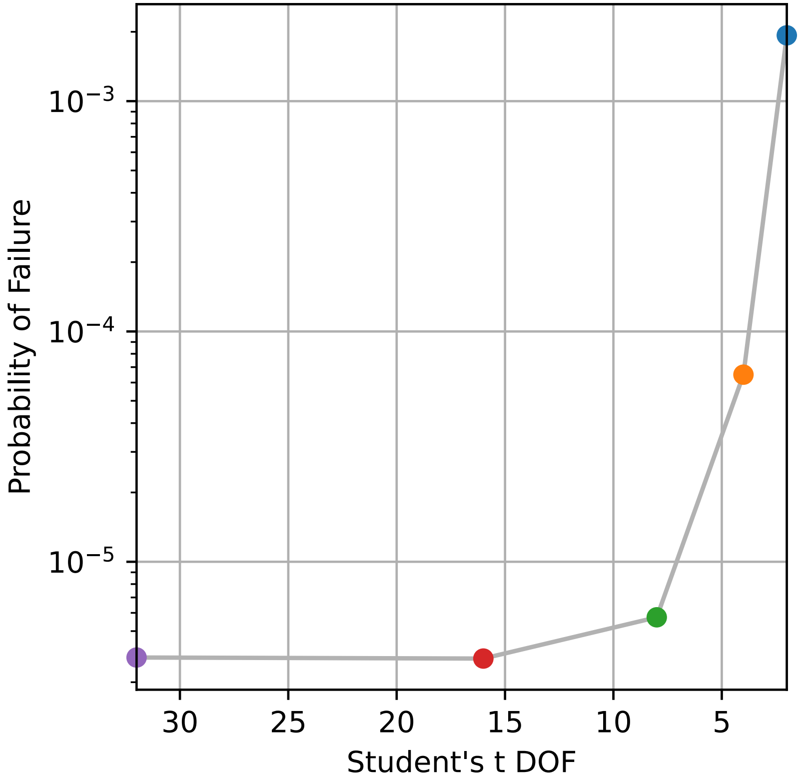


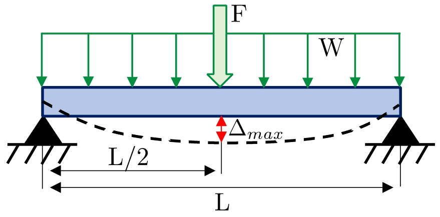


- ➢ Investigate sensitivity of any probabilistic result to error in model form and failure thresholds

Input Errors | *Fat Tails*

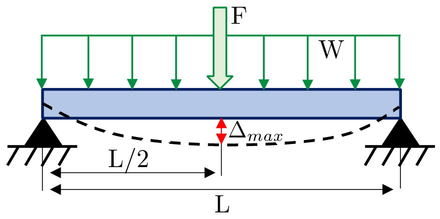


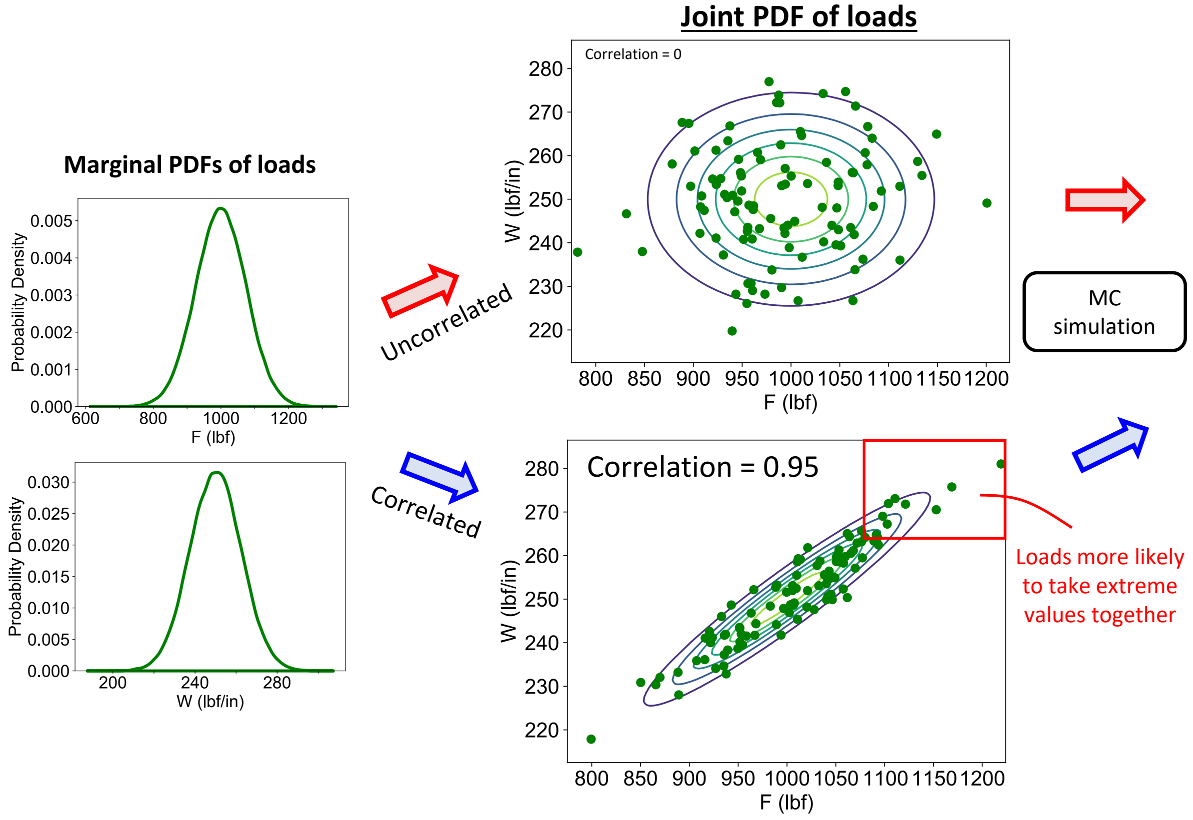


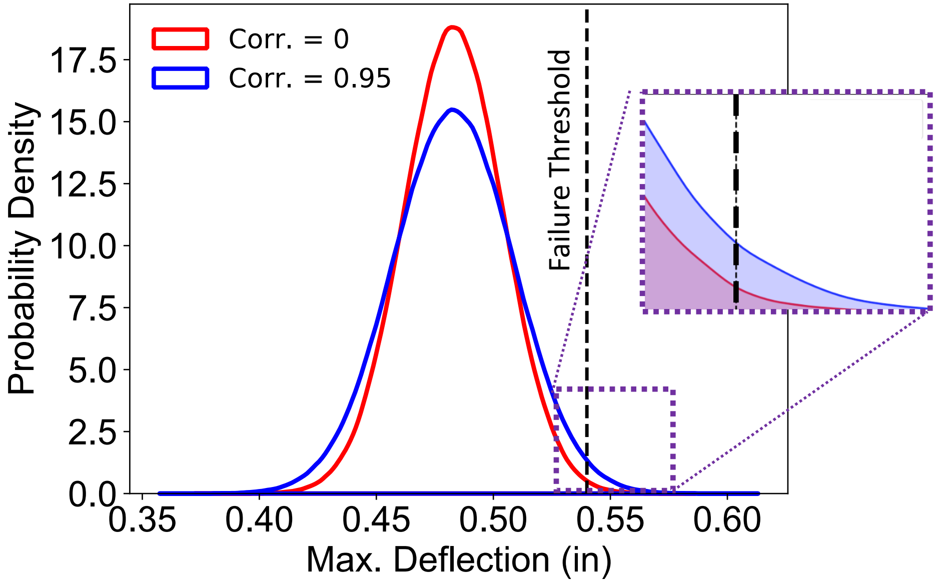


➢ Validating tails of input distributions is critical and could require large amounts of data

Input Errors | *Correlation*





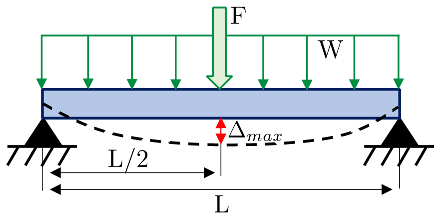


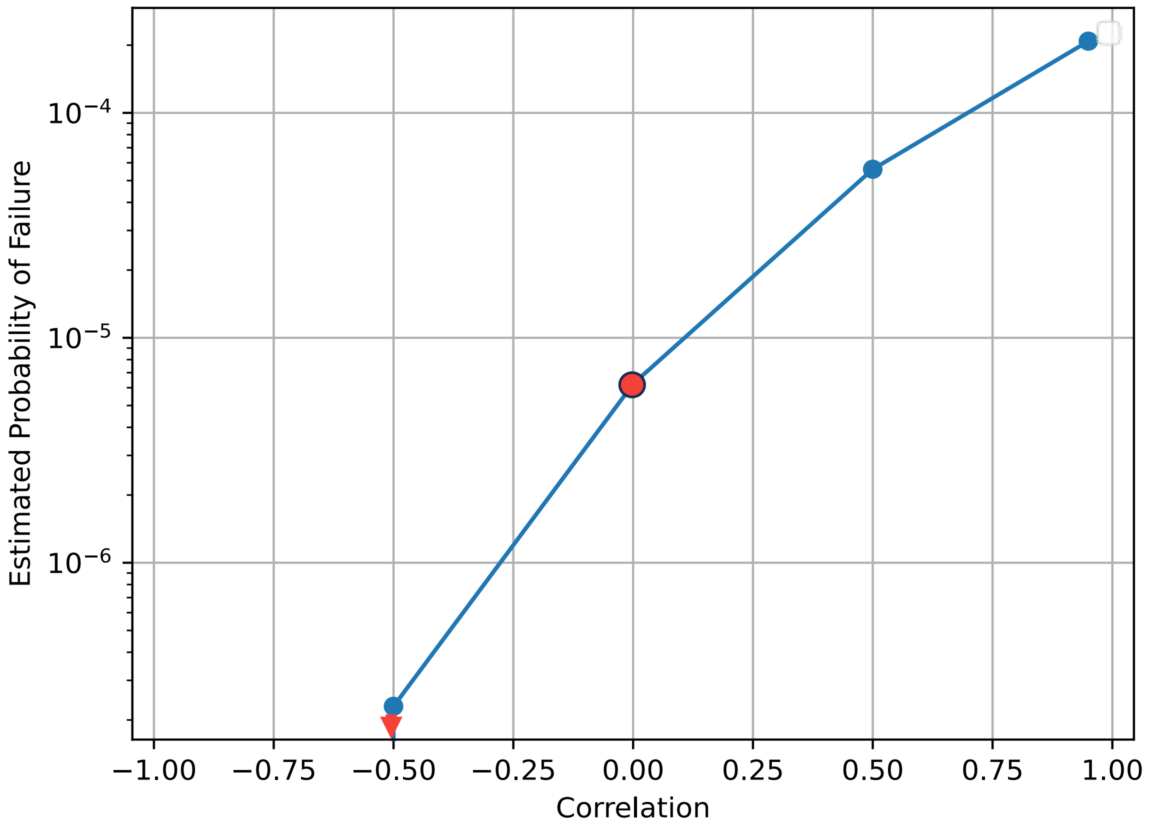
No correlation: $P(\Delta_{max}) \geq 0.54in) \approx 0.0032$

With correlation: $P(\Delta_{max}) \geq 0.54in) \approx 0.0135$

➢ **Correlated load case is over 4X more likely to fail**

Input Errors | *Correlation*

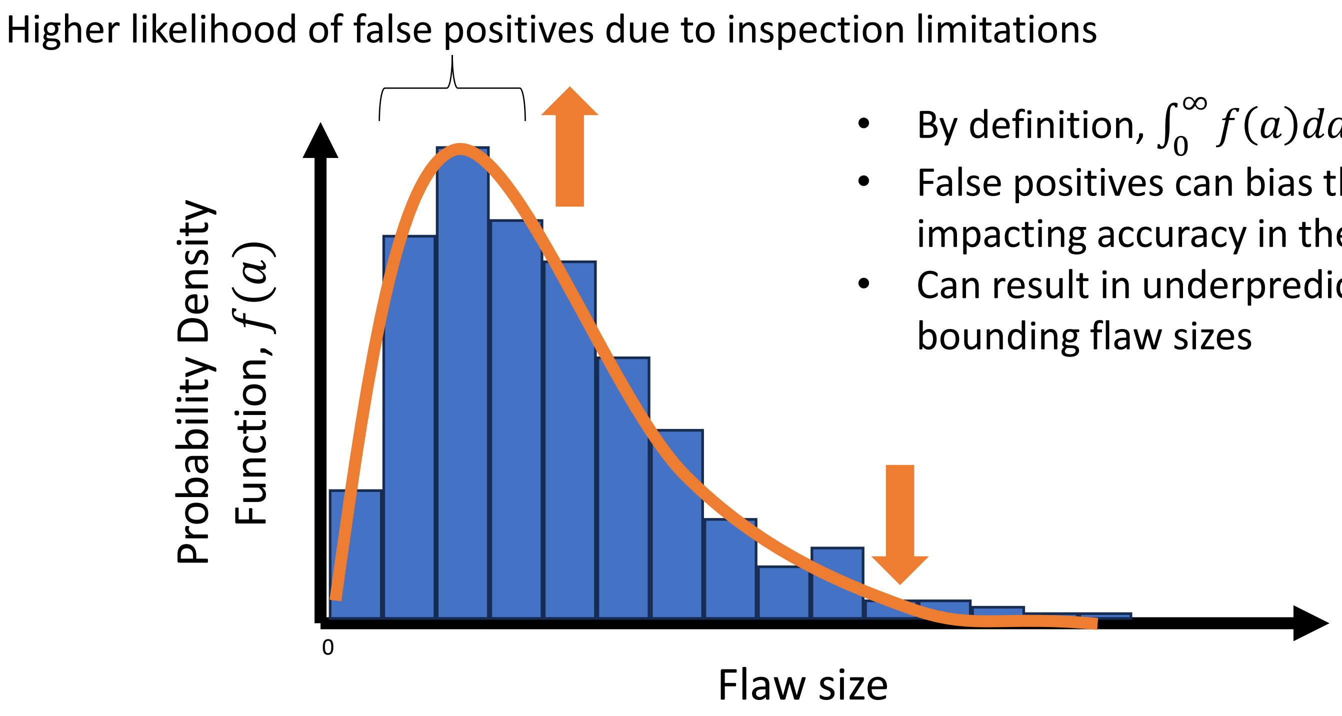




- ➢ Incorporate input correlations if they exist and consider effects of correlation in worst-case analysis

Data Contamination

Example: Estimating an inherent flaw size distribution from nondestructive inspections



- By definition, $\int_0^\infty f(a)da = 1$
- False positives can bias the density, impacting accuracy in the tails
- Can result in underpredicting bounding flaw sizes

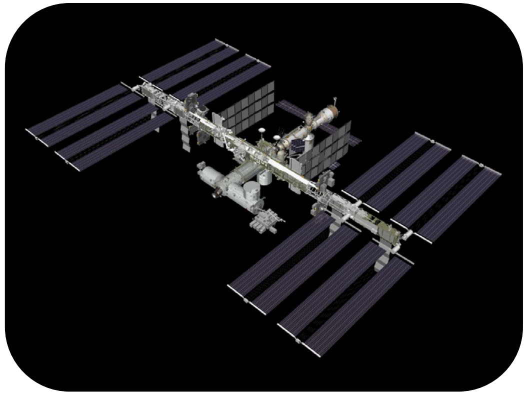
➢ Understand effects of data contamination, correct if possible, and discard data if not

Recent Applications of UQ at NASA

xEMU Spacesuit Certification

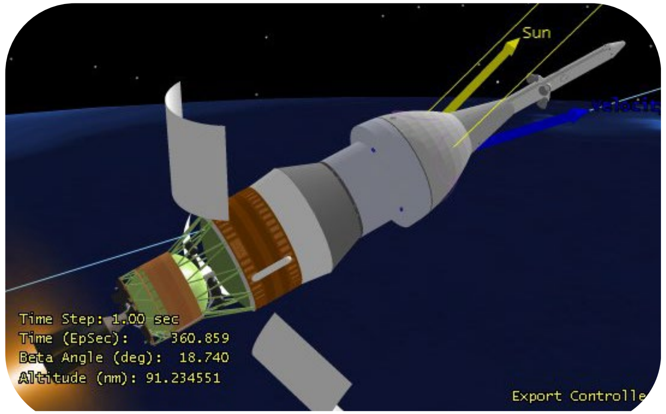
Carried out a probabilistic analysis to verify a requirement on spacesuit reliability for potential astronaut falls on the lunar surface.

ISS PrK Module Leak Investigation



Leveraged UQ approaches to identify probable root causes of crack initiation/propagation and to gauge risk of continued ISS operations.

Frangible Joint Reliability Analysis



Used probabilistic methods to estimate Orion frangible joint reliability for the successful separation of fairing panels in Artemis-1 and Artemis-2 missions.

(In Progress)

Composite Overwrapped Pressure Vessel (COPV) UQ Assessment

Demonstrating the application of UQ methods to COPV damage tolerance, and assessing the feasibility of the approach for estimating COPV reliability

(In Progress)

NASA UQ Community of Practice

Goal: Raise UQ awareness across the Agency, provide workforce development, and began forming a community of practitioners, to work towards adding state-of-the-art probabilistic and statistical methods to NASA's engineering and science toolbox.

UQ CoP Facilitator

- Mike Stanley, PhD
- Statistics, Carnegie Mellon University
- Analytical Mechanics Associates

Broader NASA Community

Feedback to the Community

- Software training/docs
- Demonstrations
- Improvements/surveys

Feedback to the Agency

- Roadmapping

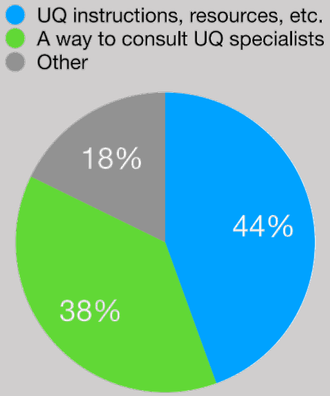
UQ Seminar Series

Facilitator

UQ COP

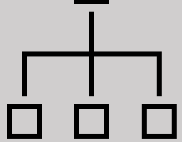
UQ Surveys

Q: What can a UQ CoP provide?



UQ Flowchart

Problem



Methods/experts

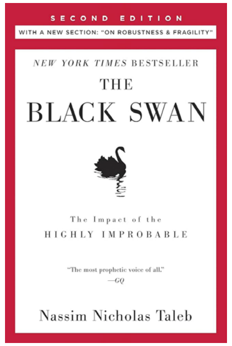
Email Mike Stanley (michael.c.stanley@nasa.gov) to join the NASA UQ CoP.

NASA UQ Seminar Series

VIP Speakers starting off the season:

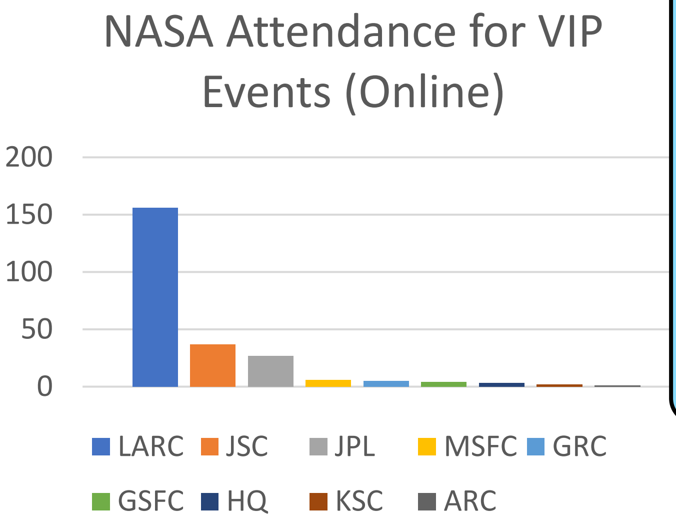
Dr. Nassim Nicholas Taleb

- Multiple New York Times Best selling author of *The Black Swan, Fooled by Randomness,* and *Antifragile*
- Discussed challenges associated with small probability and risk estimation
- ~300 attendees (online + in-person)



Dale Hall, FSA, MAAA, CFA, CERA

- Director of Research for the Society of Actuaries
- Discussed an actuarial perspective on quantifying risk and explored operational similarities between NASA and insurance companies



Additional Speakers (FY25)

- ✓ Philip Stark (UC Berkeley) – June 10
- ✓ James Berger (Duke U.) – June 24
- Kathryn Maupin (Sandia Labs) – August 12
- + A few others (TBA)

* Recordings of all talks are available

UQ Seminar Series Highlights

- Used the seminar series to foster a relationship with the Nuclear Regulatory Commission with several of its employees attending our seminars
- Record attendance for Dr. Taleb's visit with ~300 attendees
- Dramatically increased engagement with JPL (0 to 27 FY24 to FY25)
- Reached 52 branches at Langley

Email Mike Stanley (michael.c.stanley@nasa.gov) to receive seminar invites.

Summary

- UQ approaches, if properly applied, can help ensure the credibility of predictions made using modeling and simulation.
  - *Uncertainty propagation* enhances models to provide information about plausible outcomes and their relative likelihood, where different approaches for handling epistemic uncertainties exist depending on goals of the analysis.
  - For a more holistic analyses, other UQ concepts like *verification*, *validation*, *model calibration*, *sensitivity analysis*, *optimal experimental design*, *and surrogate modeling* may be required.
- Rigor is required for UQ success in practice to prevent misleading results due to model/input errors or flawed assumptions
- To learn more, consider joining the NASA UQ Community of Practice and attending future UQ Seminar Series presentations.

Further Reading

- Uncertainty Quantification (general)
  - Smith, R. C. *Uncertainty Quantification Theory, Implementation, and Applications*. 2013. [Textbook]
  - Roy, C. J. and Oberkampf, W. L. *A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing.* 2010.
  - Warner, J. E., Leser, P. E., & Schneck III, W. C. *Modern Methods in Uncertainty Quantification for NDE 4.0*. In Handbook of Nondestructive Evaluation 4.0. Springer, Cham. 2025. [Book chapter]
- Uncertainty Propagation
  - Rubinstein, R. Y. and Kroese, D. P. *Simulation and the Monte Carlo Method*., 2016.
  - Ditlevsen, O. and Madsen, H. O. *Structural Reliability Methods*. 2007 [Textbook] (Free PDF download available)
- Model Calibration
  - Kennedy, M. C. and O'Hagan, *A. Bayesian calibration of computer models*. 2002.
  - Haugh, M. B., *A Tutorial on Markov Chain Monte-Carlo and Bayesian Modeling.* 2021.
- Surrogate Modeling
  - Alizadeh, R. et al. *Managing computational complexity using surrogate models: a critical review*. 2020.
  - Gramacy, R. B. *Surrogates: Gaussian Process Modeling, Design and Optimization for the Applied Sciences*. 2020.
  - Sudret, B. et al. *Surrogate models for uncertainty quantification: An overview*. 2017.
- Model Discrepancy
  - Brynjarsdóttir, J. and O'Hagan, A. *Learning about physical parameters: The importance of model discrepancy*. 2014
  - Soize, C. *A nonparametric model of random uncertainties for reduced matrix models in structural dynamics*. 2000.
- Sensitivity Analysis
  - Saltelli, A. *Global sensitivity analysis. The primer.* [Textbook] (Free PDF download available)
  - Plischke, E. et al. *Global sensitivity measures from data*. 2013
- Software
  - Dakota: uncertainty quantification software by Sandia: https://dakota.sandia.gov/
  - SALib: open-source Python library for sensitivity analysis https://github.com/SALib/SALib
  - Scikit-learn: open-source Python library for machine learning (surrogate modeling): https://scikit-learn.org/stable/