Introduction to Uncertainty Quantification for Modeling and Simulation

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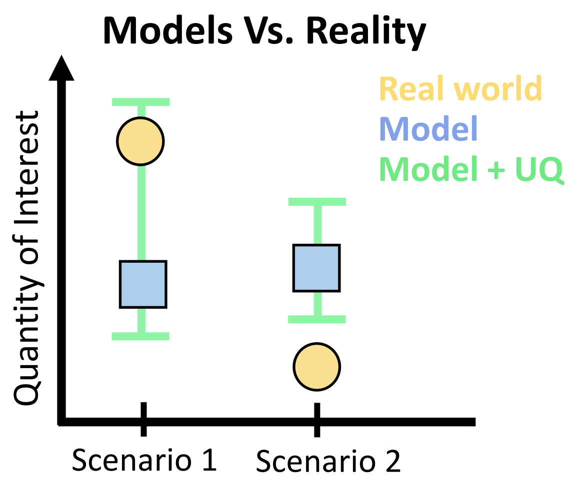
What is Uncertainty Quantification (UQ)?

"All models are wrong,
but some are useful"

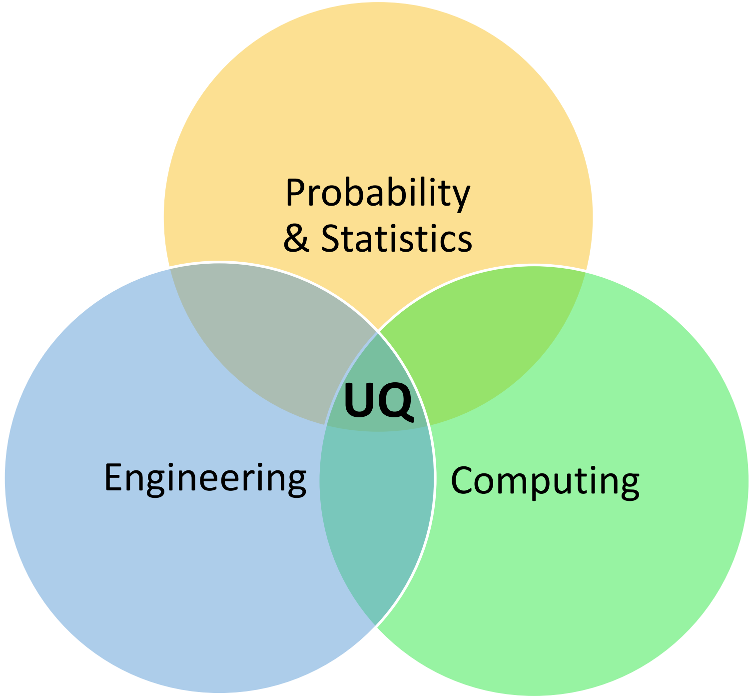
George E.P. Box



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 UQ?

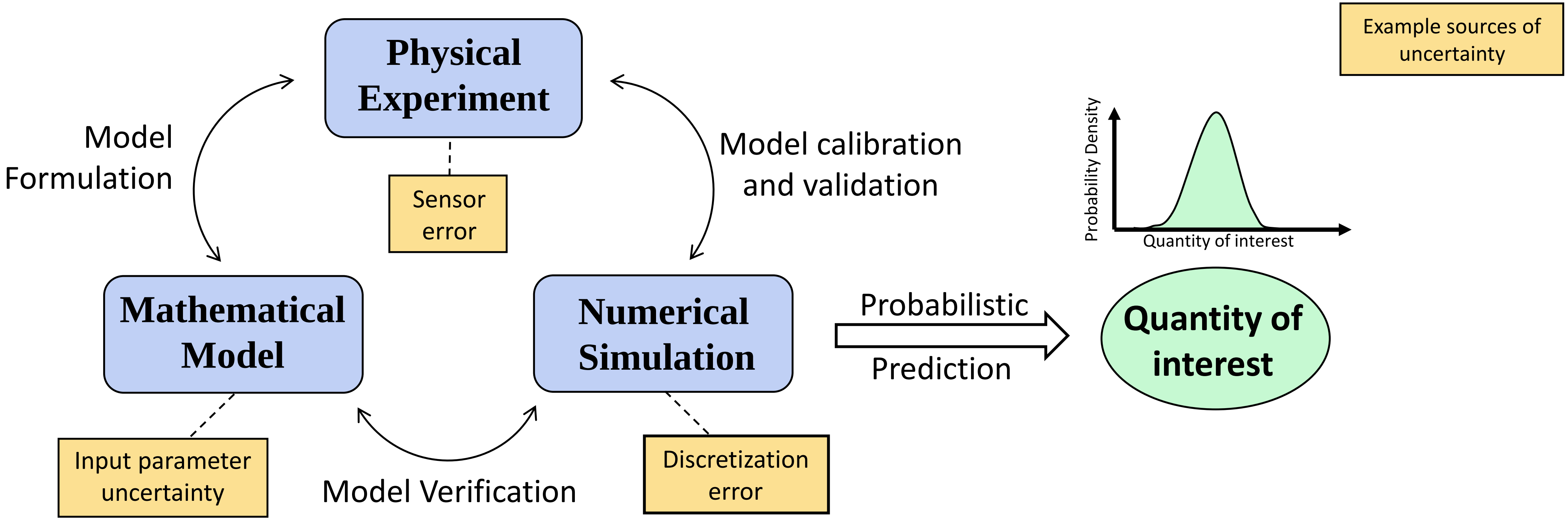


"...the science of identifying, quantifying, and reducing uncertainties associated with models, numerical algorithms, experiments, and predicted outcomes..." Smith, R. C. Uncertainty Quantification Theory, Implementation, and Applications. 2013.

⇩

Imbue our models with what we know, what we don't know, and to what degree we don't know it in order to get a more complete picture of what we're modeling.

Experiments, Models, Simulations, and UQ



- **UQ:** the quantification of the effect of various sources of error (from model, simulation, experiment) on a predicted quantity of interest
- **Model verification**: the process of quantifying the accuracy of simulation codes used to implement mathematical models (i.e. *are we solving the equations correctly*?)
- **Model validation**: the process of determining the accuracy with which mathematical models represent the physical processes of interest (i.e. *are we solving the correct equations*?)

Smith, R. C. Uncertainty Quantification Theory, Implementation, and Applications. 2013.

Computational Models: Notation and Examples

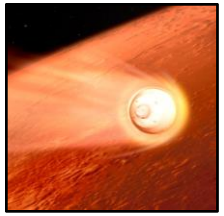
Often distinguish between *inputs* and *parameters*

Inputs X → Model $\mathcal{M}$ → Outputs Y

Often distinguish between *outputs* and *quantities of interests* (QoIs)

Trajectory Simulation

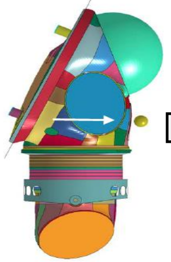
- Atmosphere conditions
- Mass properties



Landing location

Spacesuit Impact Model

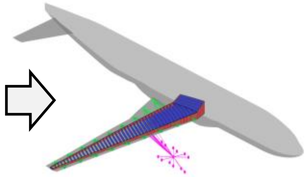
- Impact velocity
- Material properties



Max contact force

Transonic Aero Solver

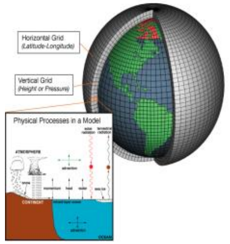
- Wing geometry
- Mach number



Lift

Weather Model

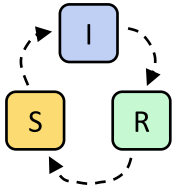
- Ocean temps.
- Initial pressures wind speeds



Storm path

Disease Dynamics Model

- Infection rate
- Birth rate
- Death rate



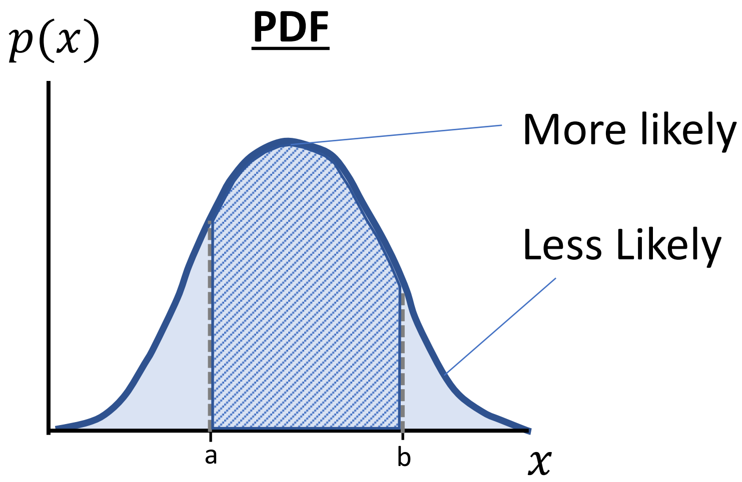
Total infected

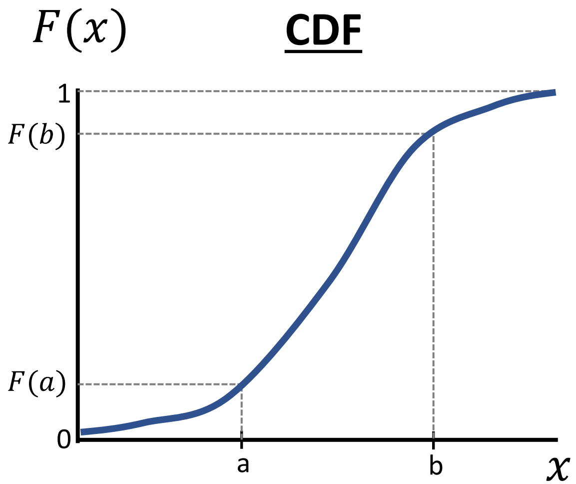
Today’s Goals and Points of Emphasis

- Provide enough information to know what to ask/search for if interested in applying UQ
  - Broad overview of the main concepts; listing common references, software, methods for further study
  - Understand “what/why/when", not necessarily “how”
- Provide parallels, results from practical NASA problems

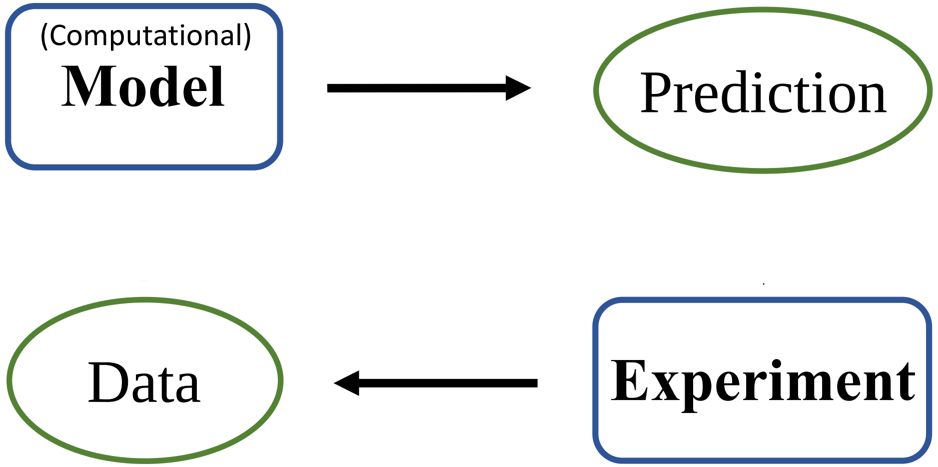
Quick Review of Terminology

- Random Variable, $\boldsymbol{X}$
  - Variable with unknown true value
- Probability Density Function (PDF), $p(x)$
  - Function describing the relative likelihood that $\boldsymbol{X}$ takes a specific value, x
- Cumulative Distribution Function (CDF), $F(x)$
  - Probability 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., $P(a \leq X \leq b)$

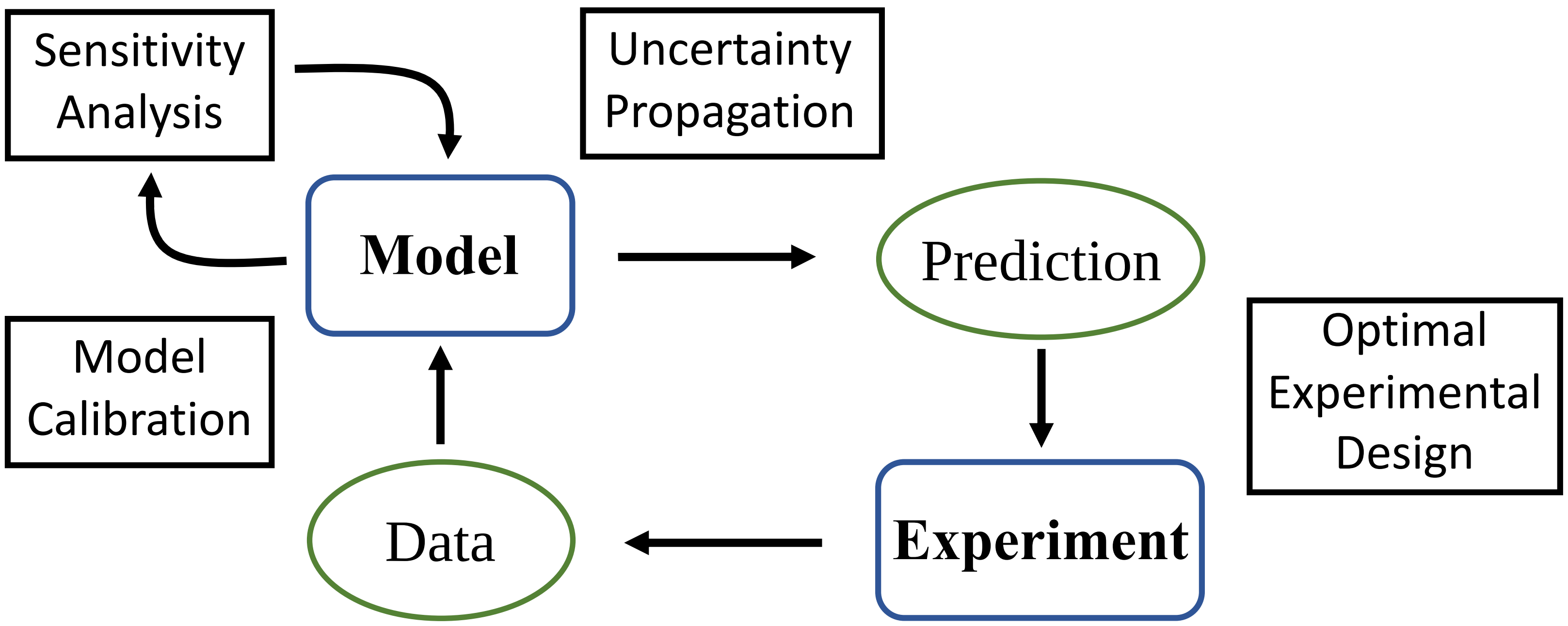




UQ Concepts

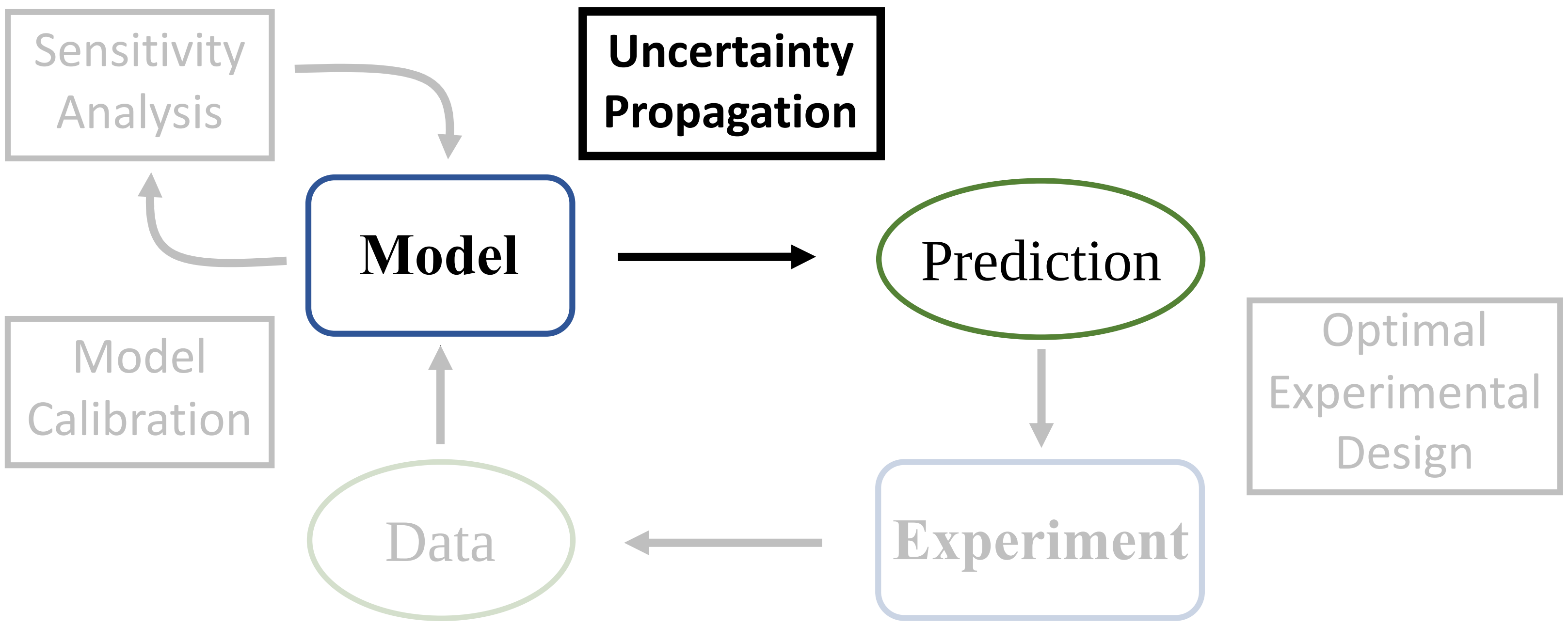


UQ Concepts



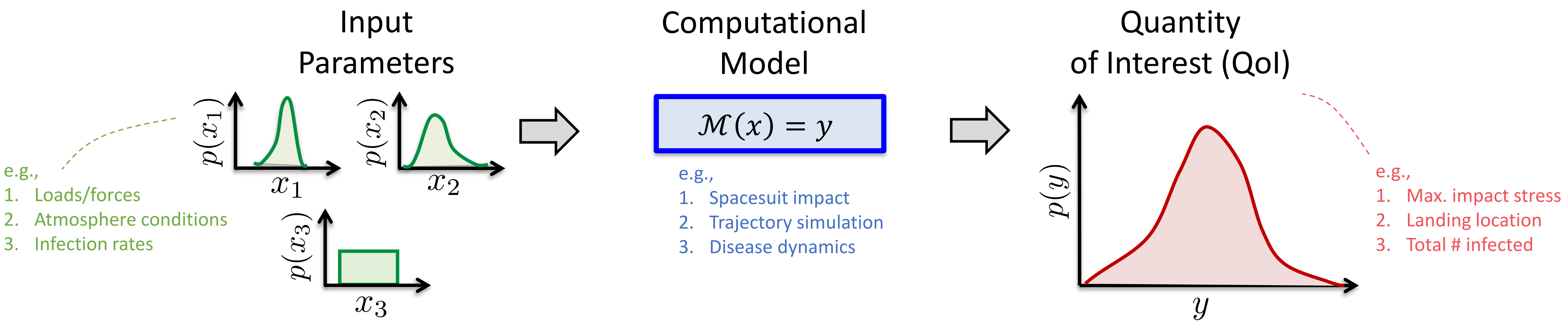
Sensitivity Analysis
Uncertainty Propagation
Model
Prediction
Model Calibration
Optimal Experimental Design
Data
Experiment

UQ Concepts: Uncertainty Propagation



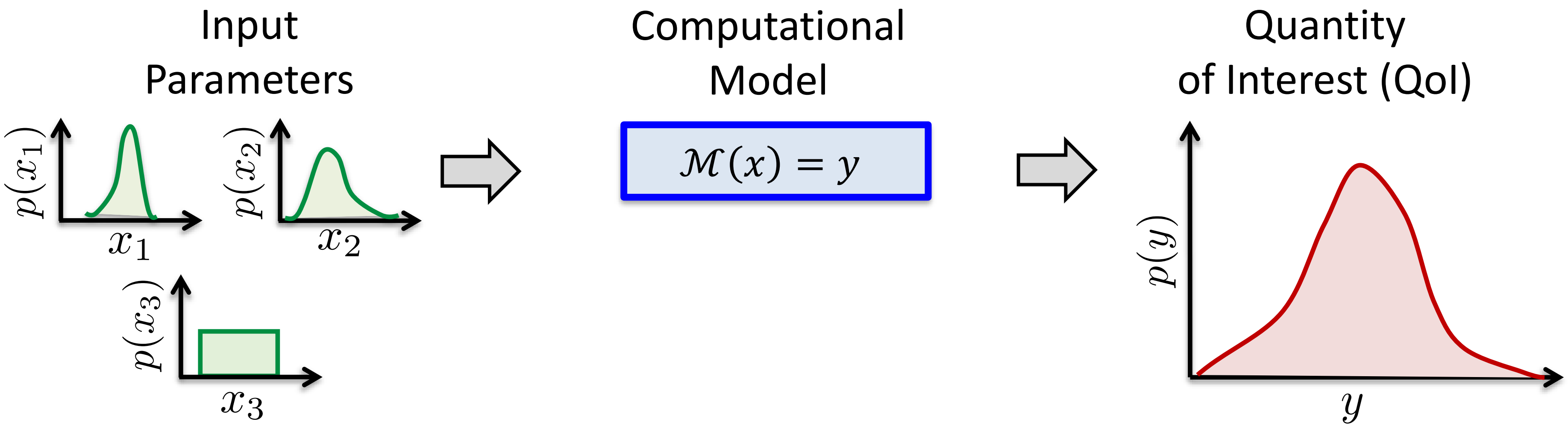
- ***Uncertainty propagation*** feeds quantified input uncertainties through our model to produce probabilistic predictions

Uncertainty Propagation



- 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% credible intervals: y_L, y_U such that $P(y_L \leq Y \leq y_U) = 0.95$
  - Probability of exceeding a critical value: $P(Y \geq y^{crit})$

Uncertainty Propagation



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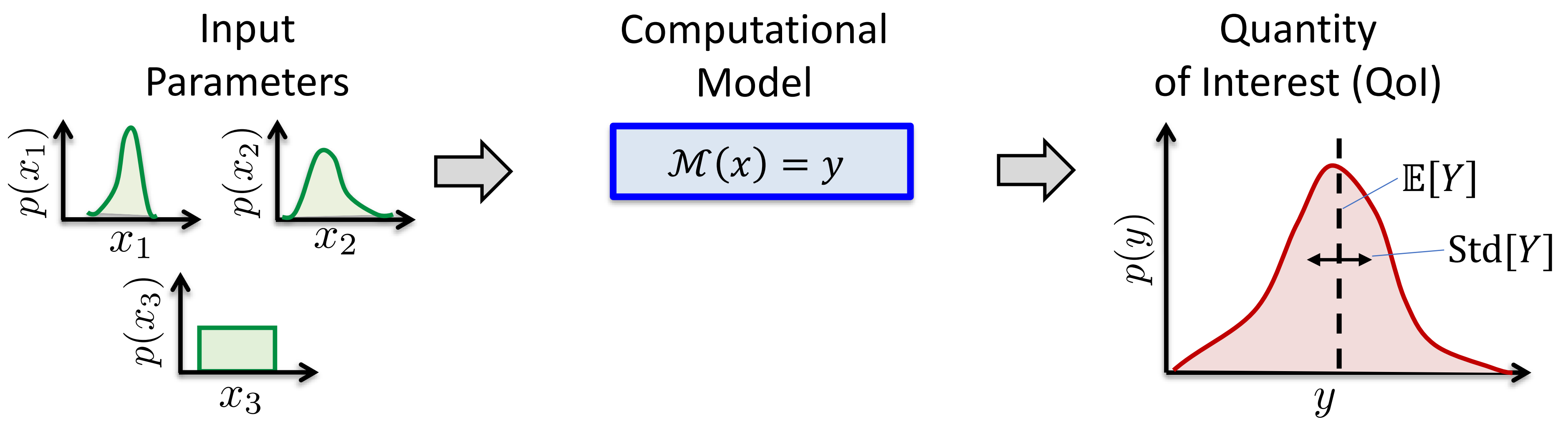

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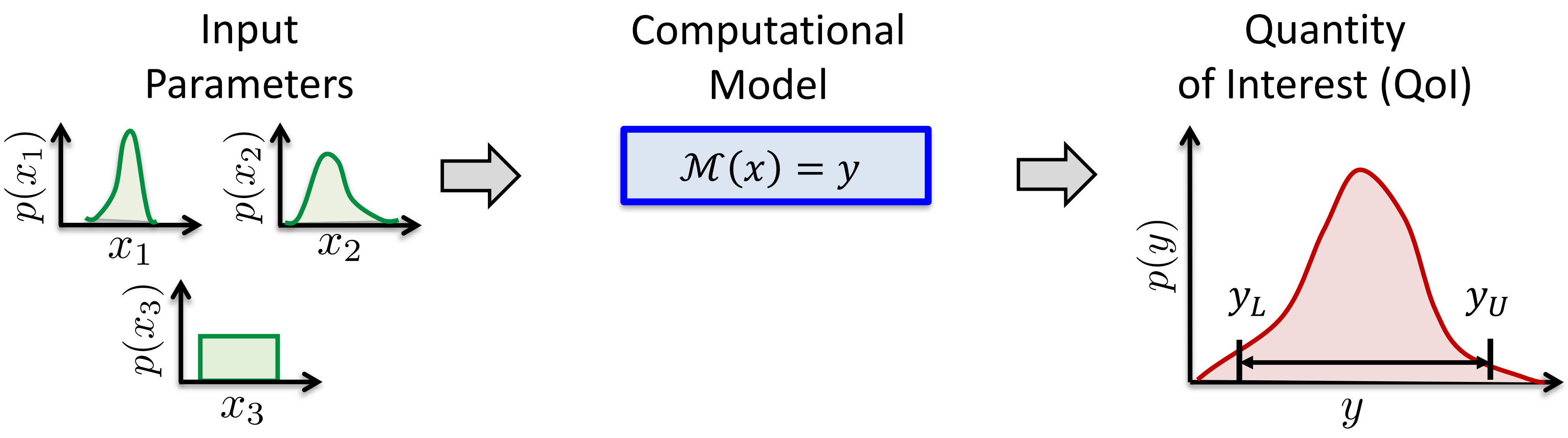

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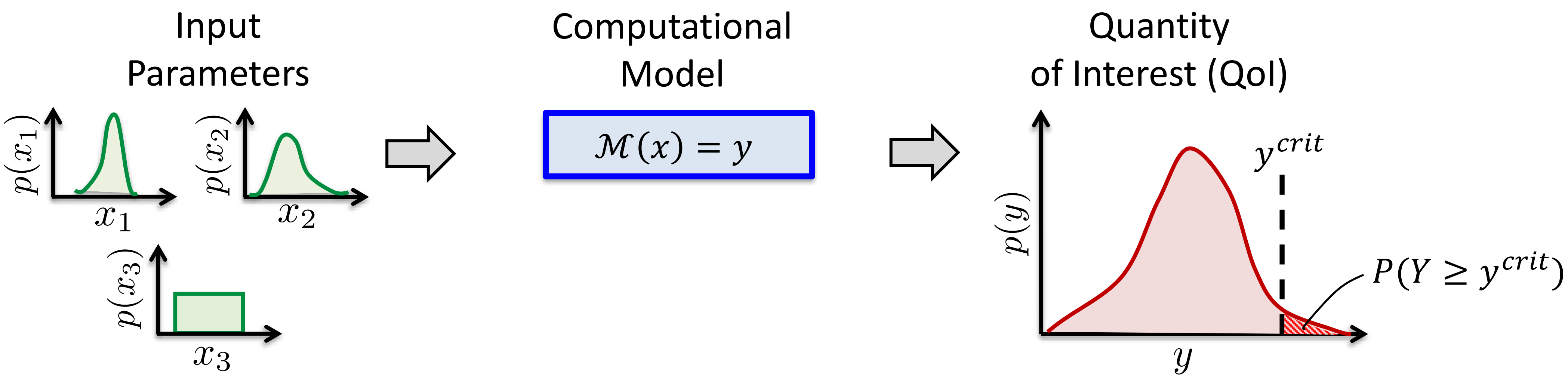

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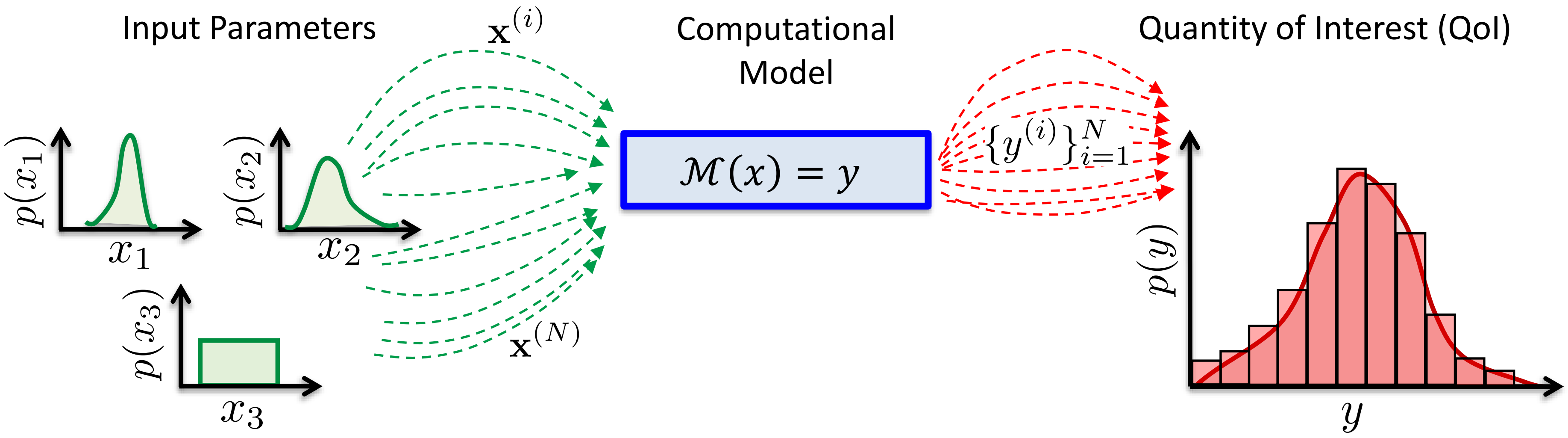
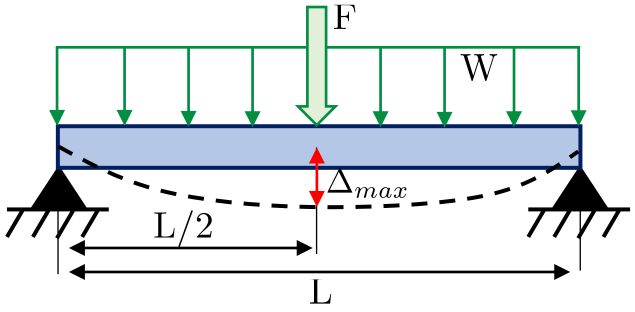
Monte Carlo (MC) Simulation



- **Procedure** – repeat following N times:
  - Generate random sample of input parameters: $x^{(i)} \sim p(x)$
  - Evaluate model & store output: $y^{(i)} = \mathcal{M}(x^{(i)})$
- **Then** – postprocess output samples $\{y^{(i)}\}_{i=1}^{N}$ to estimate PDF, statistics of QoI, etc.
  - ➢ $p(y)$ (use histogram or kernel density estimate)
  - ➢ $\mathbb{E}[Y] \approx \frac{1}{N}\sum_{i=1}^{N} y^{(i)}$ (expected value ≈ sample average)
  - ➢ $P\left(Y \geq y^{crit}\right) \approx \frac{1}{N}\sum_{i=1}^{N} \mathbb{1}(y^{i} \geq y^{crit})$ (failure probability ≈ proportion of samples that failed)

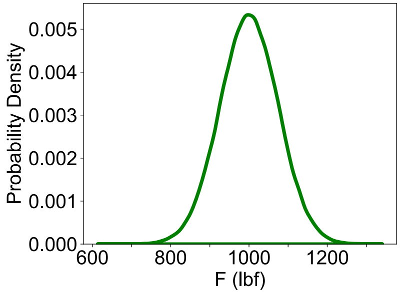
Indicator function: = 1 if True, = 0 if False

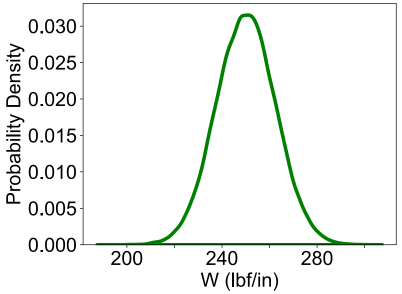
MC Example: Beam with Random Loading



- Uncertain load parameters (F, W)
- Fixed, deterministic inputs:
  - Length (L), stiffness, area

Input Parameters

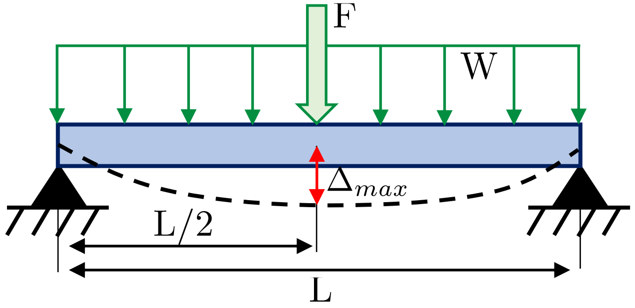




Computational Model

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

MC Example: Beam with Random Loading



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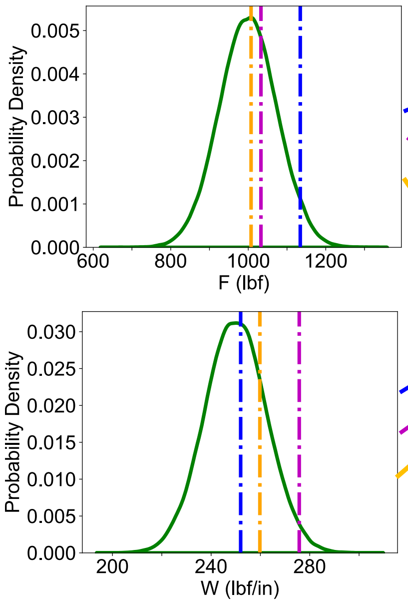
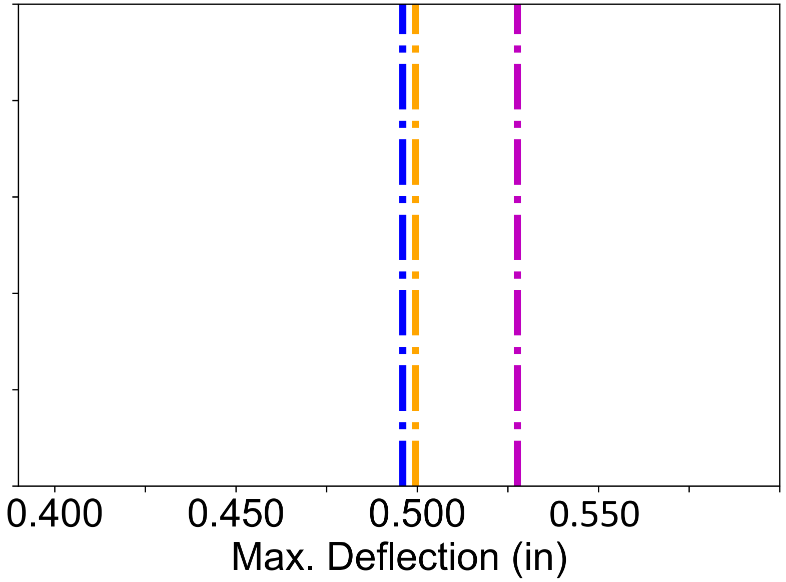


Computational Model

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

Model predictions for three randomly drawn inputs

Quantity of Interest (QoI)



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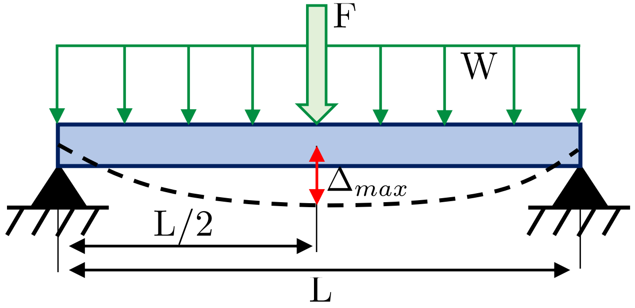

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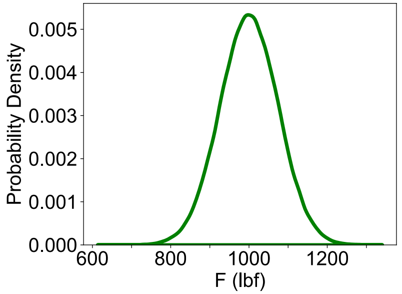
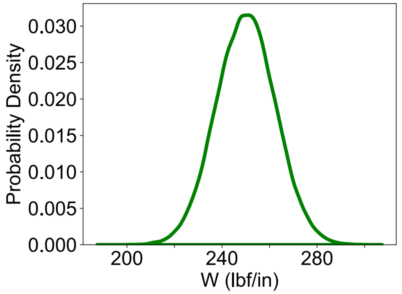




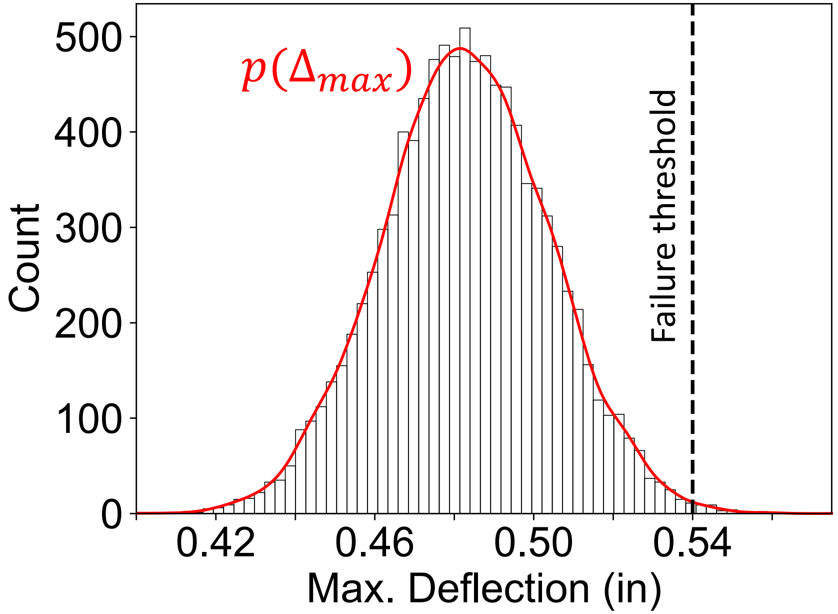
Computational Model

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

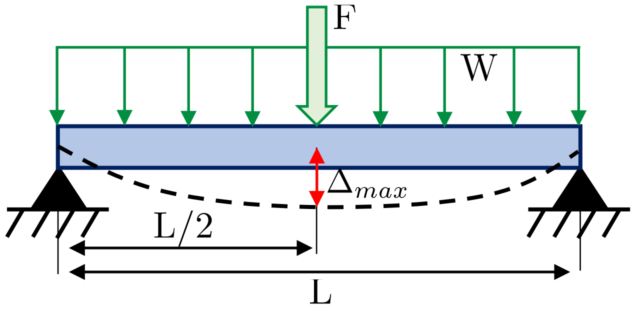
Monte Carlo simulation for N=10,000 random samples

$$\mathbb{E}[\Delta_{max})] \approx 0.4829 \text{ in}$$
$$P(\Delta_{max} \geq 0.54in) \approx 0.0032$$

Quantity of Interest (QoI)



Example: Beam with Random Loading



- Uncertain load parameters (F, W)
- Fixed, deterministic inputs:
  - Length (L), stiffness, area

- Monte Carlo implementation (e.g., Python):

```
#Specify inputs
...
#Monte Carlo simulation loop:
deflection_samples = np.zeros(N)
for i in range(N):
    F = random.normal(F_mean, F_std)
    W = random.normal(W_mean, W_std)
    deflection_samples[i] = F*L**3/(48.*E*I)+(5*W*L**4)/(384.*E*I)
#Postprocess to create histogram, estimate statistics:
plt.hist(deflection_samples)
mean = numpy.mean(deflection_samples)
failure_prob = numpy.sum(deflection_samples>=failure_threshold)/N
```

Set N, L, F_mean, F_std, …

Draw random input samples

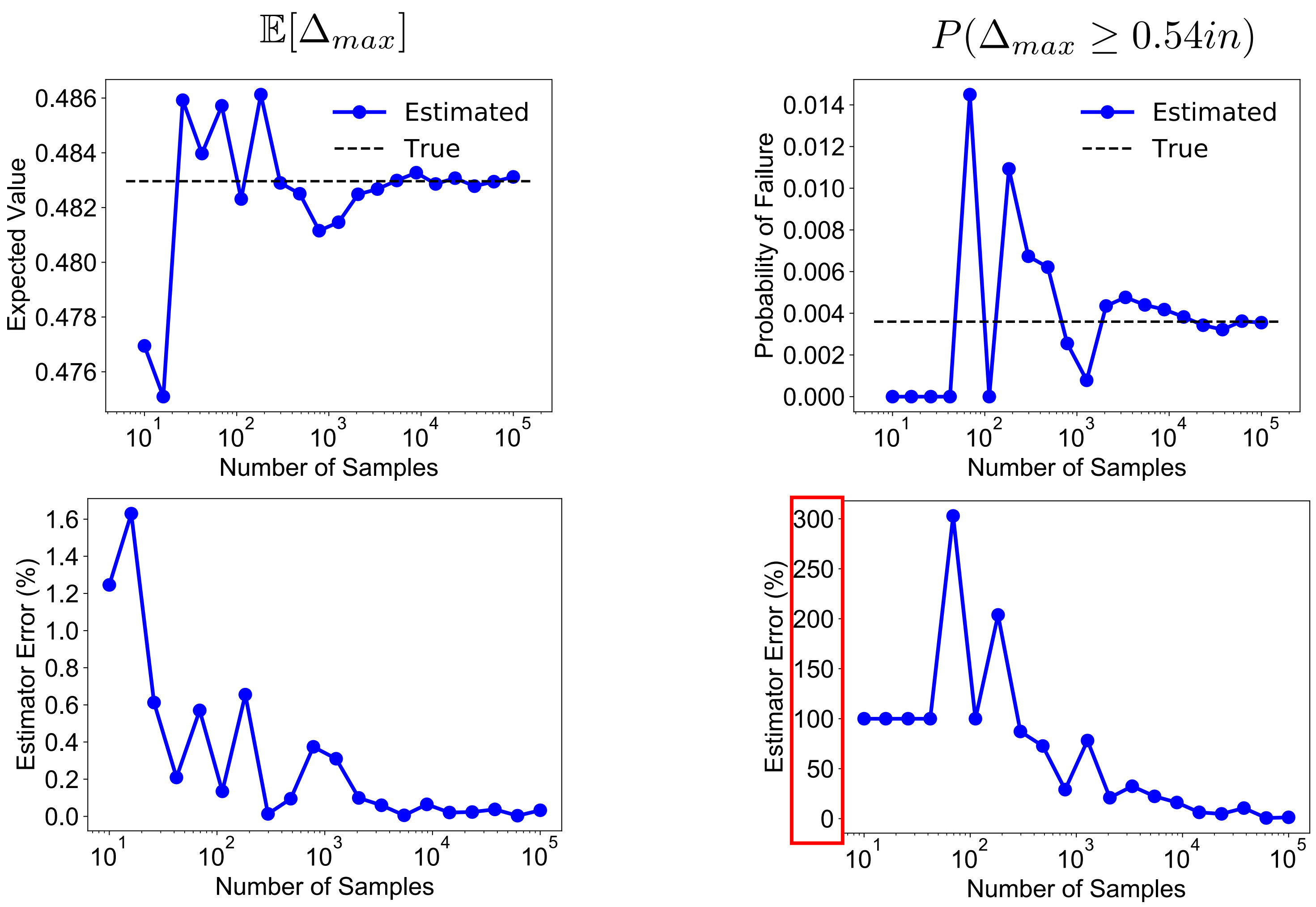
Evaluate model

$p(\Delta_{max})$

$\mathbb{E}[\Delta_{max}]$

$P(\Delta_{max} \geq 0.54in)$

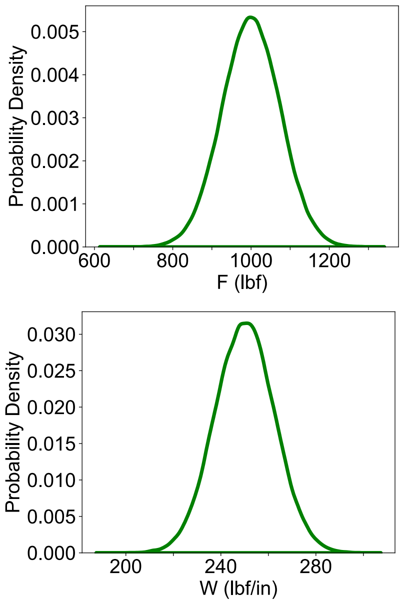
MC: Convergence



- Convergence rate is on order of $\frac{1}{\sqrt{N}}$ (via Central Limit Theorem) and is *independent* of input dimension
- Rare event (e.g., probability of failure) estimators require significantly more samples for accuracy

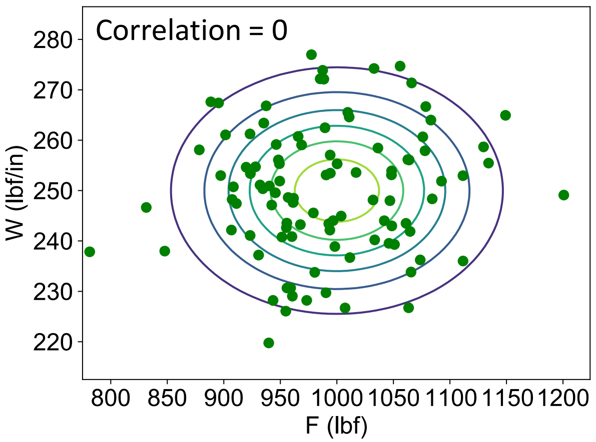
MC: Effect of Correlated Inputs

Marginal PDFs of loads

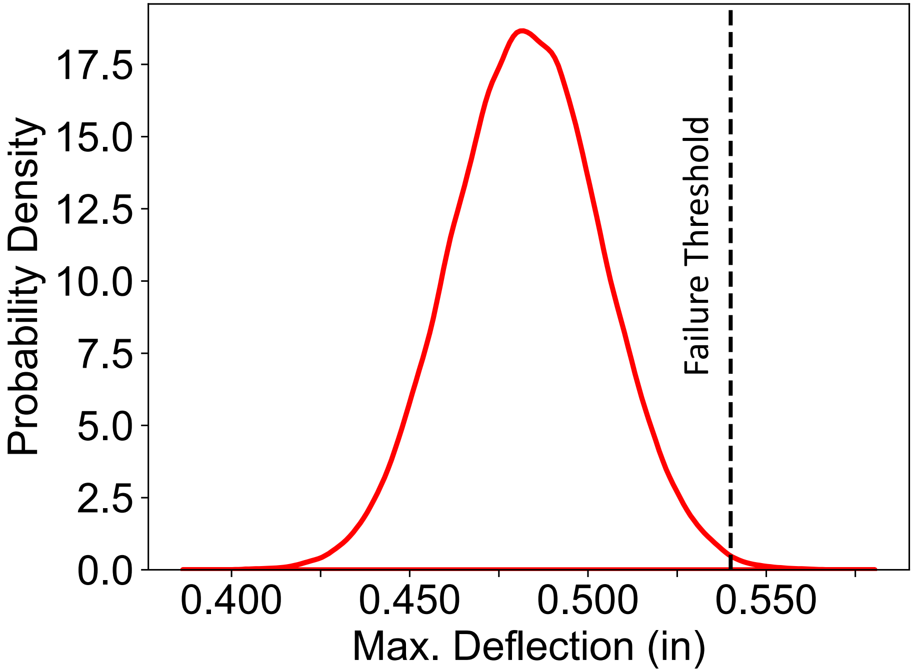


Uncorrelated

Joint PDF of loads



Monte Carlo simulation



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

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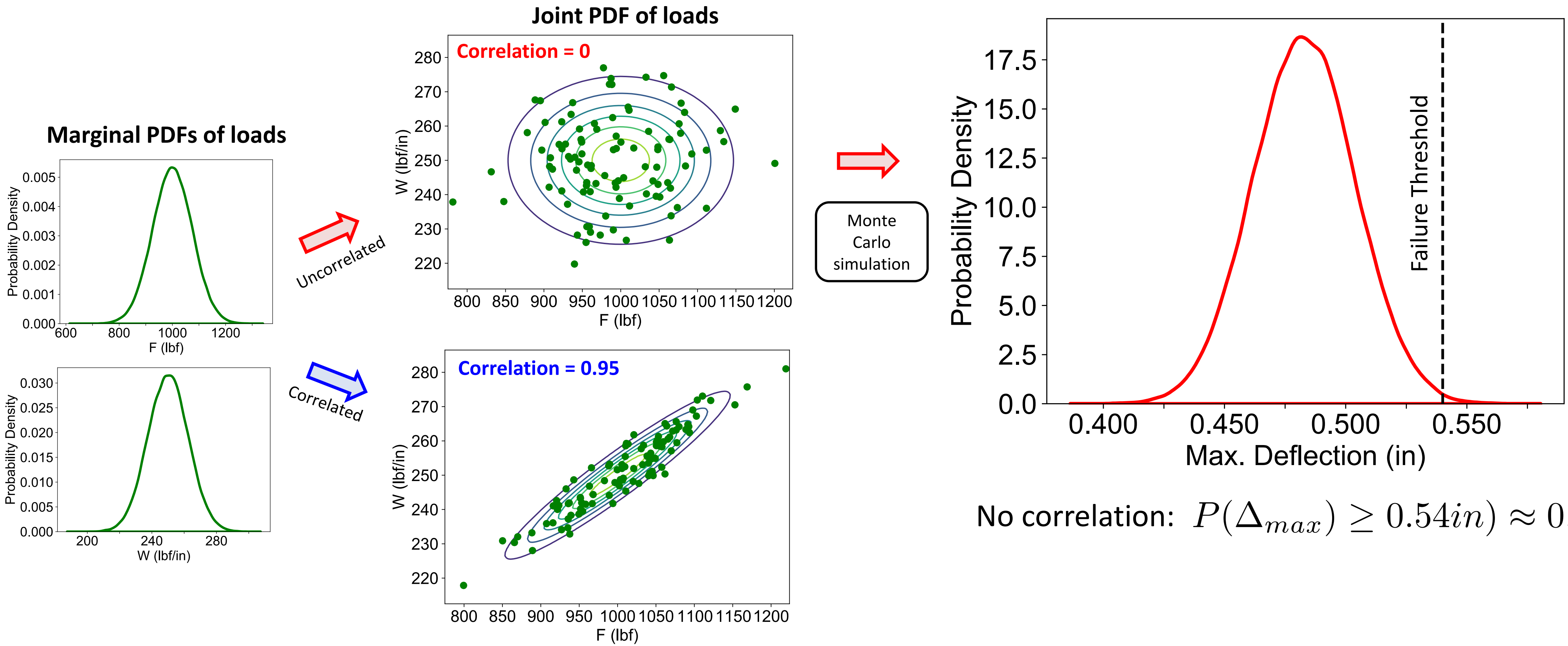

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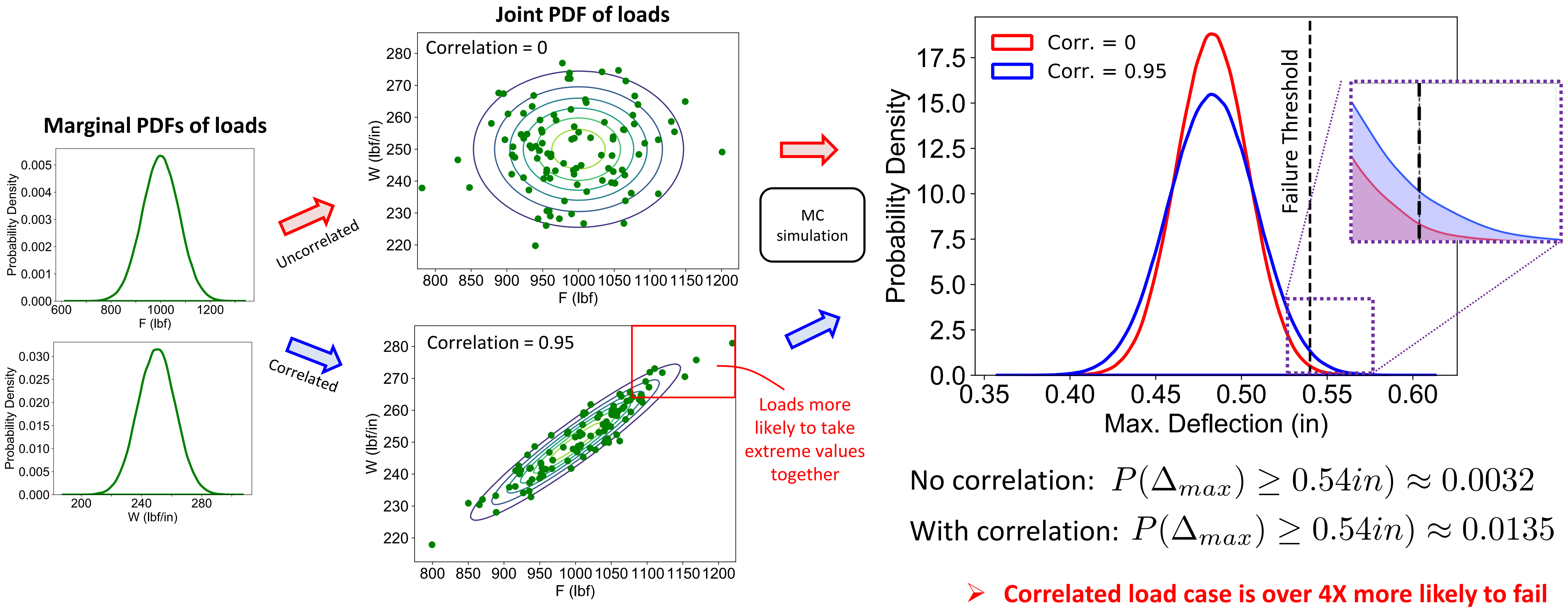


No correlation: $P(\Delta_{max}) \geq 0.54in) \approx 0.0032$

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

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

- *Important to quantify correlations; failure to do so can lead to undetected non-conservatism*

MC Takeaways

✓Non-intrusive, general-purpose, and relatively simple approach for propagating uncertainty through models

- But can be challenging/infeasible in practice when models are expensive

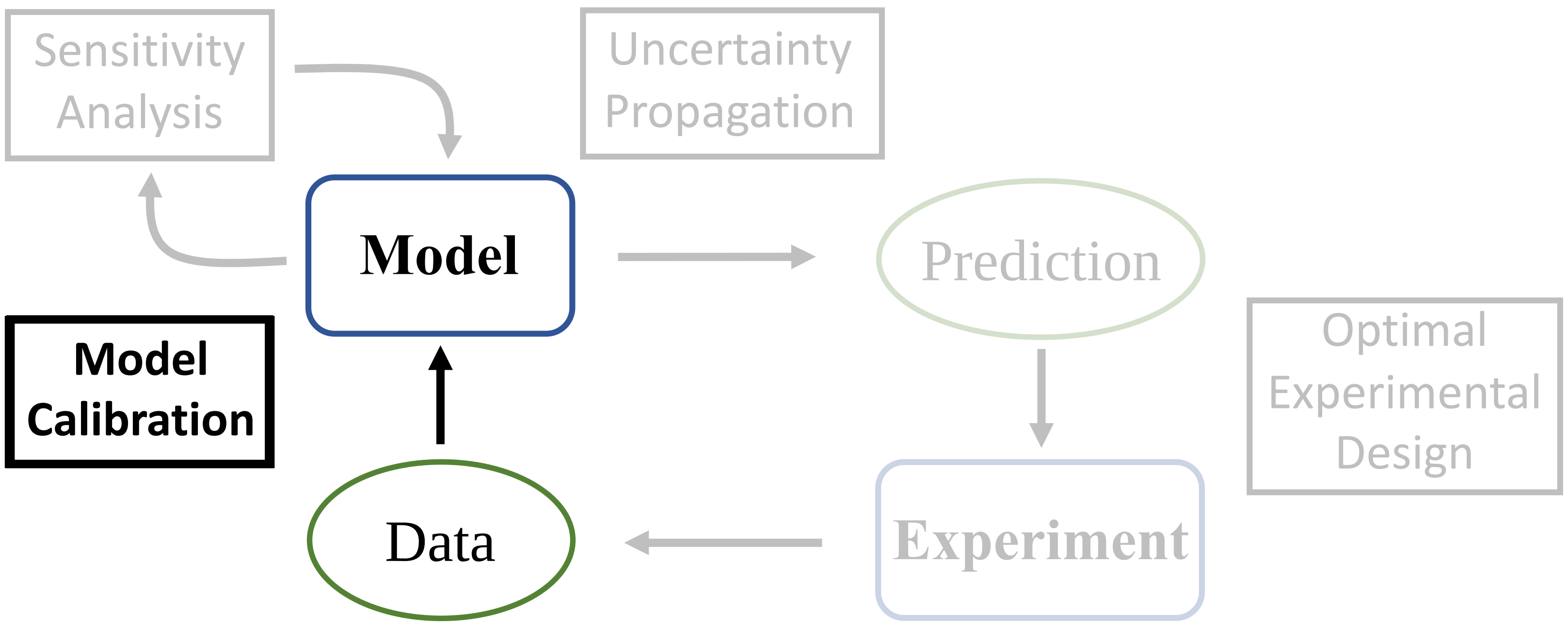
✓Exhibits provable convergence at a known rate, regardless of input dimension

✓Improperly specifying input uncertainty (e.g., parameter correlations) can have a significant impact on results

So how do we quantify input uncertainties?

1. Make estimates based on expert judgement
2. Use available data to infer uncertainty directly

UQ Concepts: Model Calibration

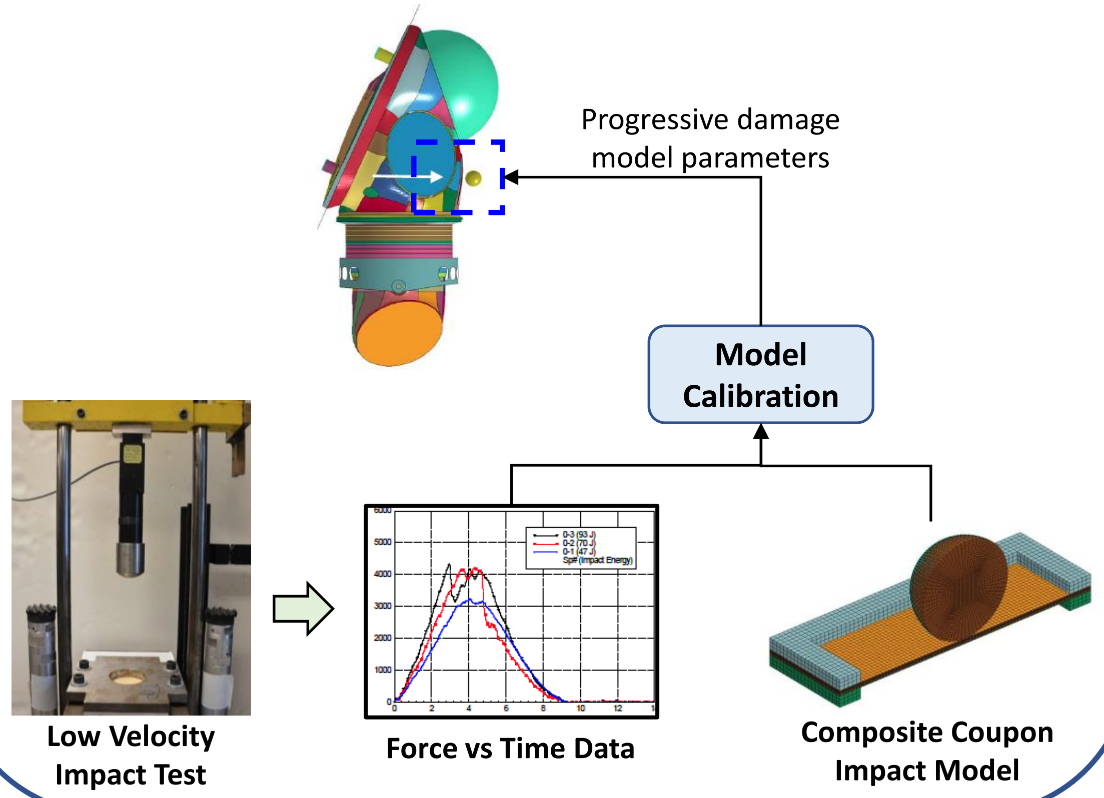


- ***Model calibration*** explicitly quantifies model input uncertainties using experimental data (can be used to improve or update initial assumptions)

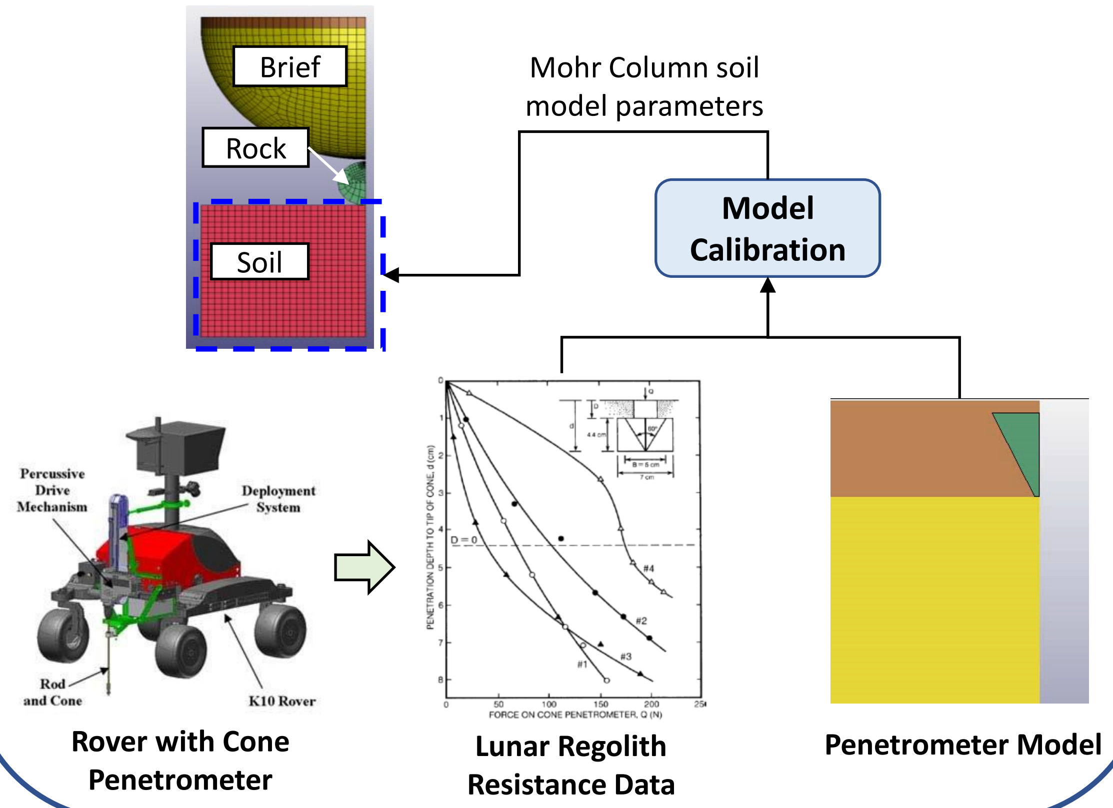
Model Calibration with Component Scale Tests

- In practice, the experimental data available for calibration is often from a simpler, component scale test
- Examples from spacesuit reliability analyses:

Modeling Progressive Impact Damage in Composites



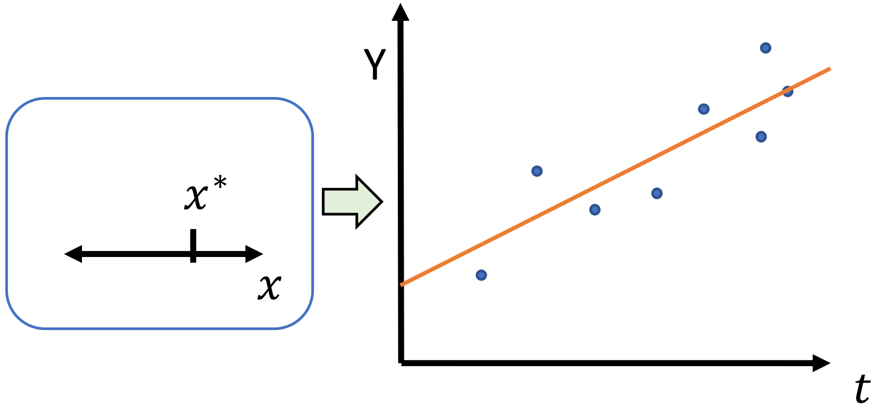
Modeling Suit Impact on Lunar Regolith



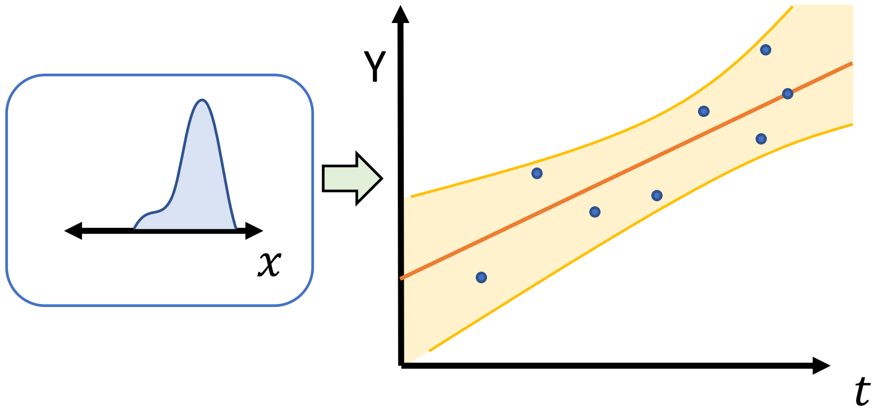
Deterministic vs. Probabilistic Calibration

- 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 $\boldsymbol{\epsilon}$

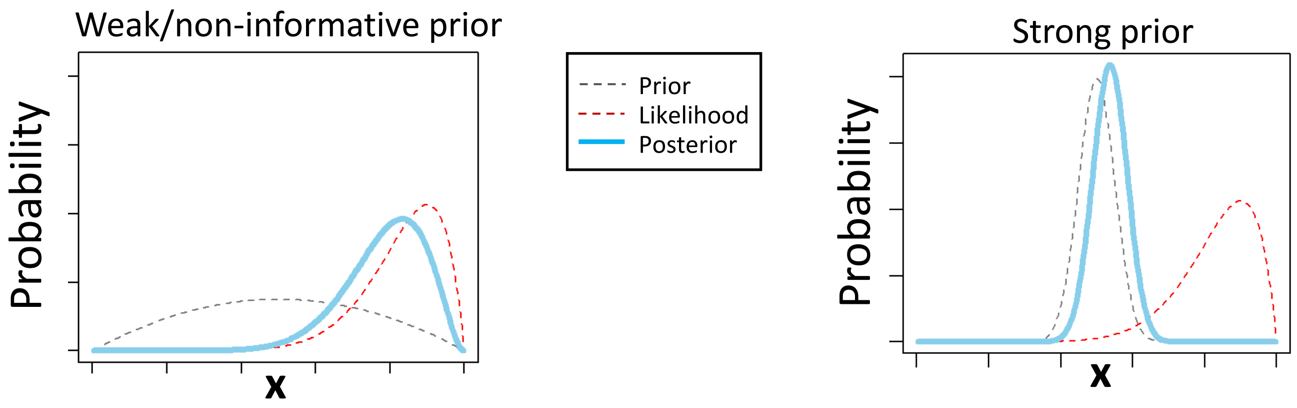


Probabilistic Calibration

How does this work in practice?

"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 $\boldsymbol{\epsilon}$"

- Formulated such that $p(x|D)$ is high when error, $||Y_{\mathcal{E}} - D||$, is low and vice versa
  - Typically implemented using <u>*Bayesian inference*</u>
  - Starts with an initial guess for uncertainty ("prior distribution") then updates it using the measurement data (with a "likelihood function")



Probabilistic Calibration Takeaways

✓Estimates input uncertainties based on data, accounting for noise

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

✓Less data → more uncertainty; more data → less uncertainty

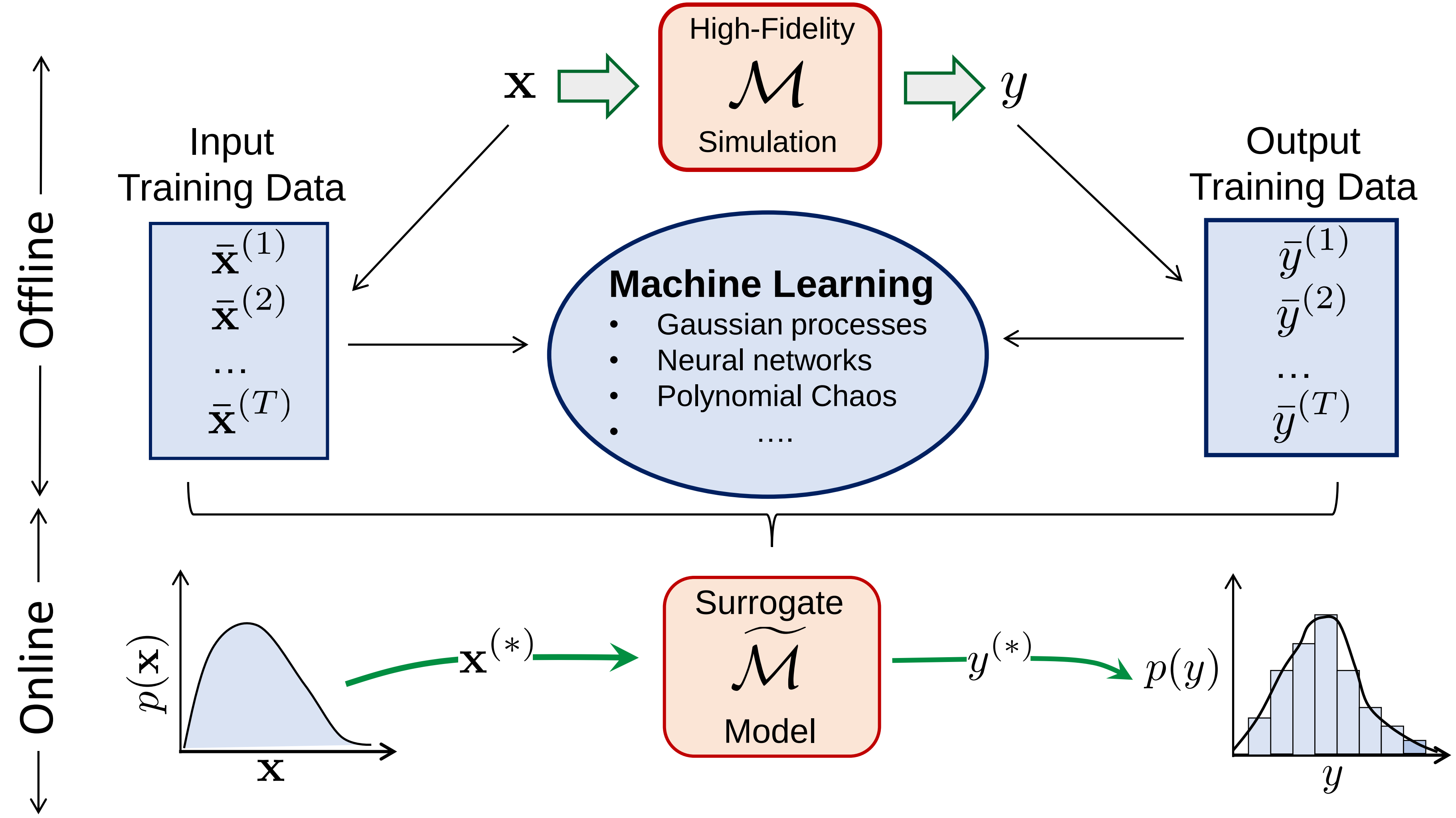
✓Variety of well-established methods exist for performing probabilistic calibration

Some notable caveats:

1. Requires specific expertise/experience
2. Prior distribution specification more nuanced than you may expect
3. Computationally expensive relative to deterministic calibration

UQ Concepts: Surrogate Modeling (AKA response surfaces, reduced order models, …)

Overcoming computational burden when the model is expensive



Orders of magnitude computational speedup possible

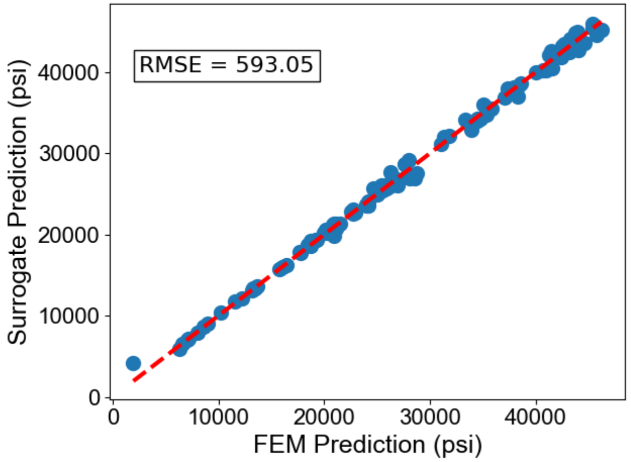
Surrogate Model Validation

- Regardless of the method used for surrogate modeling, the most important step is validating a trained model before using for UQ
- Always create a **separate** dataset for testing that is **not** used for training

(M < T)

Training		**Testing**	
$\bar{\mathbf{x}}^{(1)}$	$\bar{y}^{(1)}$	$\hat{\mathbf{x}}^{(1)}$	$\hat{y}^{(1)}$
$\bar{\mathbf{x}}^{(2)}$	$\bar{y}^{(2)}$	$\hat{\mathbf{x}}^{(2)}$	$\hat{y}^{(2)}$
…	…	…	…
$\bar{\mathbf{x}}^{(T)}$	$\bar{y}^{(T)}$	$\hat{\mathbf{x}}^{(M)}$	$\hat{y}^{(M)}$

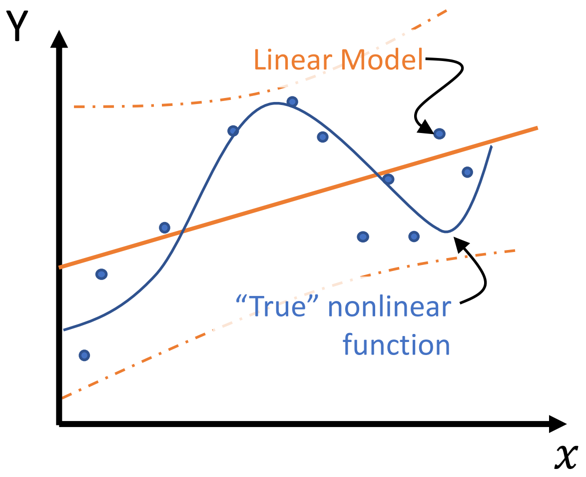
Compare predictions on test data to the original model



- If surrogate model error is <u>not</u> negligible, it can be factored into total uncertainty when making probabilistic predictions

UQ Concepts: Model Discrepancy

- *"All models are wrong,"* but our objective is to make them useful
  - Physics never perfectly represented → capture the important parts!
- In some cases, missing physics can lead to significant ***model discrepancy***
  - *Significant* meaning model form errors are on the same order as other sources of uncertainty
  - Can often be identified as a violation of assumptions about the noise in the measurements during calibration
  - Often results from a model not matching the as-built system



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  - Invalidated inverse problem formulation
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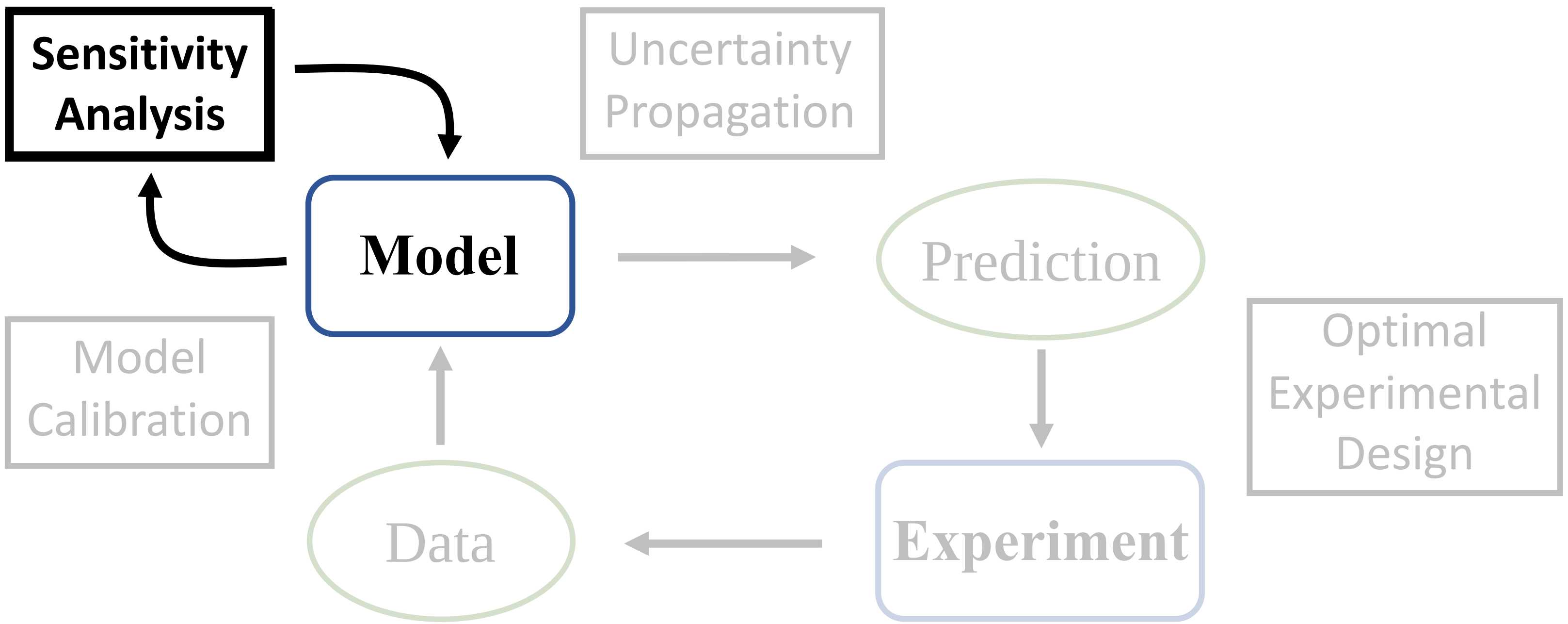
- Potential consequences:
  - Biased estimates of physical parameters
  - Invalidated inverse problem formulation
  - Inaccurate estimates of uncertainty, especially when extrapolating
- Remedies:
  - Implement an advanced calibration method to attempt to learn the discrepancy
  - ***Build a better model*** (using insights from UQ analysis); Ensure the model matches the as-built hardware as close as possible

UQ Concepts: Sensitivity Analysis

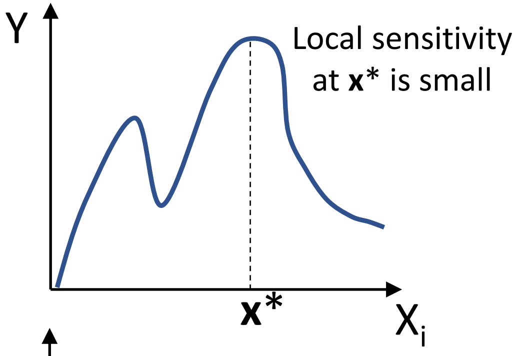


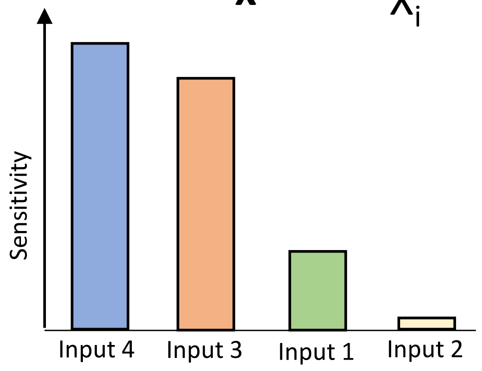
- ***Sensitivity analysis*** identifies the most influential system parameters to properly focus effort/resources in a probabilistic analysis

Sensitivity Analysis Overview

*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, model non-linearity
- Global sensitivity analysis
    - More computationally expensive
    - Holistically assesses effect of uncertainty & model behavior
    - Used to reduce dimensionality or inform additional experiments

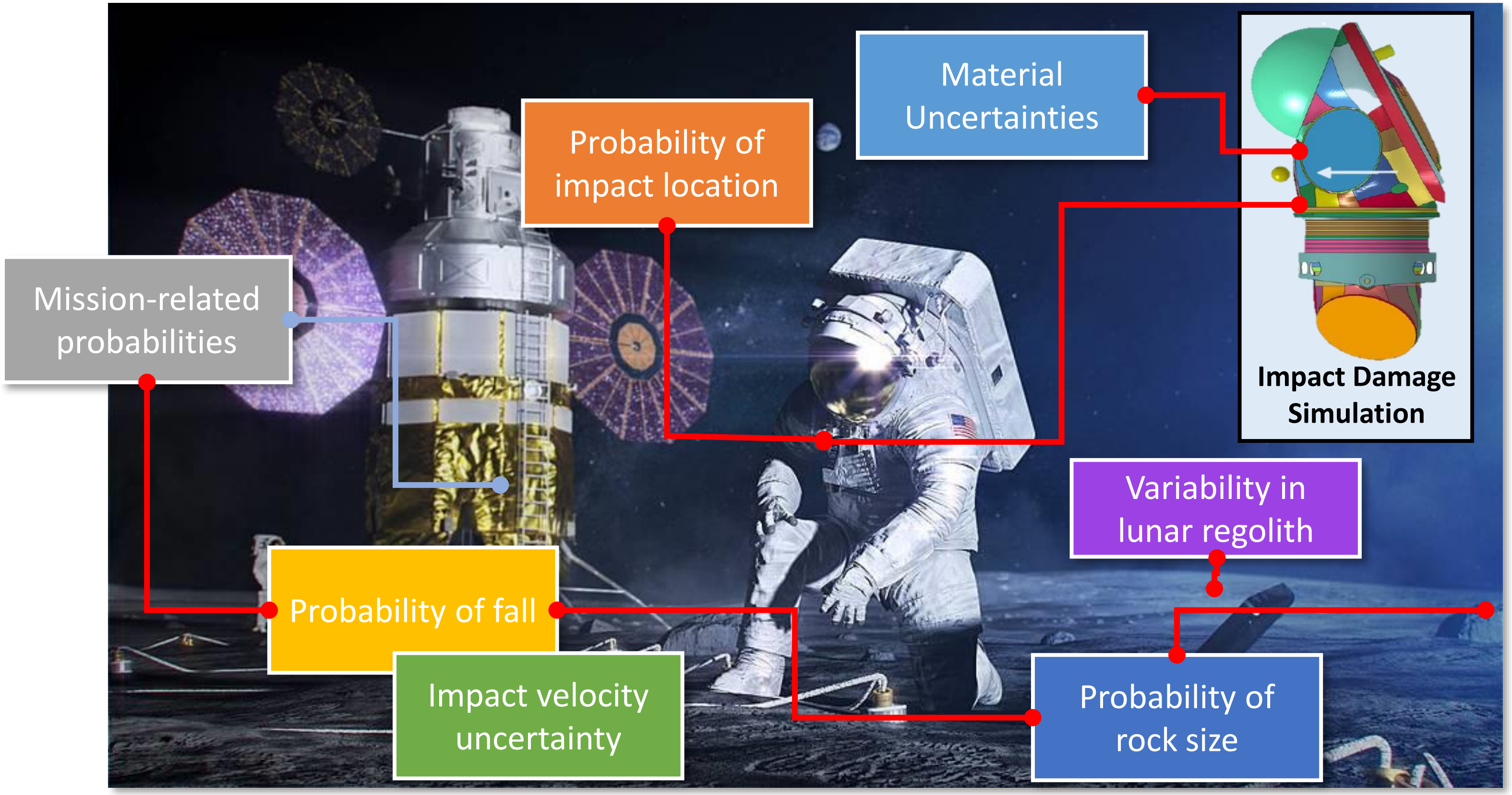




*Global sensitivity analysis. The primer. Andrea Saltelli. 2007.

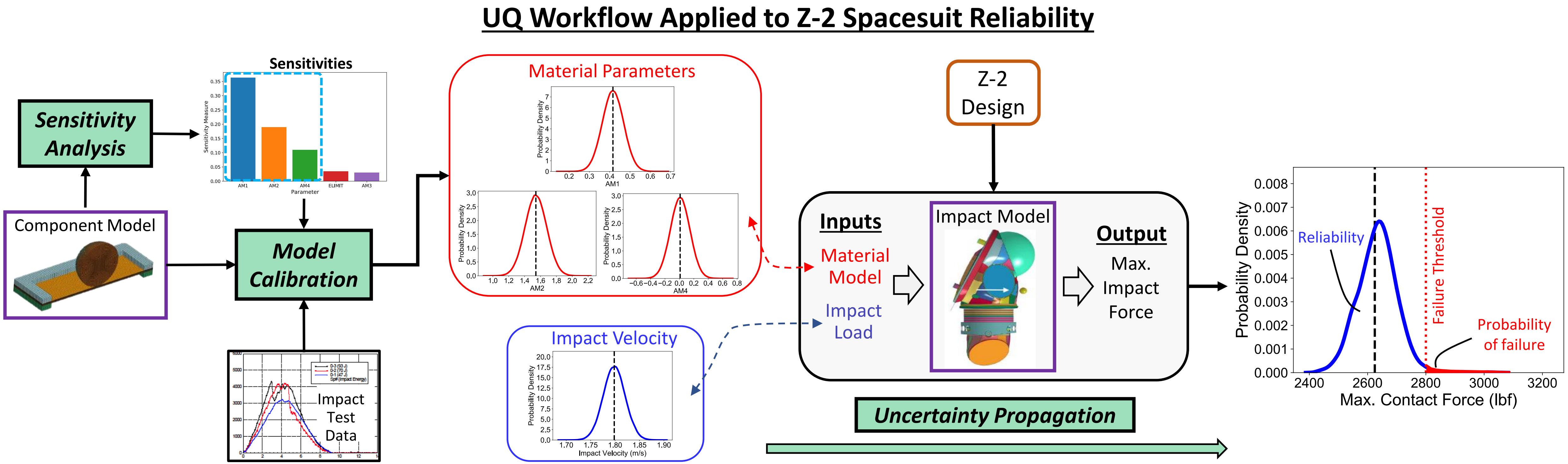
Practical Example – Spacesuit Reliability

- Estimating the reliability of a spacesuit for impact events (e.g., astronaut falls on the lunar surface) using UQ



- **Note**: this example is presented for purposes of demonstration; the reliability estimates provided here are not reflective of the true values for these projects

Z-2 Spacesuit Reliability Analysis

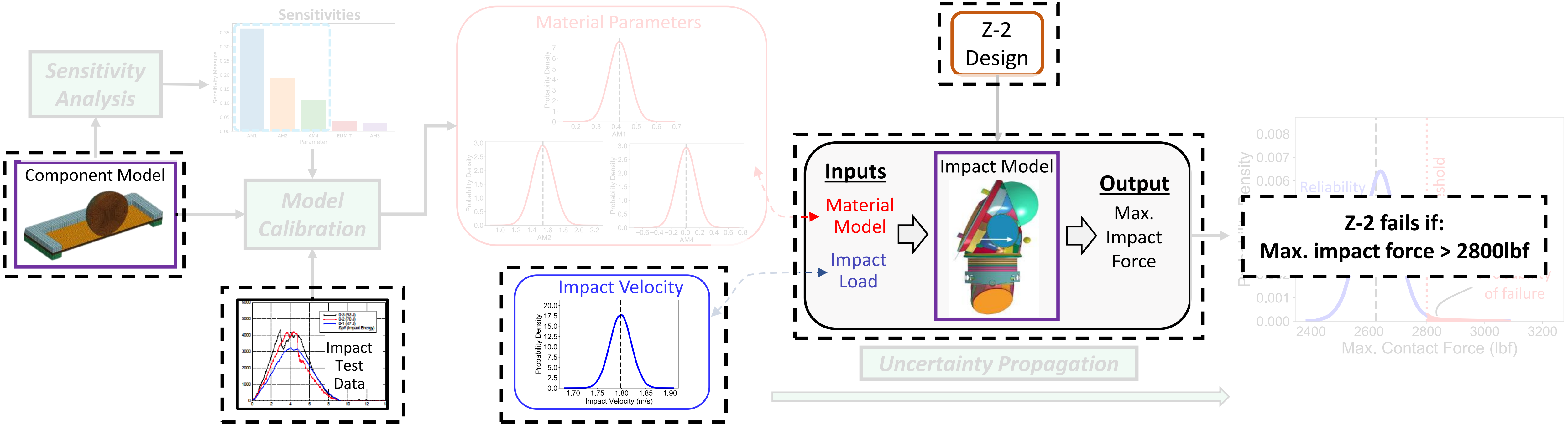


Z-2 Spacesuit Reliability Analysis

Given: candidate design, component/impact models, test data, *assumed* impact load & failure criteria

Estimate: Z-2 impact reliability

UQ Workflow Applied to Z-2 Spacesuit Reliability



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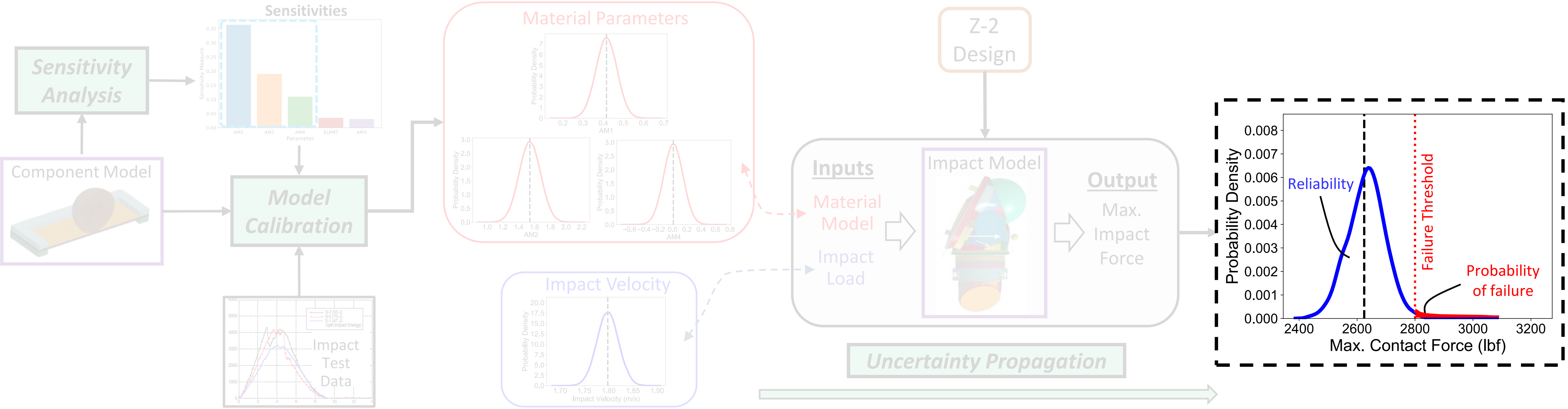

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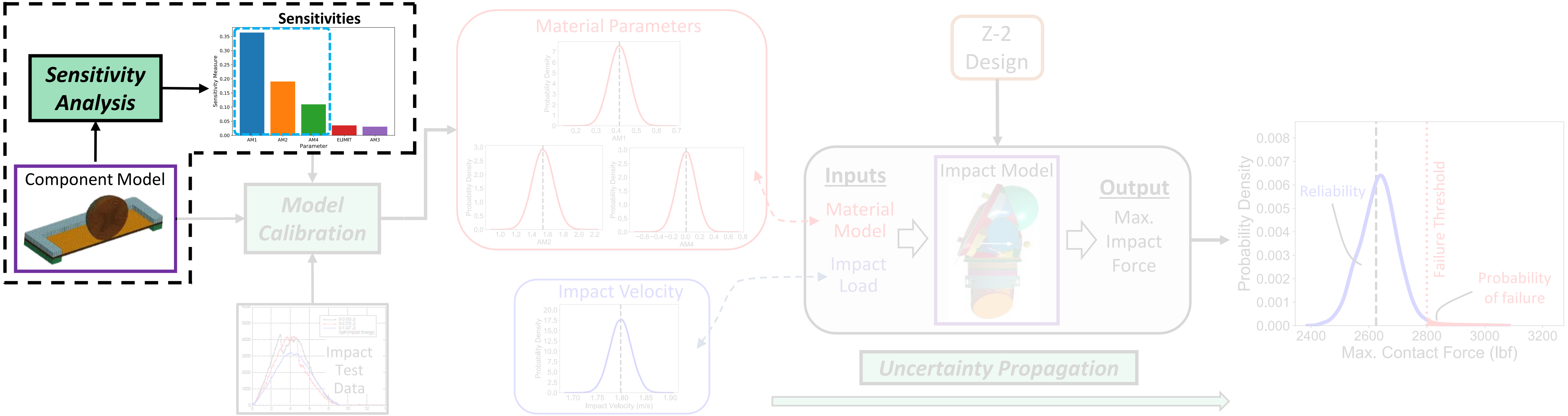


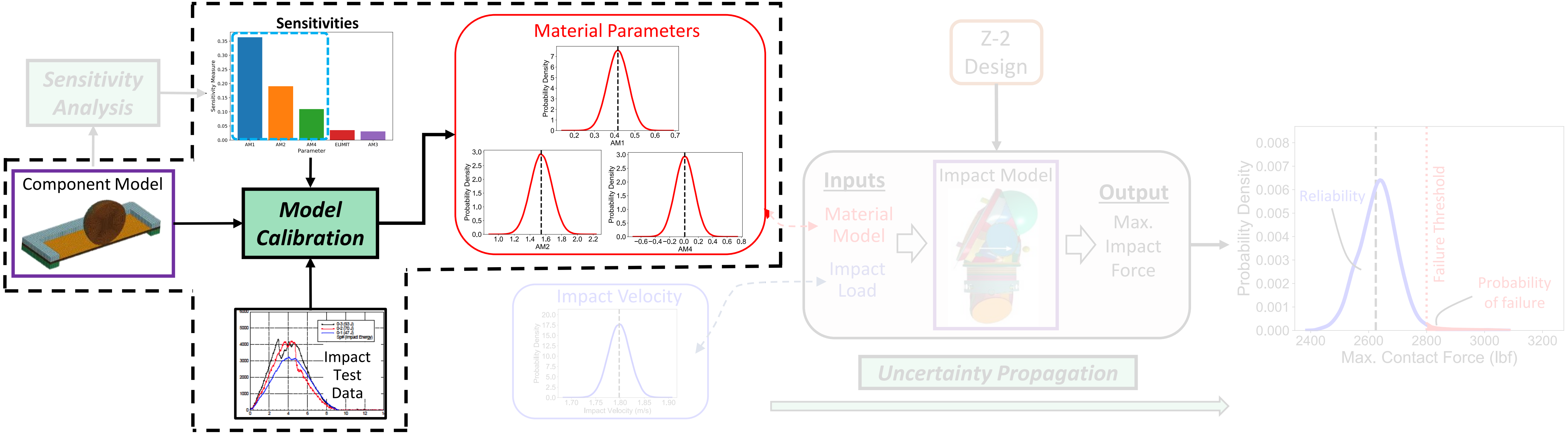
1) Applied ***sensitivity analysis*** to identify the most influential material model parameters to focus on for the remaining UQ analysis

Z-2 Spacesuit Reliability Analysis

Given: candidate design, component/impact models, test data, *assumed* impact load & failure criteria

Estimate: Z-2 impact reliability

UQ Workflow Applied to Z-2 Spacesuit Reliability

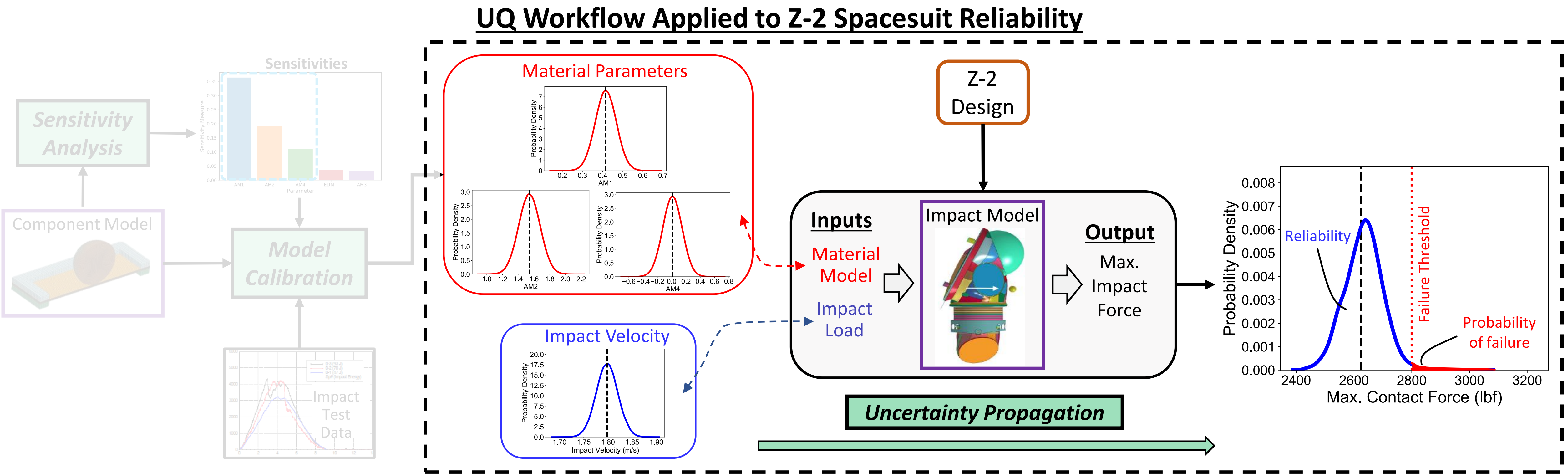


2) Used **model calibration** to quantify uncertainty in material parameters from impact test data

Z-2 Spacesuit Reliability Analysis

Given: candidate design, component/impact models, test data, *assumed* impact load & failure criteria

Estimate: Z-2 impact reliability

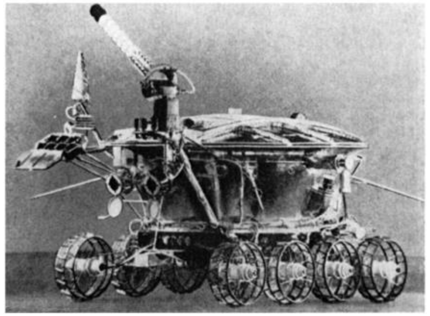


3) Used ***uncertainty propagation*** to estimate reliability given material/impact load uncertainty

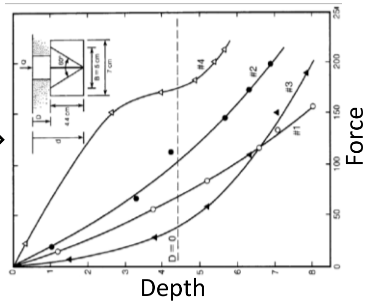
- Reliability ≈ 99.3% (*demonstration purposes only*)
- Quantified material uncertainty resulted in >10% variability in predicted max. contact force

Model Calibration – Lunar Regolith Uncertainty

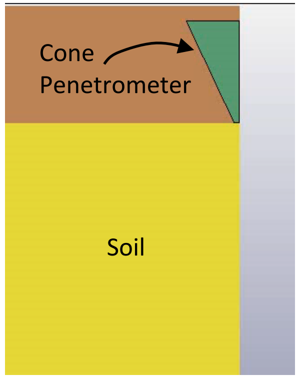
- **Lunar regolith properties**



Rover with Cone Penetrometer



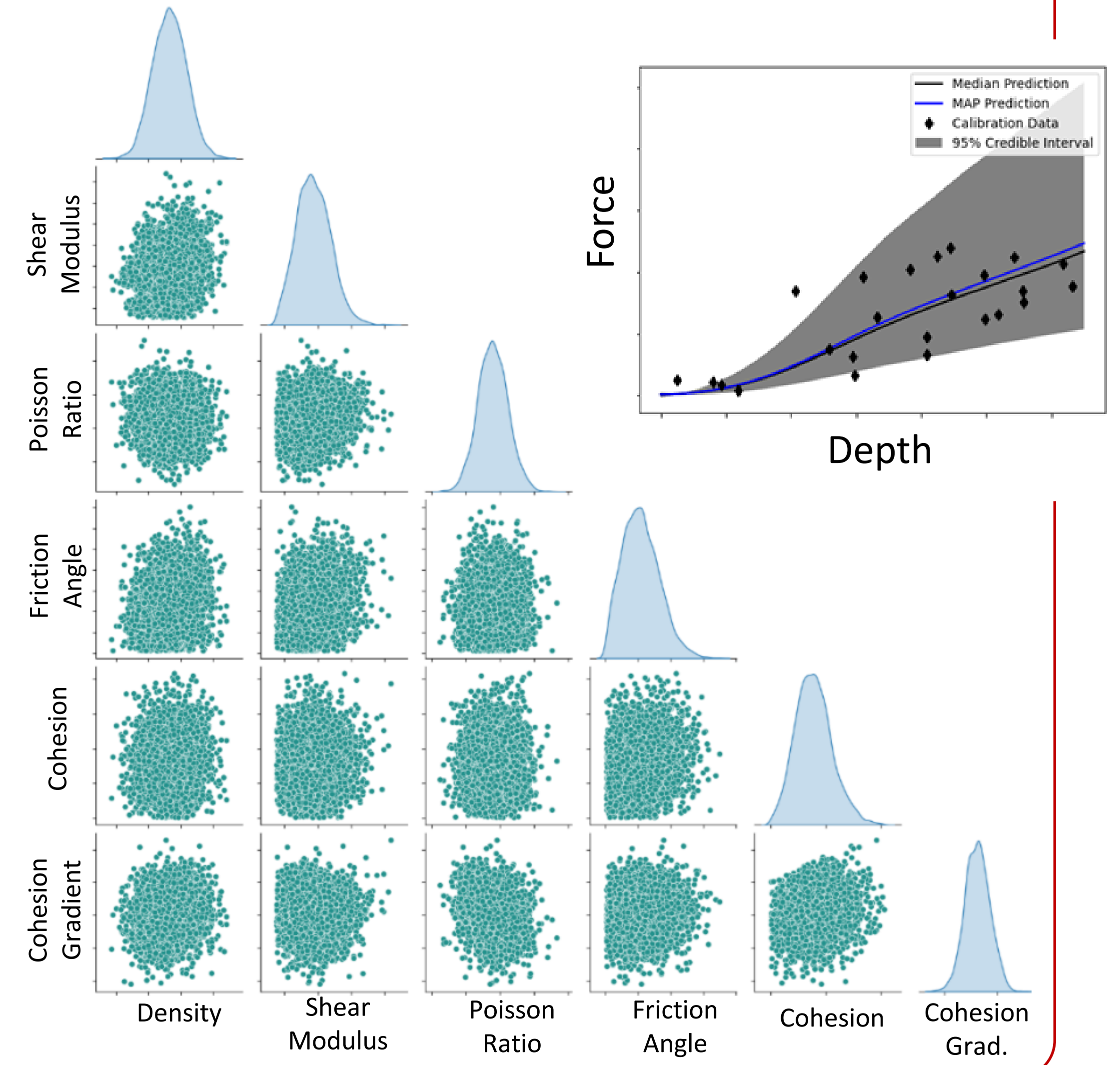
Lunar Regolith Resistance Data*



Penetrometer Model

Probabilistic Model Calibration

Soil Model Parameters



*Heiken, Grant H., David T. Vaniman, and Bevan M. French. *Lunar Sourcebook, a user's guide to the Moon*. 1991.

Summary

- UQ provides a framework to quantify what we know, what we don't know, and to what degree we don't know it, in the context of modeling & simulation
  - Monte Carlo simulation is a general-purpose, simple-to-implement method for uncertainty propagation, but:
  - It can be difficult to know which input parameters should be treated as random variables
    - ➢ Potential solution: **sensitivity analysis**
  - It can be difficult to properly assign probability distributions to input parameters
    - ➢ Potential solution: **model calibration**
  - It can be intractable for expensive, high-fidelity models
    - ➢ Potential solution: **surrogate modeling**

Summary - Common UQ Pitfalls

- Using solutions that are not converged (e.g., not enough samples for Monte Carlo)
- Assuming all input parameters are independent/uncorrelated to simplify an analysis
- Failing to validate a surrogate model (or validating using the same data it was trained on)
- Not accounting for significant model discrepancy / model form uncertainty

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. et al.: "Assessing Next-Gen Spacesuit Reliability: A Probabilistic Analysis Case Study", NASA/TM–20210019495. 2021.
- 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/

Email: james.e.warner@nasa.gov

Backup

Philosophical Points

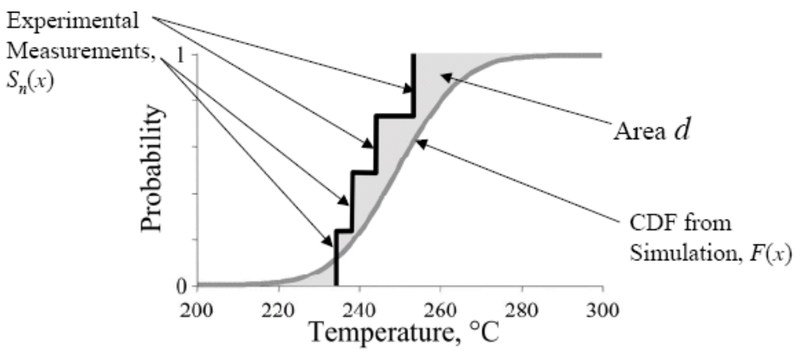
- Types of uncertainty:
  - **Aleatory uncertainty** – uncertainty due to inherent variability or randomness of a physical phenomenon
    - E.g., Variability of material properties in manufactured parts; variation in environmental load
  - **Epistemic uncertainty** – uncertainty due to a fundamental lack of knowledge or simplifying model assumptions, missing physics, measurement bias, etc. that could theoretically be reduced with additional resources/effort
    - Ex: the geometry of a *specific* manufactured part; numerical error from a coarse mesh
- Two schools of thought:
  1. **Bayesian**: probability represents degree of belief of the analyst and can be used to model both aleatory & epistemic uncertainties
  2. **Frequentist**: probability represents the frequency of occurrence and therefore is not appropriate for epistemic uncertainties; instead intervals with no associated likelihood/PDF should be used.

"The Bayesian perspective is… natural for model uncertainty quantification since it provides densities that can be propagated through models." Smith, R. C. Uncertainty Quantification Theory, Implementation, and Applications. 2013.

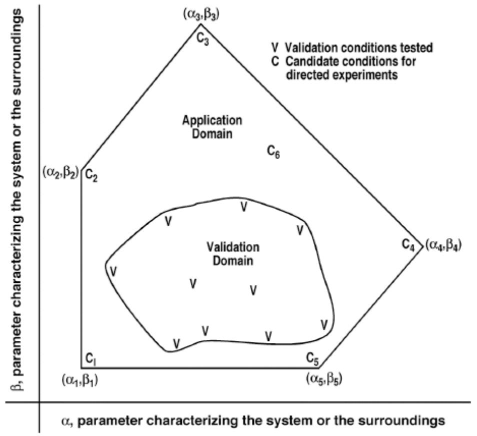
Model Discrepancy Details

- **<u>Model validation / model discrepancy / model form uncertainty</u>**

Validation metric based on experiment/simulation CDFs [1]



Validation vs. Application Domains [1]



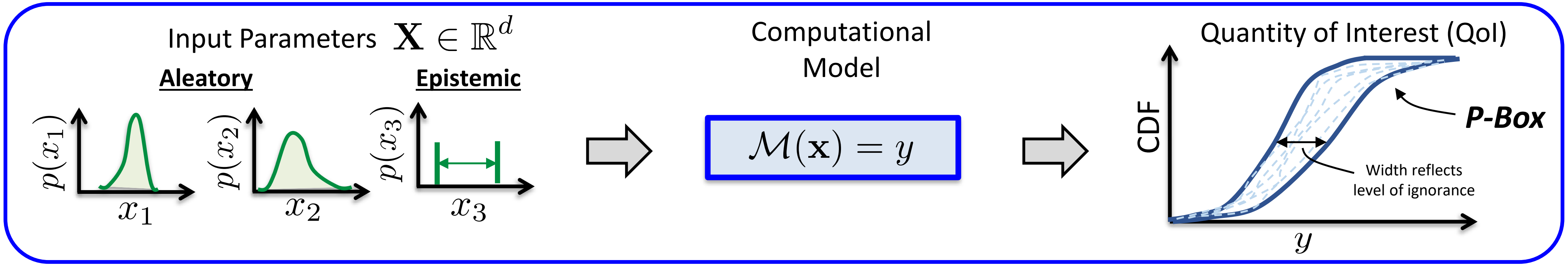
- One approach: calculate validation error metric at series of points in validation domain & build regressor to estimate model form uncertainty in application domain [1]

- References

1. Roy, C. J. and Oberkampf, W. L. *A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing.* 2010.
   - Model-form uncertainty estimation + extrapolation (images above)
2. Kennedy, M. C. and O'Hagan, A. Bayesian calibration of computer models. 2002.
   - Bayesian approach to treating model discrepancy
3. Sills, J. NESC-RP-16-01110, NASA/TM-2021-0009733. 2021.
   - Non-parametric variation approach for model form uncertainty for dynamics

Important Areas Not Covered

- **Mixed and Imprecise Probability Methods**

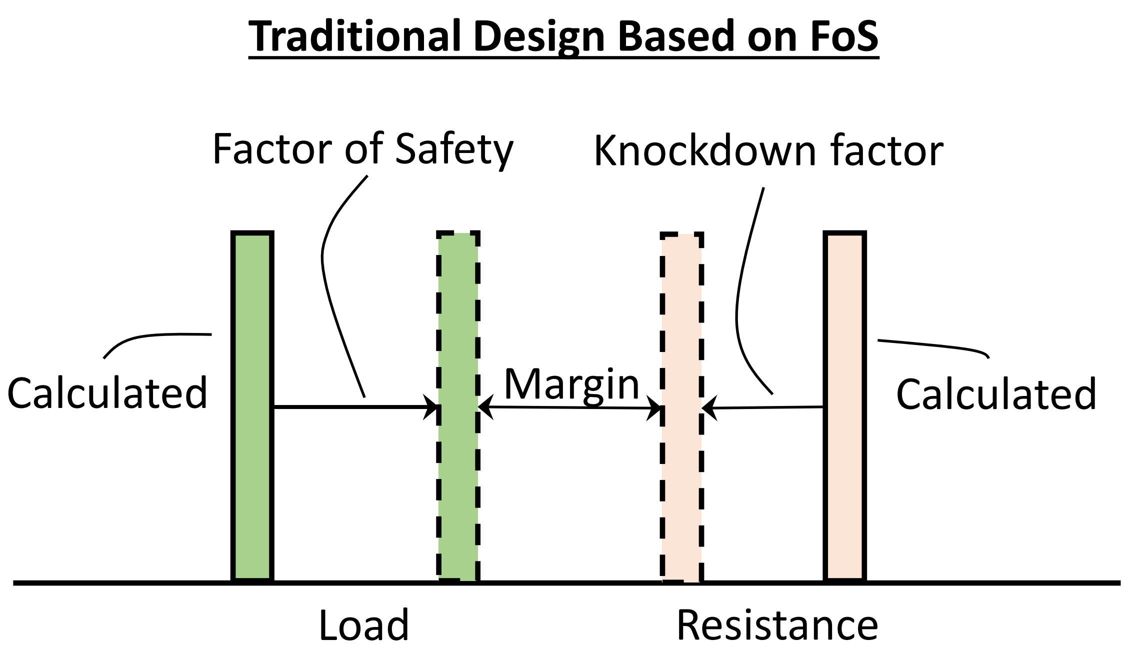


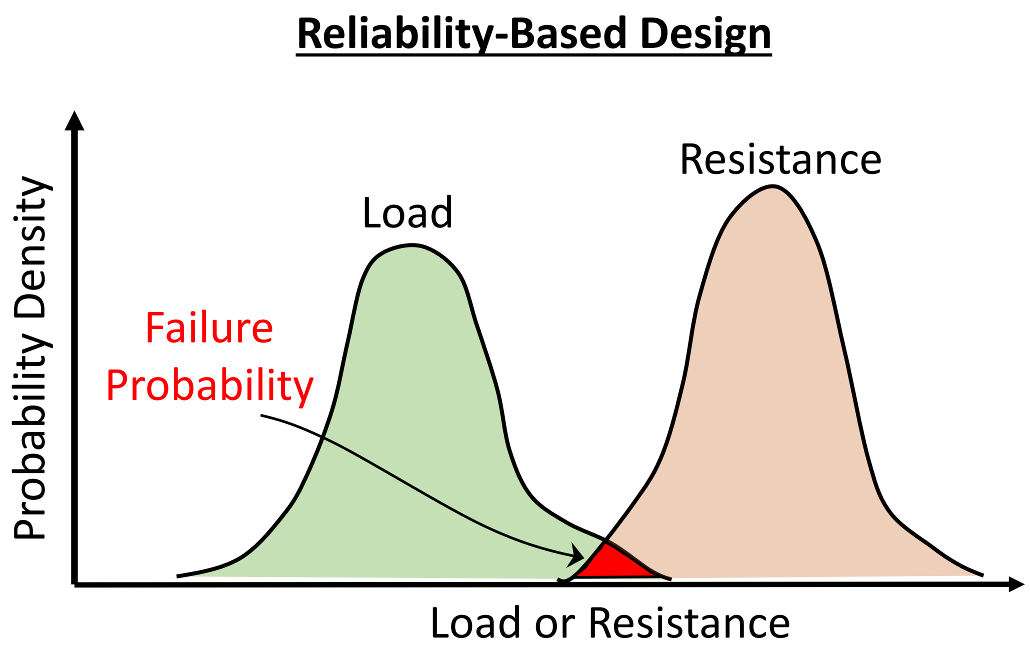
- **Philosophy**: aleatory (irreducible/stochastic) uncertainty is modeled with probability distributions, epistemic (reducible/ignorance) uncertainty is modeled with intervals with no associated probability
- **Solution approach**: double loop Monte Carlo simulation
  - Repeat: select possible epistemic variable values from intervals, perform standard Monte Carlo simulation for aleatory variables; Then: identify min/max CDFs to create P-Box solution
- Provides estimates in the form of intervals:
  - P(y < 5) = [0.2, 0.7]; Probability of failure = [0.97, 0.9999]
- Simple, efficient compromise: use worst case values for epistemic variables & use standard Monte Carlo
  - Can be challenging to identify “worst case” values for large numbers of epistemic uncertainties and complex failure criteria

- References

1. Roy, C. J. and Oberkampf, W. L. *A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing.* 2010.
2. Ferson, S. and Ginzburg, L. R. *Different methods are needed to propagate ignorance and variability*. 1996

Factor of Safety- vs. Reliability-Based Design





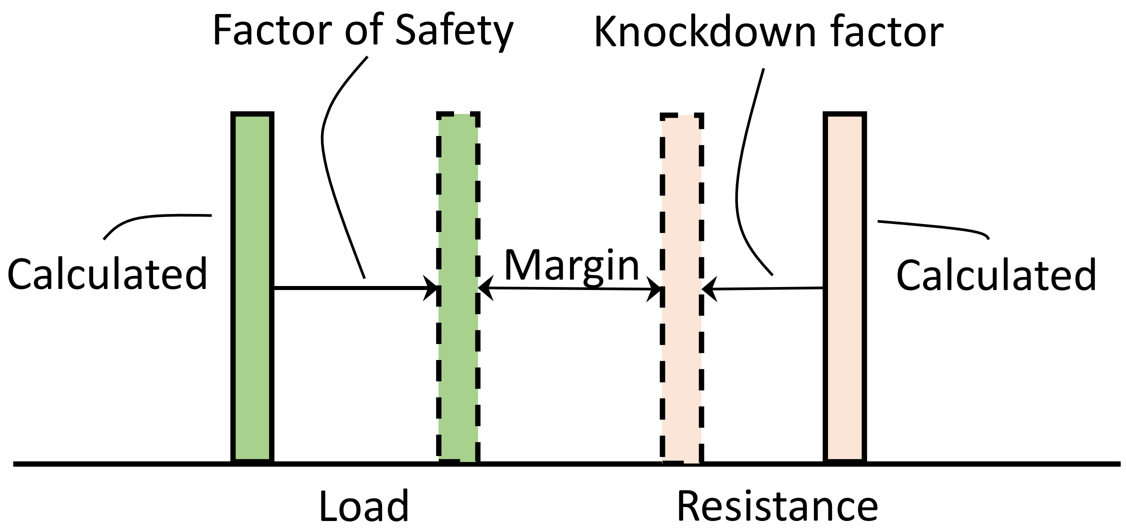
FoS Shortcomings

- Determined empirically, not necessarily based on physics/mathematics
  - Inconsistencies observed from program to program; between NASA and other external organizations
  - Difficult to specify for new vehicle types, materials, and environments
- May be sequentially applied by multiple teams
  - Can be costly, conservative, inefficient
- Does not provide measures of reliability from the design process

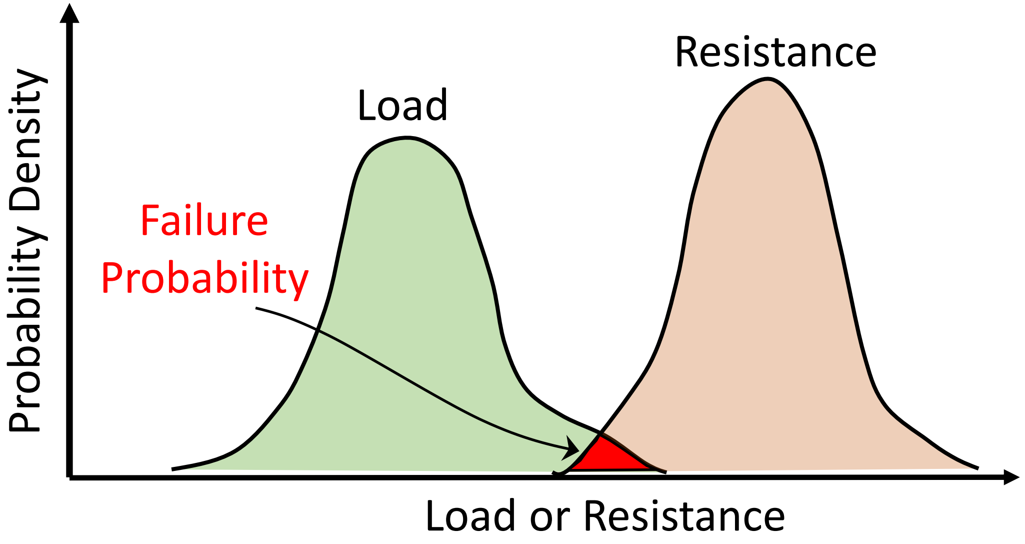
Images adapted from Raju et al. White Paper on Factors of Safety. NASA/TM-2009-215723

Factor of Safety- vs. Reliability-Based Design

Traditional Design Based on FoS



Reliability-Based Design



Reliability-Based Design

- Classical structural reliability assumes load & resistance are independent, Gaussian distributions and yields a simple analytical formula for probability of failure
- The resistance (strength) distribution can be determined directly from A/B-basis properties
- For practical problems, more general UQ methods are often needed to estimate the load (stress) distribution or the probability of failure (P[L > R]) directly – **the focus of today's slides**

Images adapted from Raju et al. White Paper on Factors of Safety. NASA/TM-2009-215723

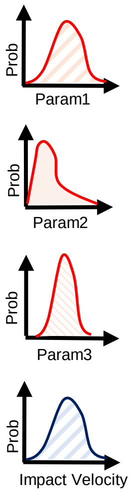
SimTools: In-House Software for Automating Simulations

Specify:
1) Number of input samples/combinations
2) Number of simulations to run in parallel
3) Number of processors to run each simulation on
4) Output metrics to compute & store

Produces:
- Processed input/output dataset

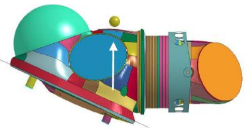
x	y	x	k	d	e	3
1	2	3	5	2	5	3
3	3	3	2	2	2	3
3	2	2	2	2	2	2
0	9	8	6	5	4	3

Input Distributions or bounds



1

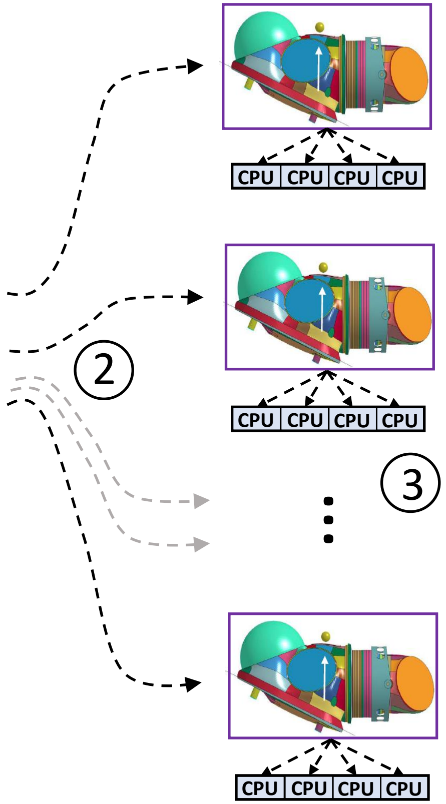
Nominal FEM model



High Performance Computing Cluster Scheduling

Inputs

AM1	…	VEL
12.4	…	1.0
14.3	…	1.4
…	…	…
13.1	…	1.1



Postprocessing & Data Management

4

Outputs

F-max	E-Max
1.2×10^3	5.4×10^3
1.8×10^3	4.9×10^3
…	…
1.6×10^3	5.8×10^3

Example: Needed to run 200 suit simulations for different inputs; Ran 15 simulations at a time on 10 processors each

➢ Performed 1+ years of serial computation time in around 1 week of wall time