

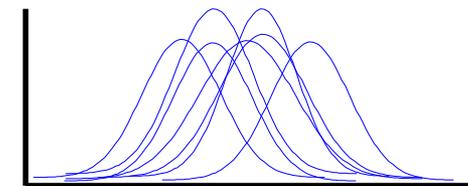
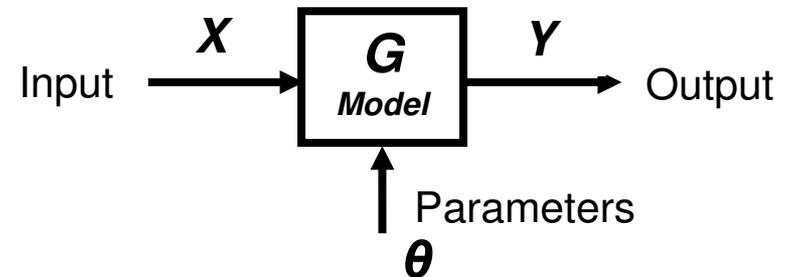
# Uncertainty Aggregation Variability, Statistical Uncertainty, and Model Uncertainty

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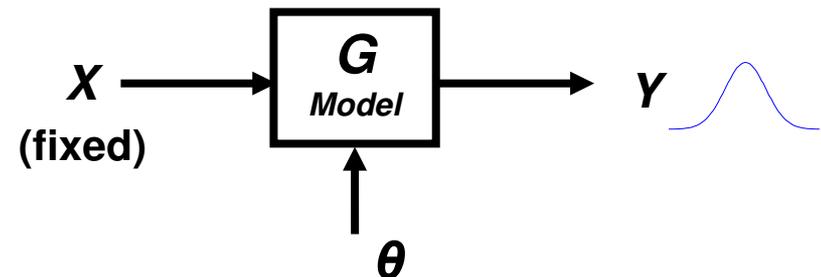
ETICS 2018  
Roscoff, France; June 4, 2018

# Sources of Uncertainty in Model Prediction

- Natural Variability (Aleatory)
  - Variation across
    - Samples → Random variables
    - Time → Random processes
    - Space → Random fields
- Input uncertainty (Epistemic)
  - Sparse data
  - Imprecise and qualitative data
  - Measurement errors
  - Processing errors
- Model uncertainty (Epistemic)
  - Model parameters
  - Solution approximation
  - Model form

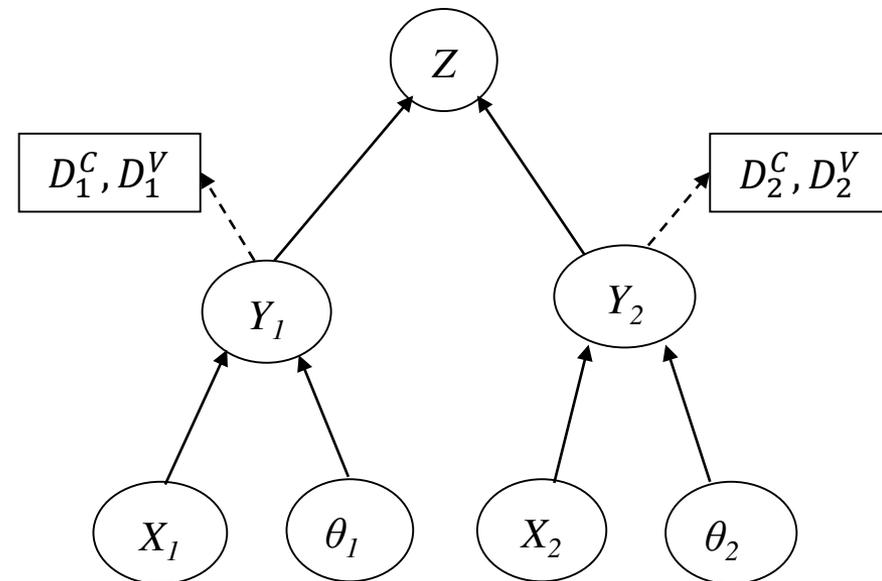


Multiple PDFs of input  $X$



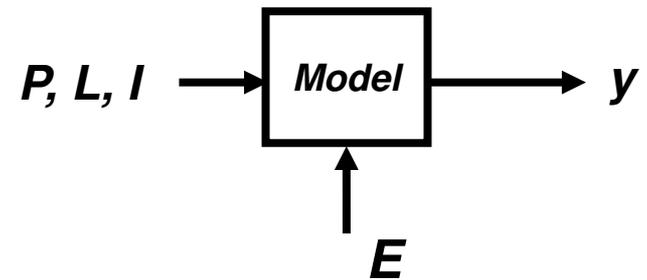
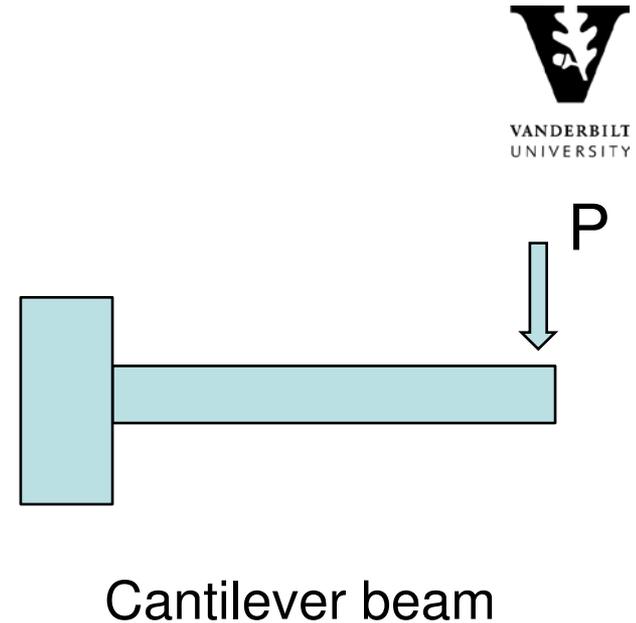
# Uncertainty aggregation

- Information at multiple levels
  - Inputs
  - Parameters
  - Model errors
  - Outputs
- Heterogeneous information
  - Multiple types of sources, formats
    - models, tests, experts, field data
  - Multiple physics, scales, resolutions
  - Different levels of fidelity and cost
- How to fuse **ALL** available information to quantify uncertainty in system-level prediction?

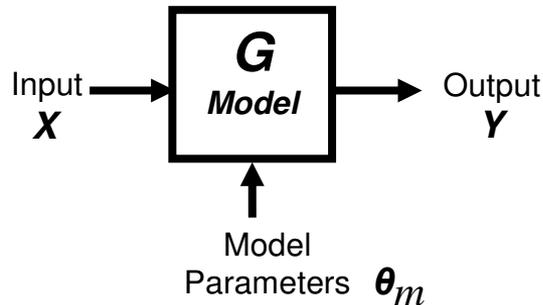


# A simple example

- Model for vertical deflection at free end (Euler-Bernoulli)  $y = \frac{PL^3}{3EI}$
- Assume  $L$  and  $I$  have only aleatory variability
- $P \rightarrow$  random variable (aleatory), but we may not know its distribution type  $D$  and parameters  $\theta_p$ , thus  $P \sim D(\theta_p)$  could have both aleatory and epistemic uncertainty
- $E \rightarrow$  model parameter (could be only epistemic, only aleatory, or both)
- Model error  $\rightarrow$  infer from tests
- Other issues
  - Boundary condition  $\rightarrow$  degree of fixity  $\rightarrow$  infer from tests
  - Spatial variability of  $E \rightarrow$  random field
  - Temporal variability of  $P \rightarrow$  random process
- Random field and random process parameters need to be inferred from data  $\rightarrow$  could have both types of uncertainty



# Treatment of Epistemic Uncertainty



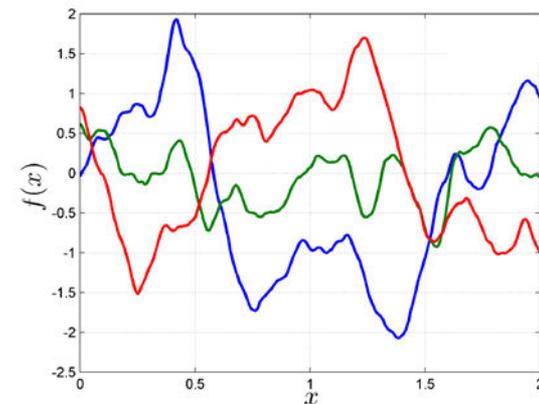
$$Y = G(X, \theta_m) + \varepsilon_M$$
$$\varepsilon_M = \varepsilon_{mf} + \varepsilon_{num}$$

- Statistical Uncertainty
  - Distribution type  $D$  and parameters  $\theta_p$  of  $X \sim D(\theta_p)$
- Model Uncertainty
  - System model parameters  $\theta_m$ 
    - uncertainty represented by probability distributions (Bayesian) ← **Calibration**
  - Model form of  $G$ 
    - Model form error  $\varepsilon_{mf}$  (quantified using validation data) ← **Validation**
  - Numerical solution error  $\varepsilon_{num}$  in  $G$ 
    - Discretization error (quantified using convergence study) ← **Verification**
    - Surrogate model error (by-product of surrogate model building)
- **Bayesian Approach** → All uncertainty/error terms represented through probability distributions

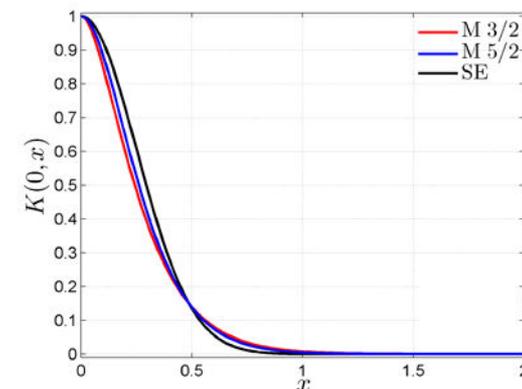
# BACKGROUND TOPICS

# Quantities varying over space and time

- Quantities expressed as random processes/fields
  - e.g., Loading at one location  $\rightarrow$  random process over time
  - e.g., material properties  $\rightarrow$  random field over space
- Aleatory uncertainty alone
  - Random process/field parameters are deterministic
    - e.g., **Gaussian process**  $w(x) \sim \text{GP}(m(x), C(x, x'))$
    - $m(x) = a + bx + cx^2 \dots$
    - $C(x, x') = \text{Cov}(w(x), w(x'))$ ,
      - e.g., **Squared exponential (SE)**
  - $$C(r, l) = \sigma^2 \exp(-r^2 / l^2)$$
- With epistemic uncertainty
  - Random process/field parameters are uncertain

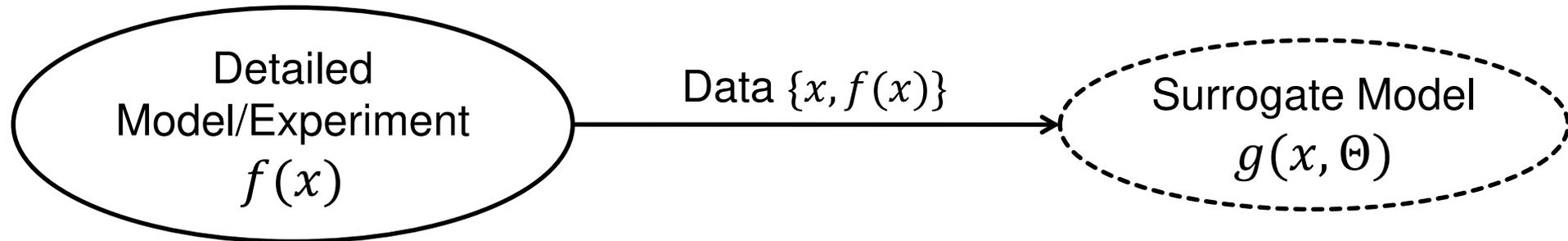


Random process realizations



Correlation functions

# Surrogate Modeling

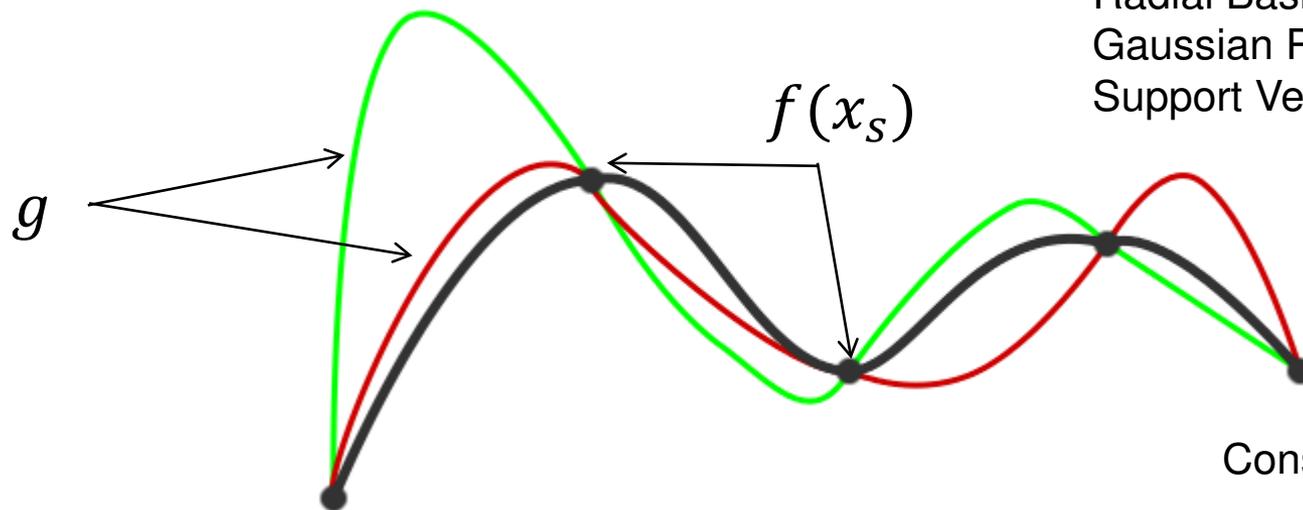


- ❖ Uncertainty quantification of the output
- ❖ Multiple runs of expensive system analysis
- ❖ Unknown functional form

- ❖ Inexpensive to evaluate at any location

- ❖ Examples:

Polynomial Chaos Expansions  
Radial Basis Functions  
Gaussian Process Models  
Support Vector Machines



**Surrogate model output has uncertainty**

Consistent Reconstruction  
 $g(x_s) = f(x_s)$

# Global Sensitivity Analysis

- $Y = G(\mathbf{X})$
- $\mathbf{X} \rightarrow$  random variables
- $Y \rightarrow$  calculated through uncertainty propagation
- Apportion variance of  $Y$  to inputs  $\mathbf{X}$
- Analyze sensitivity of output over the entire domain rather than (1) suppressing a variable completely (2) using local derivatives
- Individual effects  $S_I$  & Total effects  $S_T$  (i.e., in combination with other variables)

$$S_I = \frac{V_{X_i}(E_{X_{\sim i}}(Y | X_i))}{V(Y)} \quad S_T = \frac{E_{X_{\sim i}}(V_{X_i}(Y | X_{\sim i}))}{V(Y)}$$

- Single loop sampling approaches exist in literature to calculate  $S_I$  and  $S_T$

# Parameter estimation: Least Squares



- Linear regression  $Y = X\theta$ 
  - $\theta \rightarrow$  model parameters (m by 1)
  - “n” ordered input – output observations
    - Each input observation is a vector (1 by m)
    - Each output observation is a scalar
  - Construct  $X \rightarrow$  matrix of inputs (n by m)
  - Construct  $Y \rightarrow$  vector of outputs (n by 1)

$$\hat{\theta} = (X^T X)^{-1} (X^T Y)$$

Coefficient of determination  $R^2$   
Proportion of variance explained by the linear regression model  
High Value  $\neq$  Accurate Prediction

- Non-linear model  $Y = G(X, \theta)$ 
  - Simple least squares  $\rightarrow$  Minimize  $S(\theta) = \sum_{i=1}^n (y_i - G(x_i, \theta))^2$
  - $\alpha$ -level confidence intervals on  $\theta$  using F-statistic  $S(\theta) \leq S(\hat{\theta}) \left\{ 1 + \frac{m}{n-m} F_{m, n-m}^\alpha \right\}$
- Advanced methods  $\rightarrow$  weighted, generalized, moving, iterative
  - Unbiased, convergent estimates
  - Applicable to multiple output quantities
- Disadvantages
  - Based on assumption of normally distributed residuals
  - Difficult to include other types of uncertainty in input/output (imprecision, no ordered pairs)

# Likelihood function

Likelihood → Probability of observing the data, given specific values of parameters

## Example

- Random variable  $X$ ; Available data points  $x_i$  ( $i = 1$  to  $n$ )
- Suppose we fit a normal distribution to  $X$

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Likelihood function

$$L(\mu, \sigma) = P(\text{observing data } x_i \mid (\mu, \sigma)) \propto f_X(x_i)$$

Considering all  $n$  data points,

$$L(\mu, \sigma) \propto \prod_{i=1}^n f_X(x_i)$$

Maximum likelihood estimate (MLE)

→ Maximize likelihood function and estimate parameters  $(\mu, \sigma)$

# Bayesian estimation

- Maximum Likelihood Estimate
  - Maximize  $L(\theta) \rightarrow$  Point estimate of  $\theta$
- To account for uncertainty regarding  $\theta$ 
  - Bayesian approach  $\rightarrow$  probability distribution of  $\theta$
  - Assume a uniform prior over the domain of  $\theta$

$$f(\theta) = \frac{L(\theta)}{\int L(\theta)}$$

- Calculate marginal distributions of individual parameters
- PDF of  $X \rightarrow f_X(x/\theta)$ 
  - Distribution of  $\theta \rightarrow f(\theta)$
  - Each sample of  $\theta \rightarrow$  PDF for  $X$
  - Family of PDFs for  $X$

# Bayes' Theorem

- Theorem of Total Probability

$$P(A) = \sum_{i=1}^n P(A | E_i) P(E_i)$$

(Events  $E_i$  are mutually exclusive and collectively exhaustive)

- Bayes theorem

$$P(A | B) = \frac{P(B | A) P(A)}{P(B)}$$

$$P(E_i | A) = \frac{\overset{\text{likelihood}}{P(A | E_i)} \overset{\text{prior}}{P(E_i)}}{\underset{\text{normalizing constant}}{P(A)}}$$

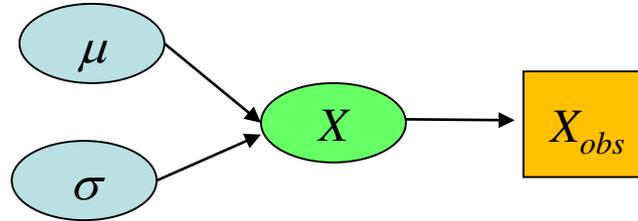
- In terms of probability densities (continuous variables):

- $\theta$  : parameter to be updated
- $\mathbf{D}$  : experimental data
- $\Pr(\mathbf{D}|\theta)$  : likelihood function of  $\theta$
- $\pi(\theta)$  : prior PDF of  $\theta$
- $\pi(\theta|\mathbf{D})$  : posterior PDF of  $\theta$

$$\pi(\theta | \mathbf{D}) = \frac{\Pr(\mathbf{D} | \theta) \pi(\theta)}{\int \Pr(\mathbf{D} | \theta) \pi(\theta) d\theta}$$

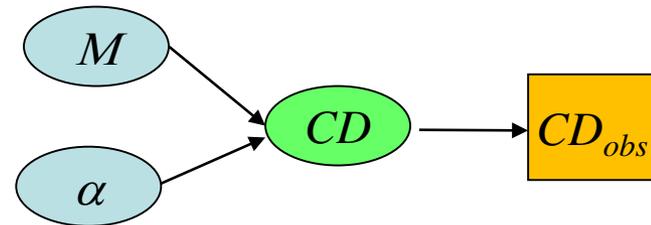
# Three examples of Bayesian inference

- Distribution parameters of a random variable → Statistical uncertainty



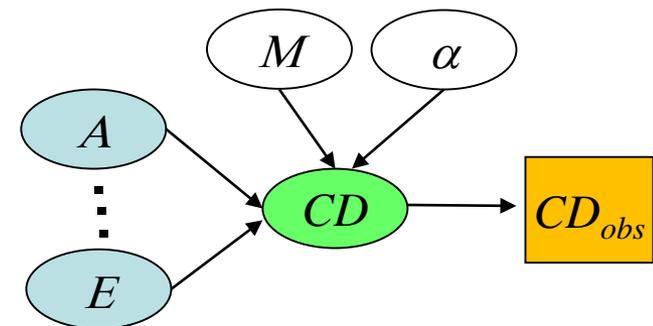
- Distributions of unmeasured test inputs

$$CD = 0.05 - 0.015 * M + 4.0e-004 * \alpha - 7.04e-004 * M * \alpha + 1.45e-003 * M^2 + 4.6e-004 * \alpha^2$$



- Distributions of model coefficients  
**(Bayesian regression)**

$$CD = 0.05 - A * M + B * \alpha - C * M * \alpha + D * M^2 + E * \alpha^2$$



# Construction of posterior distribution

$$\pi(\theta | \mathbf{D}) = \frac{\Pr(\mathbf{D} | \theta)\pi(\theta)}{\int \Pr(\mathbf{D} | \theta)\pi(\theta)d\theta}$$

- Conjugate distributions → Prior and posterior have same distribution type; only the parameters change.
- Sampling-based methods
  - **Markov Chain Monte Carlo methods**
    - Metropolis
    - Metropolis-Hastings
    - Gibbs
    - Slice sampling
    - Adaptive improvements
  - **Particle filter methods**
    - Sequential importance re-sampling (SIR)
    - Rao-Blackwellization

# Statistical Uncertainty: Bayesian Inference of Distribution Parameters



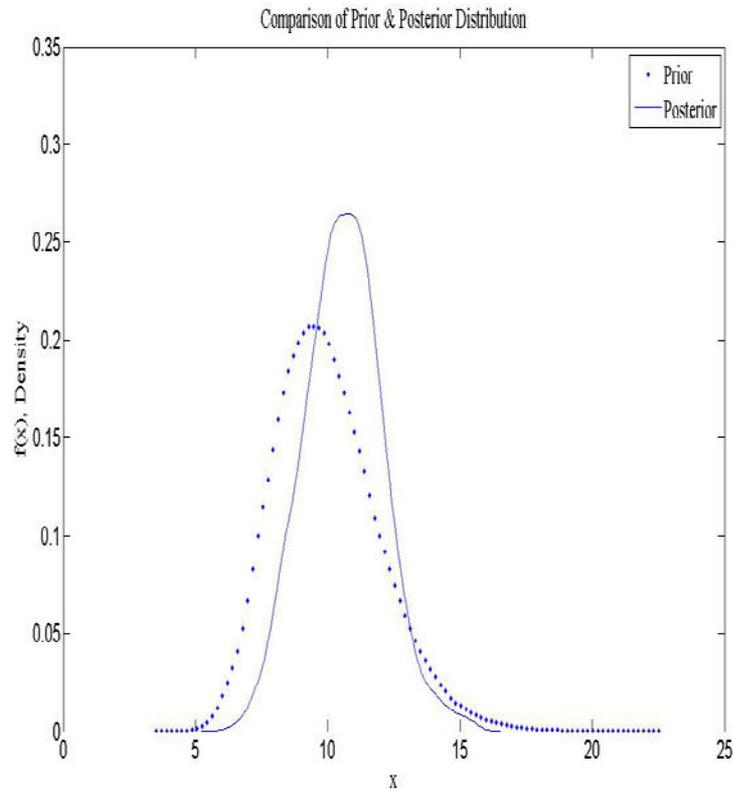
- An RV 'X' has a known 'pdf' type  $\rightarrow X \sim f_X(x | \theta)$
- Unknown parameters  $\theta$
- Observe instances of 'X' through experiments
- Assume prior distributions for  $\theta$  and update them

$$L(\theta) = \prod_{i=1}^n f_X(x_i | \theta)$$

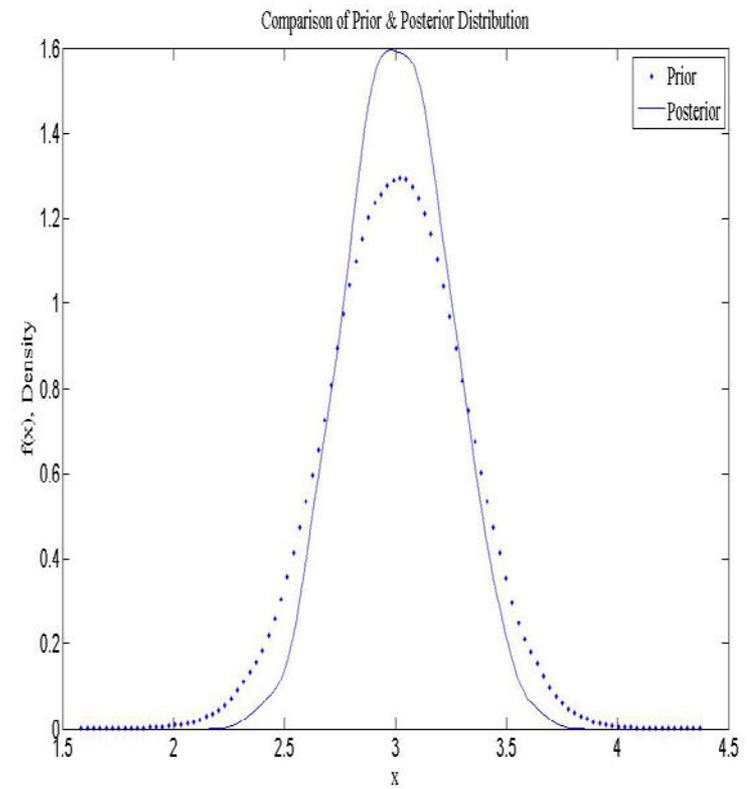
**X ~ N( $\mu, \sigma$ )     $\theta = \{\mu, \sigma\}$     Observed Values of X = {12, 14}**

Parameter No.	Parameter Name	Prior Distribution			Posterior Distribution	
		PDF Type	Mean	Moments	Mean	Variance
1	$\mu$	Log Normal	10	4	10.57	2.19
2	$\sigma$	Johnson	3	0.085 -0.006 0.017	3.03	0.05

# Comparison of densities



Prior & Posterior of  $\mu$



Prior & Posterior of  $\sigma$

# Model Uncertainty: Bayesian Inference of Model Inputs

- Consider a model  $y = g(\mathbf{x}) + \varepsilon$
- Assume prior distributions for  $\mathbf{x}$
- Observe  $y$  through experiments ( $y_i, i = 1$  to  $n$ )
- Update distributions for  $\mathbf{x}$
- $\varepsilon$  is assumed to be a normal random variable with zero mean and  $\sigma^2$  variance, which is calculated from instances of  $y$  observed through experiments.

$$L(x) = \prod_{i=1}^n \exp\left(-\frac{(y_i - g(x))^2}{2\sigma^2}\right)$$

# Model Uncertainty: Bayesian Inference of Model Coefficients

- Consider a model  $y = b_0 + b_1 \cdot X_1 + b_2 \cdot X_2 + \dots + \varepsilon$
- The model coefficients  $\mathbf{b}$  are unknown
- Model calibration data are collected  $(x_i, y_i)$  ( $i = 1$  to  $n$ )
- Prior distributions are assumed for  $\mathbf{b}$  and updated.
- $\varepsilon$  is assumed to be a normal random variable with zero mean and  $\sigma^2$  variance
- This method is applicable irrespective of whether the model is linear or not  $\rightarrow y = g(\mathbf{x}, \mathbf{b})$

$$L(\mathbf{b}) = \prod_{i=1}^n \exp\left(-\frac{(y_i - g(x_i, \mathbf{b}))^2}{2\sigma^2}\right)$$

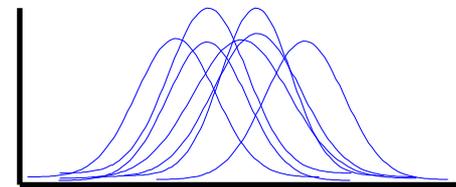
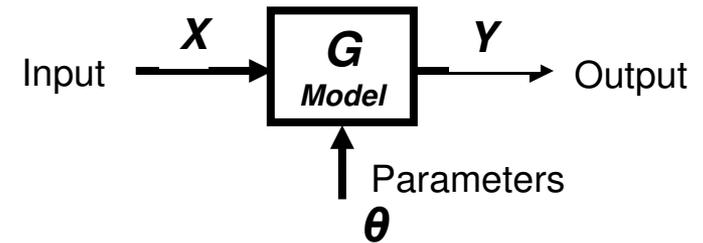
# Summary of Background Topics

- Aleatory vs. epistemic uncertainty
  - In random variables and random processes/fields
- Surrogate modeling
  - Adds to the uncertainty in prediction
- Sensitivity analysis
  - Variance-based
- Parameter estimation
  - Distribution parameters (statistical uncertainty)
  - Model parameters (model uncertainty)
  - Likelihood, Bayes' theorem, and MCMC

# STATISTICAL UNCERTAINTY

# Input uncertainty due to data inadequacy

- Sources of data inadequacy
  - Sparsity
  - Imprecision (i.e., interval)
  - Vagueness, ambiguity
  - Missing
  - Erroneous, conflicting
  - Measurement noise
  - Processing errors



Multiple PDFs of input  $X$

- Data inadequacy leads to epistemic uncertainty in the quantification of model inputs and parameters
  - Value of a deterministic variable
  - Value of distribution parameter of a random variable
  - Values of parameters of random process or random field

# Topics



- Parametric approach
  - Family of distributions
  - Model selection
  - Ensemble modeling
- Non-parametric approach
  - Kernel density
  - General approach with point and interval data
- Separating aleatory and epistemic uncertainty

# Non-Probabilistic Methods to handle epistemic uncertainty



- Interval analysis
- Fuzzy sets / possibility theory
- Evidence theory
- Information gap theory

# Probabilistic Methods



- Frequentist  $\rightarrow$  confidence bounds
- P-boxes, imprecise probabilities
- Family of distributions
- Bayesian approach

Statistical uncertainty

$\rightarrow$  Distribution type

$\rightarrow$  Distribution parameters

# Family of distributions



- Johnson
- Pearson
- Beta
- Gamma

Four-parameter families

# Johnson family of distributions

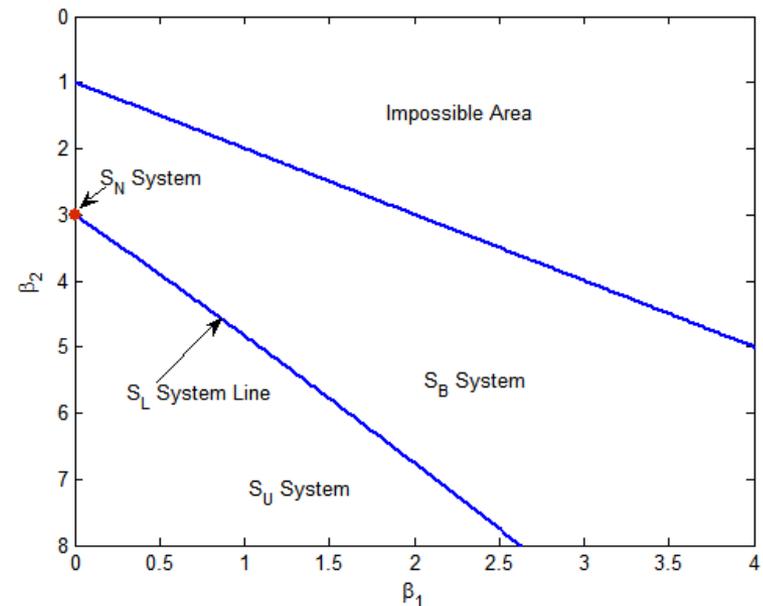
PDF: 
$$f_x(x) = \frac{\delta}{\lambda\sqrt{2\pi}} g'\left(\frac{x-\xi}{\lambda}\right) \exp\left\{-\frac{1}{2}\left[\gamma + \delta \cdot g\left(\frac{x-\xi}{\lambda}\right)\right]^2\right\}$$

CDF: 
$$F(x) = \Phi\{\gamma + \delta \cdot g[(x - \xi) / \lambda]\}$$

Inverse CDF: 
$$Z = \gamma + \delta \cdot g[(x - \xi) / \lambda]$$

Z - standard normal variate

$g(y) = \ln(y)$ , for lognormal ( $S_L$ )  
 $= \ln\left[y + \sqrt{y^2 + 1}\right]$ , for unbounded ( $S_U$ )  
 $= \ln\left[y / (1 - y)\right]$ , for bounded ( $S_B$ )  
 $= y$ , for normal ( $S_N$ )



$$\beta_1 \equiv m_3^2 / m_2^3 \qquad \beta_2 \equiv m_4 / m_2^2$$

# Statistical uncertainty: Parametric approach

## Case 1: Known distribution type

- Estimate distribution parameters of  $X$
- Assume distribution type is known  
 $\rightarrow f_X(x|P)$
- Data  $D \rightarrow m$  point data ( $x_i, i = 1$  to  $m$ )

$$L(P) = \text{Prob}(D | P) = \text{Prob}(x_i | P)$$

$$= \int_{x_i - \frac{\varepsilon}{2}}^{x_i + \frac{\varepsilon}{2}} f_X(x | P) dx = \varepsilon f_X(x_i | P) \propto f_X(x_i | P)$$

$$L(P) \propto \prod_{i=1}^m f_X(x_i | P)$$

- Consider an interval  $(a, b)$  for  $X \rightarrow$

$$\begin{aligned} L(P) &\propto \text{Prob}(D | P) \\ &= \text{Prob}(x \in [a, b] | P) \\ &= \int_a^b f_X(x | P) dx \end{aligned}$$

- Likelihood can include both point data and interval data

$$L(P) \propto \left( \prod_{i=1}^m f_X(x_i | P) \right) \left( \prod_{i=1}^n \int_{a_i}^{b_i} f_X(x | P) dx \right)$$

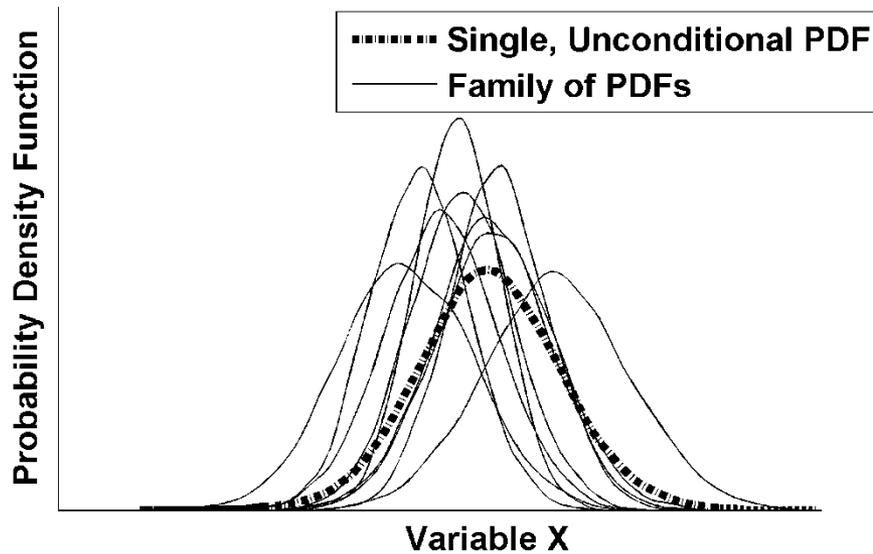
# Estimation of Parameters

- Maximum Likelihood Estimate
  - Maximize  $L(\mathbf{P})$
- To account for uncertainty in  $\mathbf{P}$ 
  - Bayesian updating  $\rightarrow$  Joint distribution of  $\mathbf{P}$
  - Assume a uniform prior over the domain of  $\mathbf{P}$

$$f(\mathbf{P}) = \frac{L(\mathbf{P})}{\int L(\mathbf{P})}$$

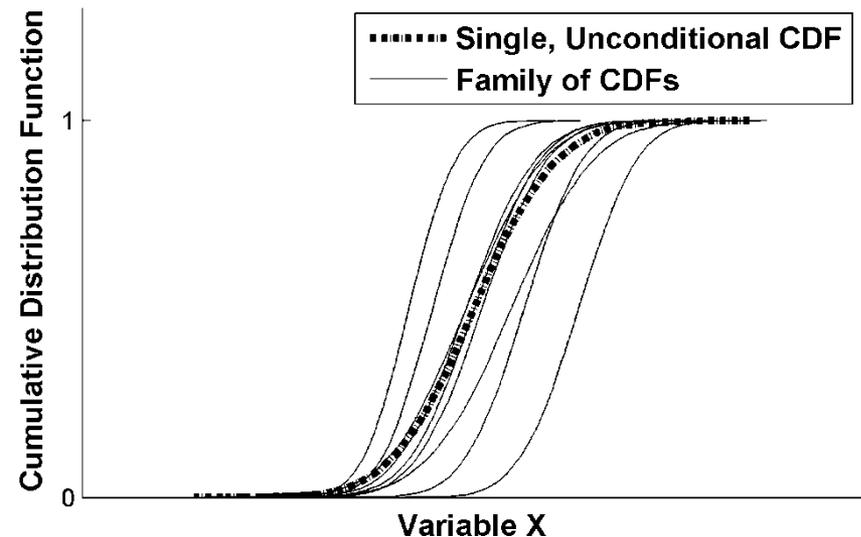
- Calculate marginal distributions of individual parameters
- PDF of  $X \rightarrow f_X(x/\mathbf{P}) \rightarrow$  Two loops of sampling
  - Distribution of  $\mathbf{P} \rightarrow f(\mathbf{P})$
  - Each sample of  $\mathbf{P} \rightarrow$  PDF for  $X$
  - Family of PDFs for  $X$

# Family vs. Single



Single distribution spreads over the entire range

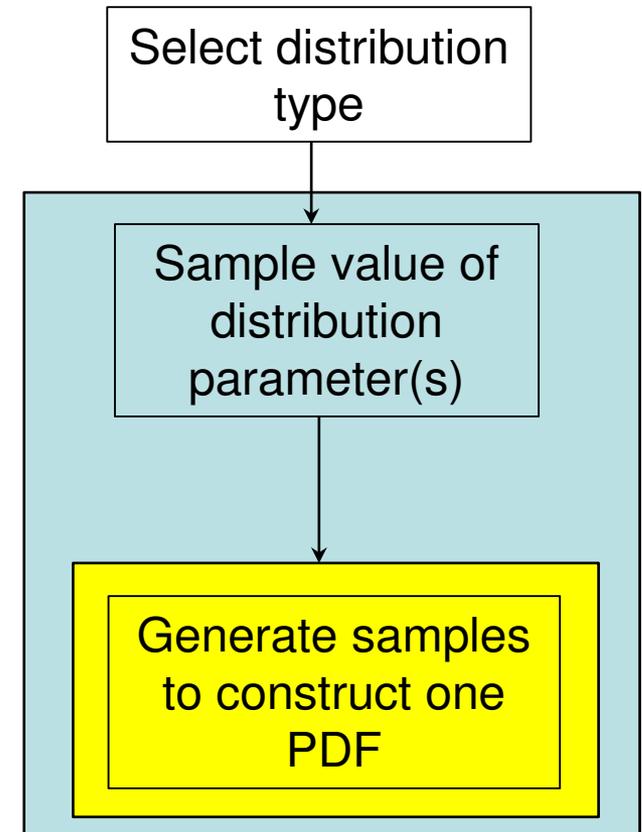
Includes both types of uncertainty: aleatory and distribution parameter (epistemic)



# Case 2: Uncertain Distribution Type

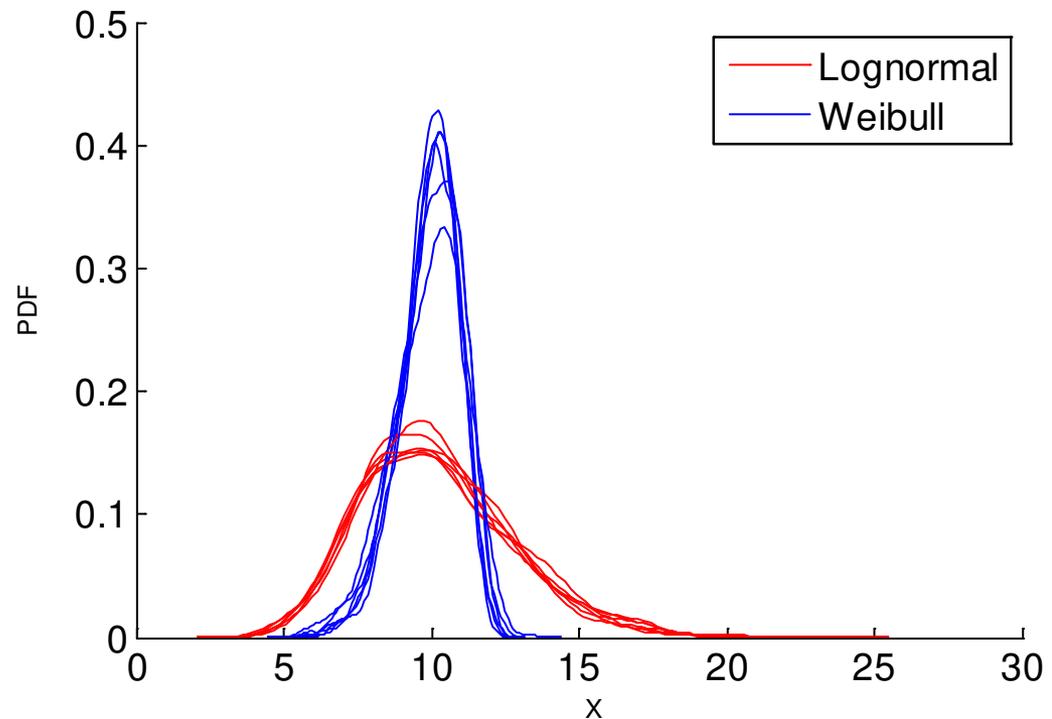
## Parametric Approach

- Distribution type  $\rightarrow T_1$  or  $T_2$ 
  - Uncertainty  $\rightarrow P(T_1)$  and  $P(T_2)$
- Given a distribution type, parameters are uncertain
  - Sample value of distribution parameter(s)
- Conditioned on the distribution type, value of parameters
  - Sample random values by inverting CDF
- Can collapse all three loops into a single loop for sampling



# Example

- Variable  $X$  is either Lognormal or Weibull
- Lognormal
  - $\lambda \sim N(2.3, 0.23)$
  - $\xi \sim N(0.1, 0.01)$
- Weibull
  - $a \sim N(10.5, 1.05)$
  - $b \sim N(11.7, 1.17)$



# Quantify distribution type uncertainty



- How to quantify uncertainty in a particular distribution type ?
- Compare two possible distribution types
- Two approaches
  - Bayesian model averaging → Ensemble modeling
  - Bayesian hypothesis testing → Model selection

Sankararaman & Mahadevan, MSSP, 2013

# Bayesian model averaging

- Suppose  $f^1$  and  $f^2$  are two competing PDF types for  $X$
- The corresponding parameters are  $\phi$  and  $\theta$
- BMA assigns weight to each PDF type

$$f_X(x | w, \phi, \theta) = wf_X^1(x | \phi) + (1 - w)f_X^2(x | \theta)$$

- Estimate PDFs of  $w$ ,  $\phi$  and  $\theta$  simultaneously
  - Construct likelihood  $\rightarrow L(w, \phi, \theta)$  using data (D)
    - Point values  $\rightarrow$  product of pdf's
    - Intervals  $\rightarrow$  product of ranges of cdf values over intervals
  - Bayesian inference  $\rightarrow f(w, \phi, \theta | D)$

# Uncertainty representation

- Physical variability  $\rightarrow$  Expressed through the PDF

$$f_X(x | w, \phi, \theta)$$

- Distribution type uncertainty  $\rightarrow w$
- Distribution parameter uncertainty  $\rightarrow \phi$  and  $\theta$
- Unconditional distribution  $\rightarrow$  collapsing into single loop

$$f_X(x) = \int \int \int f_X(x | w, \phi, \theta) f(w, \phi, \theta | D) dw d\phi d\theta$$

# Bayesian Hypothesis Testing

## Comparing two hypotheses

Bayes' Theorem  $\longrightarrow$  
$$\frac{P(H_0 | D)}{P(H_1 | D)} = \frac{P(D | H_0)P(H_0)}{P(D | H_1)P(H_1)}$$

Bayes Factor  $\longrightarrow$  
$$B = \frac{P(D | H_0)}{P(D | H_1)}$$

Compute based on  
 $f_Y(y|H_0)$  &  $f_Y(y|H_1)$

### Confidence in Model

$P(H_0) + P(H_1) = 1$ ; No prior knowledge  $\rightarrow P(H_0) = P(H_1) = 0.5$   
Probability(Model being correct) =  $P(H_0|D) = B/B+1$

# Distribution type uncertainty

- Two competing distribution types
  - $M_1$  with parameter  $\Phi$
  - $M_2$  with parameter  $\theta$

$$B = \frac{P(D | M_1)}{P(D | M_2)} = \frac{L(M_1)}{L(M_2)}$$

- Straightforward to calculate
  - $L(M_1, \Phi)$  and  $L(M_2, \theta)$

$$P(D | M_1) \propto \int P(D | M_1, \phi) f'(\phi) d\phi$$

- Necessary to calculate
  - $L(M_1)$  and  $L(M_2)$
  - By integrating out  $\Phi$  and  $\theta$

$$P(D | M_2) \propto \int P(D | M_2, \theta) f'(\theta) d\theta$$

- Simultaneously obtain posterior PDFs  $f(\phi)$  and  $f(\theta)$
- Inherently these PDFs are conditioned on  $M_1$  and  $M_2$  respectively

# Aleatory and epistemic uncertainty

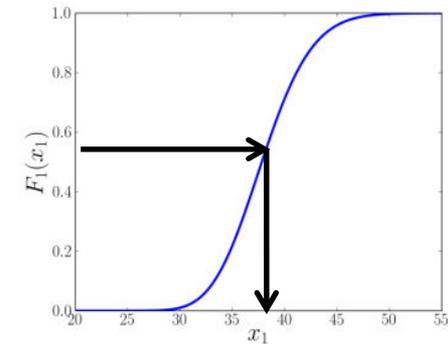
- Distribution parameter uncertainty



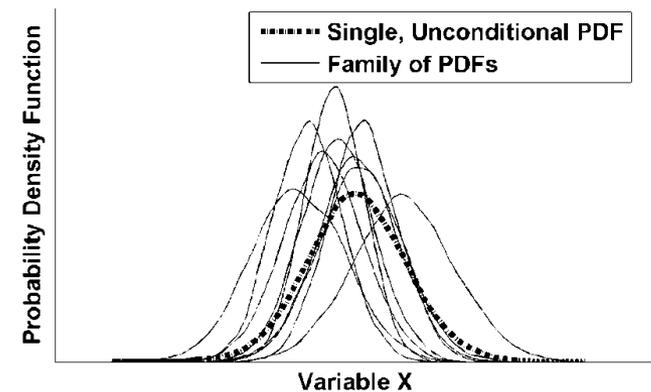
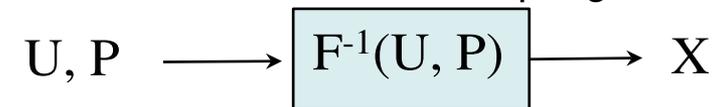
- Introduce auxiliary variable  $U \rightarrow$  CDF of  $X$

$$U = \int_{-\infty}^X f_X(x | P) dx$$

Uncertainty propagation  $\rightarrow$  single loop sampling of aleatory and epistemic uncertainty



Monte Carlo Sampling



# Distribution type uncertainty

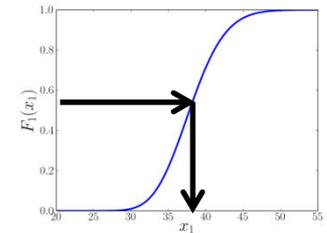
For a given distribution type  $D$

$U \rightarrow$  auxiliary variable

$$\mu_X, \sigma_X \rightarrow \begin{matrix} f_X(x) & F_X(x) \\ \text{PDF} & \text{CDF} \end{matrix}$$



$$X = F_X^{-1}(U \mid \mu_X, \sigma_X) = h(U, \mu_X, \sigma_X)$$



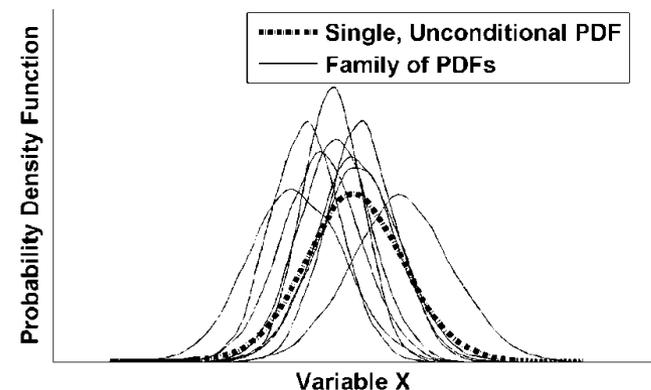
Multiple competing distributions ( $D_k$ ) each with parameters  $\theta_k$

$$X = h(U, D, \theta)$$

Composite distribution

$$f_{X|\Theta}(x|\theta) = \sum_{k=1}^N w_k f_{X|\Theta_k}(x|\theta_k)$$

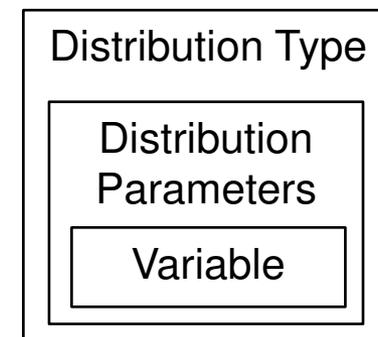
Sankararaman & Mahadevan, MSSP, 2013  
Nannapaneni & Mahadevan, RESS, 2016



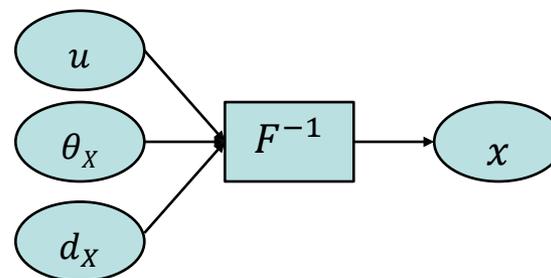
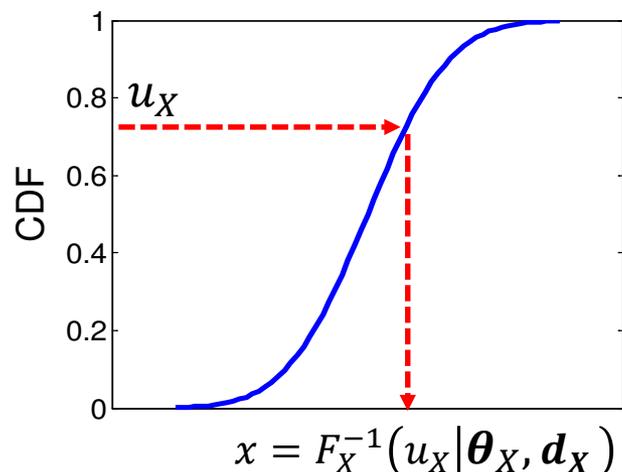
# Sampling the input for uncertainty propagation

## Inputs with aleatory + epistemic uncertainty

- Brute force approach - Nested three-loop sampling
  - Computationally expensive



## Auxiliary variable approach $\rightarrow$ single loop sampling

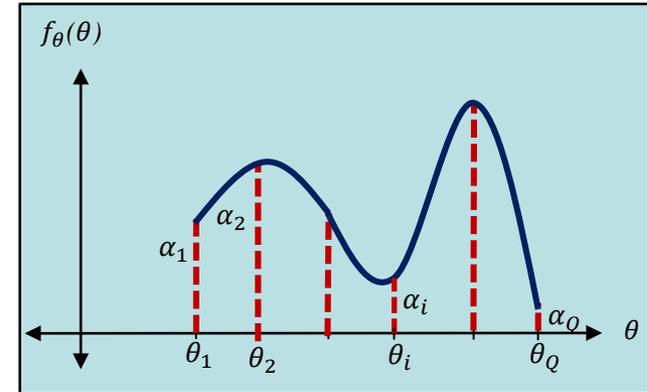


$$f_{X|\theta}(x|\theta) = \sum_{k=1}^N w_k f_{X|\theta_k}(x|\theta_k)$$

# Sampling the multivariate input

## Correlation uncertainty

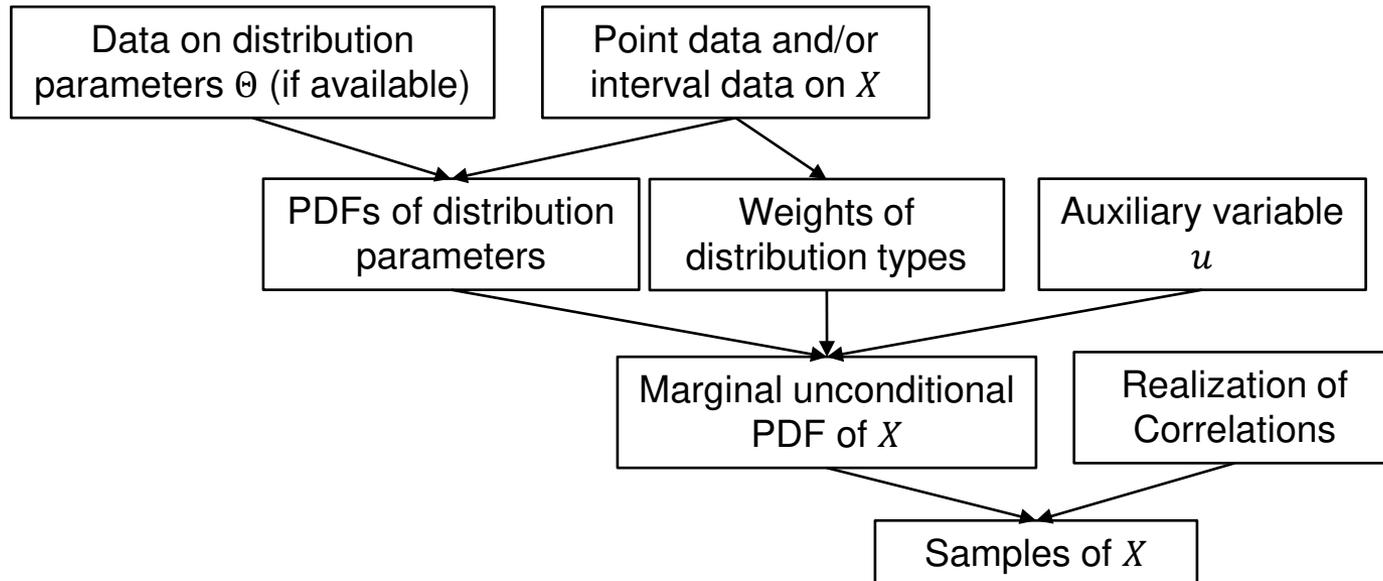
- Data on correlation coefficients
- Construct a non-parametric distribution
- Likelihood



$$L(\alpha) = \prod_{i=1}^r f_{\Theta}(\theta = \theta_p^i | \alpha) \prod_{j=1}^s [F_{\Theta}(\theta = \theta_b^j | \alpha) - F_{\Theta}(\theta = \theta_a^j | \alpha)]$$

- Use MLE to construct PDF of correlation coefficient
- Sample the correlation coefficient from the non-parametric distribution
- Multivariate sampling
  - Transform the correlated non-normal variables to uncorrelated normal variables
  - Sample the uncorrelated normals; then convert to original space

# Summary of parametric approach



- Fitting parametric probability distributions to sparse and interval data
- Auxiliary variable
  - Distinguish aleatory and epistemic contributions
  - Facilitates sensitivity analysis
  - Supports resource allocation for further data collection

# Case 2: Uncertain Distribution Type

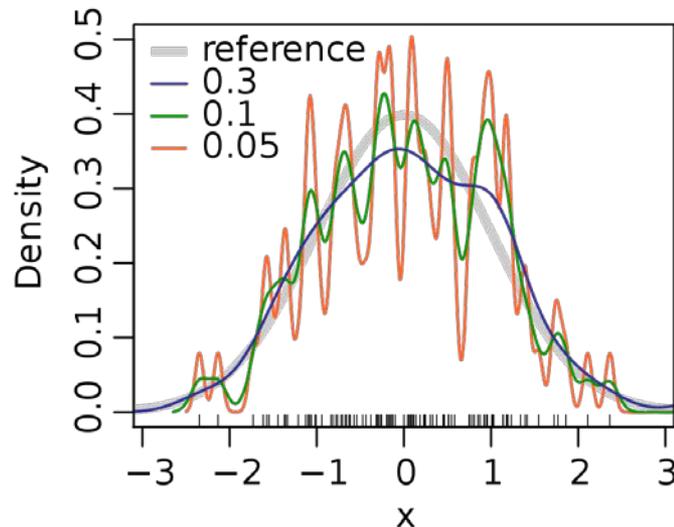
## Kernel density estimation

- Non-parametric PDF

- $x_1, x_2, x_3 \dots x_n$  are i.i.d samples from a PDF to be determined

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^n K\left(\frac{x - x_i}{h}\right)$$

- $K \rightarrow$  kernel function  $\rightarrow$  symmetric and must integrate to unity
- $h \rightarrow$  smoothing parameter  $\rightarrow$  “bandwidth”



- Larger the  $h$ , smoother the PDF
- Optimal  $h$  for normal PDF  $\rightarrow h = \left(\frac{4\hat{\sigma}^5}{3n}\right)^{\frac{1}{5}}$
- MATLAB
  - `[f, x] = ksdensity (samples)`
  - `plot (x, f)  $\rightarrow$  PDF`
- Multi-variate kernel densities available

# Case 2: Uncertain Distribution Type

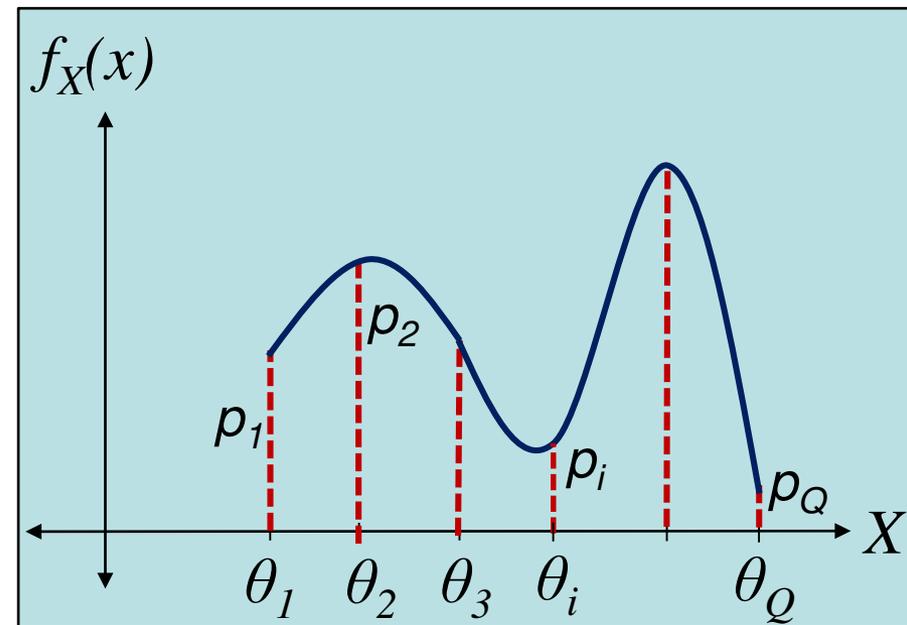
## Likelihood-based Non-Parametric Approach

- Discretize the domain of  $X \rightarrow \theta_i, i = 1$  to  $Q$
- PDF values at each of these  $Q$  points known
  - $f_X(x = \theta_i) = p_i$  for  $i = 1$  to  $Q$
- Interpolation technique
  - Evaluate  $f(x)$  over the domain

- Construct likelihood

$$L \propto \left( \prod_{i=1}^n \int_{a_i}^{b_i} f_X(x) dx \right) \left( \prod_{i=1}^m f_X(x_i) \right)$$

- Maximize  $L \rightarrow$  Find  $p_i$



Sankararaman & Mahadevan, RESS, 2011

# Pros/cons of non-parametric approach

- Flexible framework
  - Integrated treatment of point data and interval data
  - Fusion of multiple types of information
    - Probability distributions
    - Probability distributions of distribution parameters
    - Point data, interval data
- Results in a single distribution
  - Not a family, as in the parametric approach
  - Smaller number of function evaluations for uncertainty propagation
- Cannot distinguish aleatory and epistemic uncertainty

# Statistical Uncertainty: Summary



- Epistemic uncertainty regarding parameters of stochastic inputs → represented by probability distributions → family of distributions
- Three options discussed
  - Use 4-parameter distributions (families of distributions)
  - Introduce auxiliary variable to separately capture aleatory uncertainty
  - Use non-parametric distributions
- Above discussion covered sparse and imprecise data

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# MODEL UNCERTAINTY

# Activities to address model uncertainty

- Model Verification → Numerical Error
- Model Calibration → Model parameters
- Model Selection → Model form uncertainty
- Model Validation → Model form uncertainty

# Model Verification

## Code verification

- Method of manufactured solutions
- Code to code comparisons

## Solution verification

- $\epsilon_{num}$  → Numerical error
- $\epsilon_h$  → Discretization error
- $\epsilon_{in-obs}$  → Input obs error
- $\epsilon_{y-obs}$  → Output obs error
- $\epsilon_{su}$  → Surrogate model error
- $\epsilon_{uq}$  → UQ error
- $\epsilon_{mf}$  → Model form error

$$\begin{aligned}y_{obs} &= y_{pred} + \epsilon_{pred} - \epsilon_{y-obs} \\ &= y_{pred} + \epsilon_{num} + \epsilon_{mf} - \epsilon_{exp} \\ &= g(x, \epsilon_h, \epsilon_{su}, \epsilon_{in-obs}, \epsilon_{uq}) + \epsilon_{mf} - \epsilon_{y-obs}\end{aligned}$$

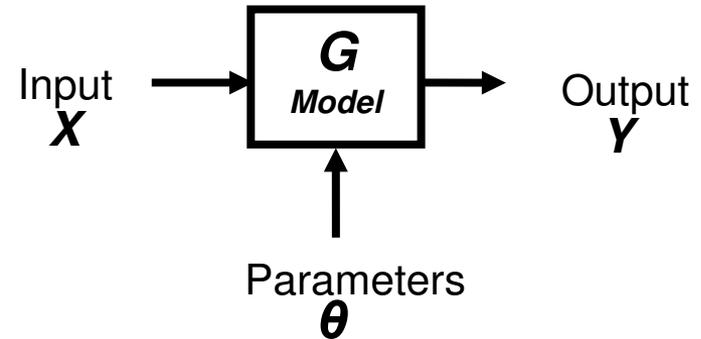
Rebba, Huang & Mahadevan, RESS, 2006  
Sankararaman, Ling & Mahadevan, EFM, 2011

## Use Bayesian network for systematic aggregation of errors

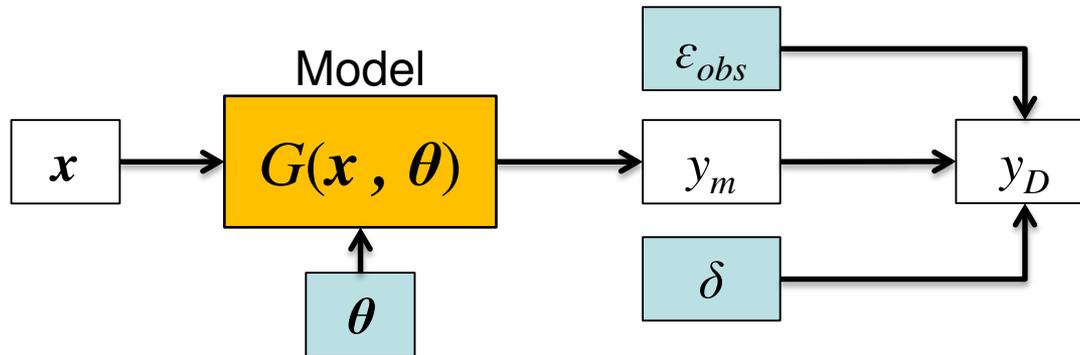
- Deterministic error (bias) → Correct where it occurs
- Stochastic error → Sample and add to model prediction

# Model Calibration (Parameter estimation)

- 3 techniques
  - Least squares
  - Maximum likelihood
  - Bayesian
  
- Issues
  - Identifiability, uniqueness
  - Precise or Imprecise data
  - Ordered or un-ordered input-output pairs
  - Data at multiple levels of complexity
  - Dynamic (time-varying) output
  - Spatially varying parameters



# Model discrepancy estimation



$$y_D = y_m + \delta + \varepsilon_{obs}$$

$$= G(x; \theta) + \delta(x) + \varepsilon_{obs}$$

Kennedy and O'Hagan,  
JRS, 2001

- Several formulations possible for model discrepancy:

1.  $\delta_1$  as Constant
2.  $\delta_2$  as i.i.d. Gaussian random variable with fixed mean and variance
3.  $\delta_3$  as independent Gaussian random variable with input dependent mean and variance  $\delta_3 \sim N(\mu(x), \sigma(x))$

4.  $\delta_4$  as a stationary Gaussian process
5.  $\delta_5$  as a non-stationary Gaussian process

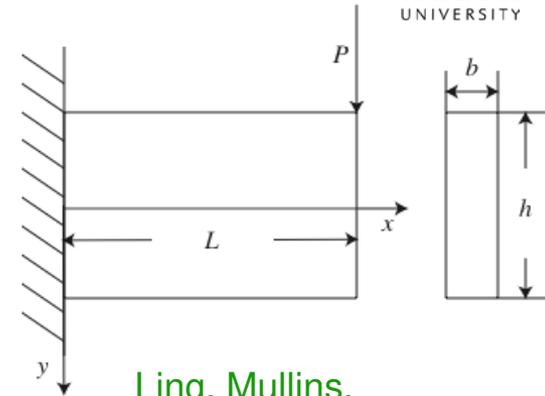
$$\delta \sim N(m(x), k(x, x'))$$

- Result depends on formulation

Ling, Mullins, Mahadevan, JCP, 2014

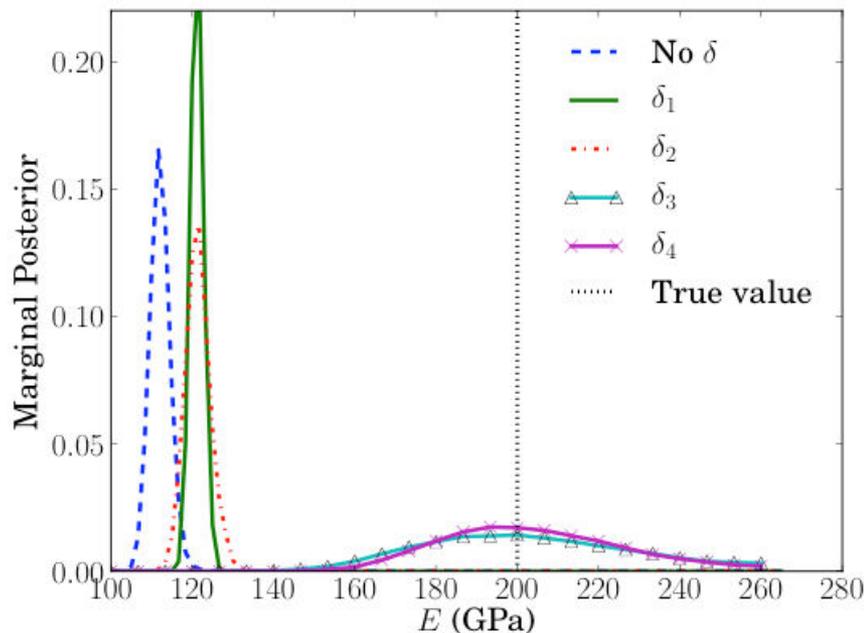
# Discrepancy options with KOH

- Calibrate Young's modulus using Euler-Bernoulli beam model
- Synthetic deflection data generated using Timoshenko beam model with  $P = 2.5 \mu\text{N}$



Ling, Mullins,  
Mahadevan, JCP 2014

## Calibration



## Prediction at $P = 3.5 \mu\text{N}$

Discrepancy	MR	MR
No d	0.5	0.5
IID Gauss	0.66	0.65
Input-dep Gauss	0.55	0.6
Stationary GP	0.36	0.95
Non-stationary GP	0.34	0.93

Input-dependent

# Multi-fidelity approach to calibration

(if models of different fidelities are available)

- Need surrogate models in Bayesian calibration
- High-fidelity (HF) model is expensive
- Build surrogate for Low-fidelity (LF) model
- Use HF runs to “correct” the LF surrogate

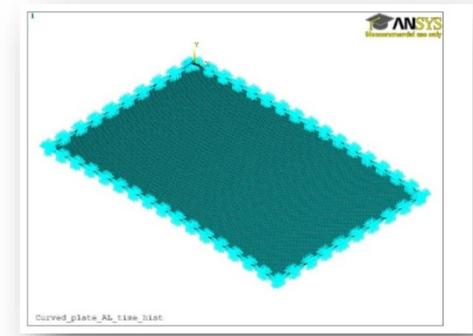
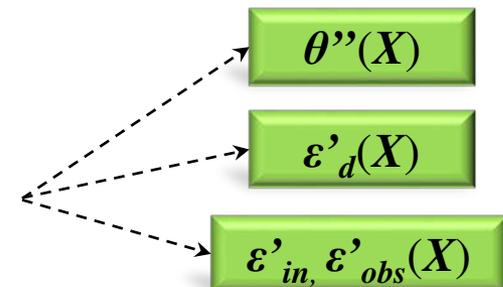
$$Y_{HF} = S_I(X + \varepsilon_{in}, \theta(X)) + \varepsilon_{surr} + \delta_{2,I}(X)$$

- Pre-calibration of model parameters  $\rightarrow$  Stronger priors
- Estimation of HF-LF discrepancy

$$LF_{corr} = S_I(X + \varepsilon_{in}, \theta'(X)) + \varepsilon_{surr} + \delta'_{2,I}(X)$$

- Use experimental data to calibrate model parameters and discrepancy

$$Y_{exp} = S_I(X + \varepsilon_{in}, \theta'(X)) + \varepsilon_{surr} + \delta'_{2,I}(X) + \varepsilon_d(X) + \varepsilon_{obs}(X)$$



**Hypersonic panel**

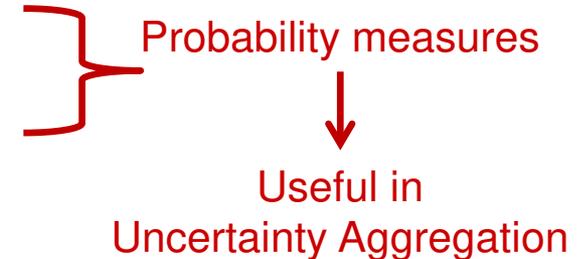
Absi & Mahadevan,  
MSSP, 2015

Absi & Mahadevan,  
MSSP, 2017

# Model Validation

## Quantitative Methods

1. Classical hypothesis testing
2. Bayesian hypothesis testing (equality and interval)
3. Reliability-based method (distance metric)
4. Area metric
5. K-L divergence



## Bayesian hypothesis testing

- Comparison of two hypotheses ( $H_0$  and  $H_1$ )
  - $H_0$ : model agrees with data,  $H_1$ : otherwise
- Validation metric → Bayes factor

$$B = \frac{P(D | H_0)}{P(D | H_1)} \quad D \rightarrow \text{obs data}$$

**P(model agrees with data)**

$$\Pr(H_0|D) = B / B+1$$

## Model reliability metric

- Pred  $\rightarrow y$       Obs  $\rightarrow z$
- $H_0 \rightarrow |y - z| \leq \delta$
- Compute  $P(H_0)$
- $P(H_1) = 1 - P(H_0)$

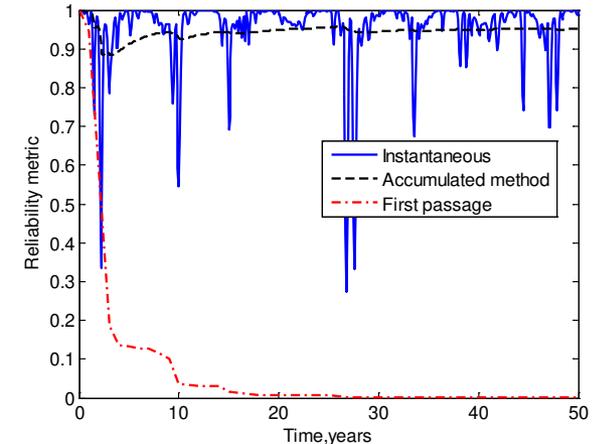
Rebba et al, RESS 2006;  
Rebba & Mahadevan, RESS 2008  
Mullins et al, RESS, 2016.

# Model reliability metric

- Multi-dimensional → Mahalanobis distance

$$M_R = P \left( \sqrt{(\mathbf{z} - \mathbf{D}_i)^T \boldsymbol{\Sigma}_z^{-1} (\mathbf{z} - \mathbf{D}_i)} < \sqrt{\boldsymbol{\lambda}^T \boldsymbol{\Sigma}_z^{-1} \boldsymbol{\lambda}} \right)$$

- Input-dependent
  - Expected value
  - Random variable
  - Random field
- Time-dependent (dynamics problems)
  - Use time-dependent reliability methods
    - Instantaneous
    - First-passage
    - Cumulative



# Prediction Uncertainty Quantification



## From calibration to prediction

- Same configuration and QOI  $\rightarrow$  can estimate discrepancy
  - Create surrogate for discrepancy or observation
- Different configuration or QOI  $\rightarrow$  KOH discrepancy cannot be propagated
- Embedded discrepancy calibration + propagation  $y_D = G(x; \theta + \delta(x)) + \varepsilon_{obs}$
- Combine calibration and validation results
  - Uncertainty aggregation across multiple levels
  - Able to include relevance

Sankararaman & Mahadevan,  
RESS, 2015

Li & Mahadevan,  
RESS, 2016

## Bayesian state estimation

- Model form error directly quantified using state estimation
- Able to transfer to prediction
  - Estimation of discrepancy at unmeasured locations
  - Estimation of discrepancy for untested, dynamic inputs
  - Translation of model form errors to untested (prediction) configurations

Subramanian & Mahadevan,  
JCP, MSSP, submitted

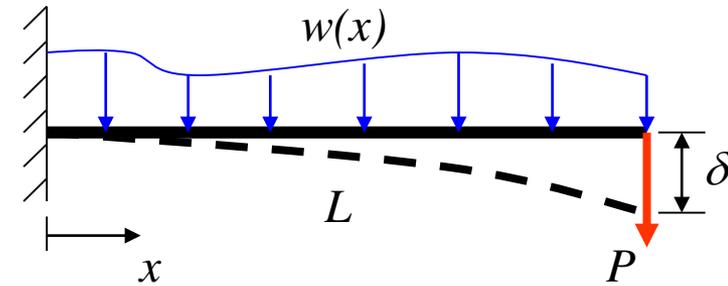
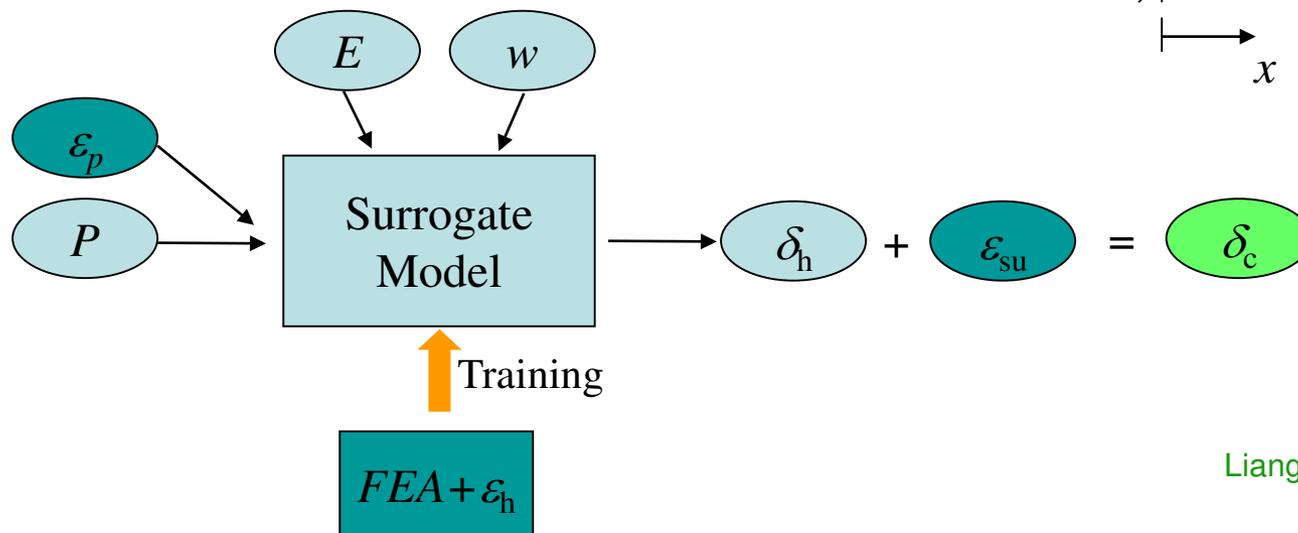
# Model Uncertainty: Summary

- Several activities to address model uncertainty
  - Calibration
  - Validation
  - Selection
  - Verification (Error quantification)
- Bayesian approach to calibration and validation highlighted
- Approaches to quantify various model errors
- Rigorous approach to error combination (differentiate stochastic and deterministic errors)
- Various error/uncertainty sources can be systematically included in a Bayesian network

# UNCERTAINTY AGGREGATION

# Error combination: rigorous approach

- Current methods use RMS

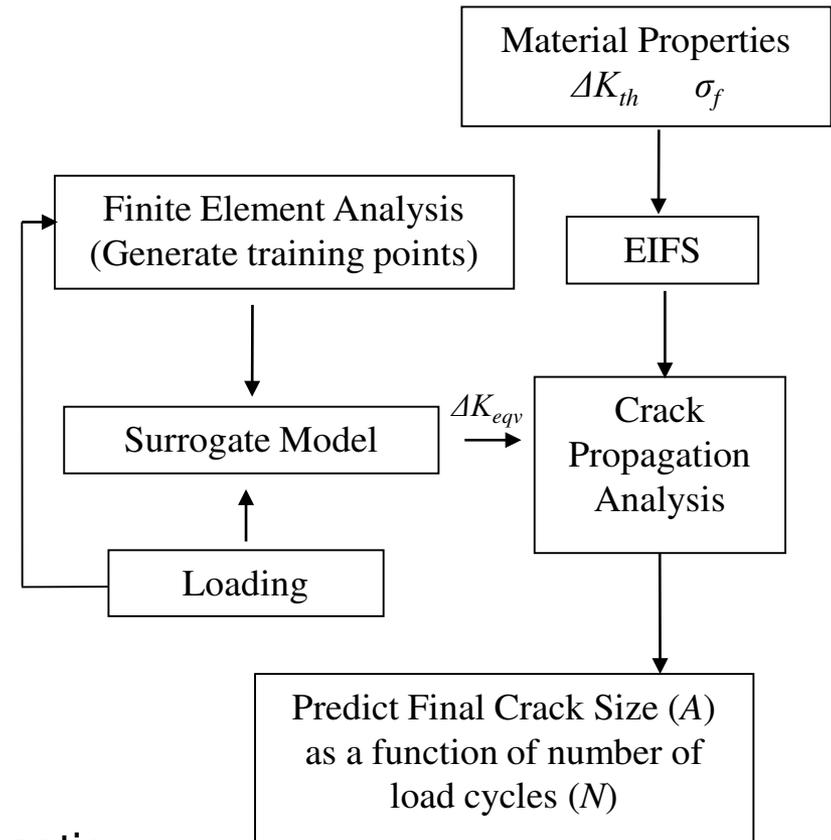


Liang & Mahadevan, IJUQ, 2011

- Correct for deterministic errors; sample stochastic errors
- Surrogate model: e.g., 2<sup>nd</sup> order polynomial chaos expansion (PCE)
- Corrected model prediction:  $\delta_c = \text{PCE}_h(P + \varepsilon_p, E, w) + \varepsilon_{su}$

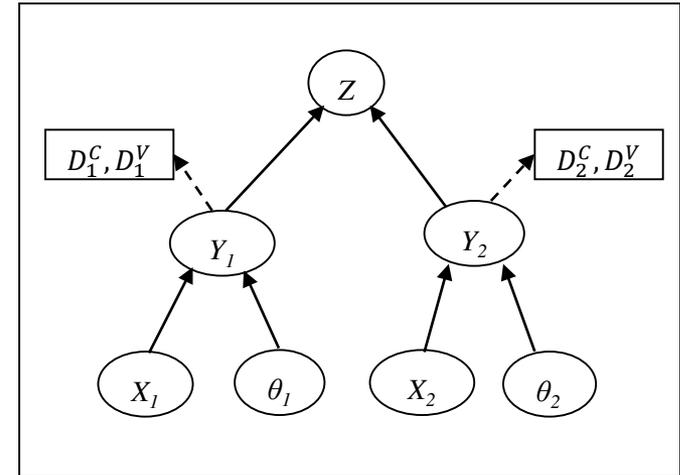
# Multiple sources of uncertainty in crack growth prediction

- Physical variability
  - Loading
  - Material Properties
- Data uncertainty
  - Sparse input data
  - Output measurement
- Model uncertainty/errors
  - Finite element discretization error
  - Gaussian process surrogate model
  - Crack growth law
- Complicated interactions
  - Some errors deterministic, some stochastic
  - Combinations could be non-linear, nested, or iterative
  - **Need systematic approach (e.g., Bayesian network) to aggregate uncertainty**



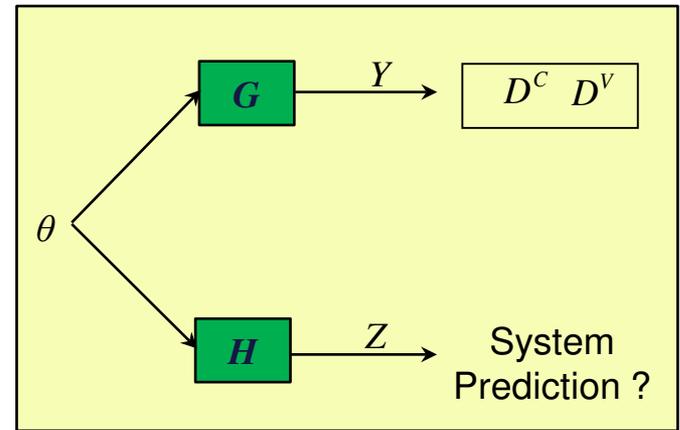
# Aggregation of Calibration, Verification and Validation Results

- Verification  $\rightarrow$  Numerical errors
  - “Correct” the model output
- Calibration data ( $D^C$ )  $\rightarrow$  PDF's of  $\theta$
- Validation data ( $D^V$ )  $\rightarrow$   $P(H_0|D^V)$
- System-level prediction  $\rightarrow$  PDF of  $Z$

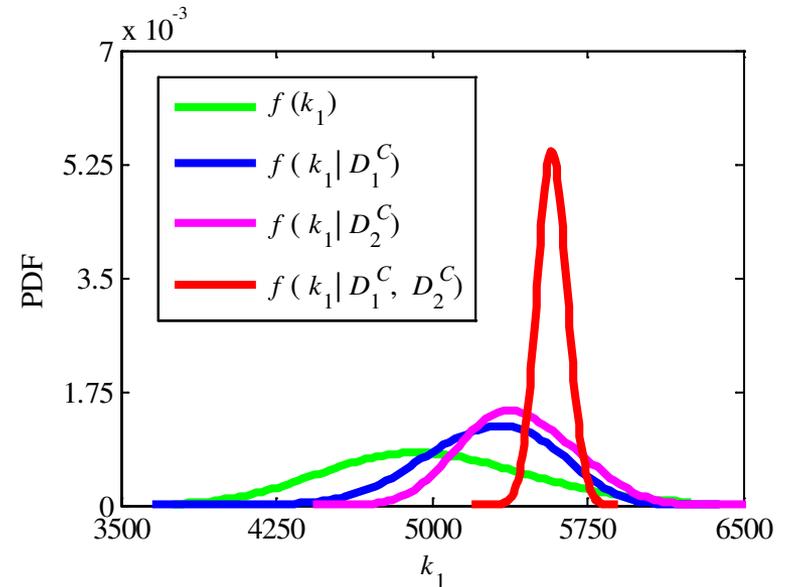
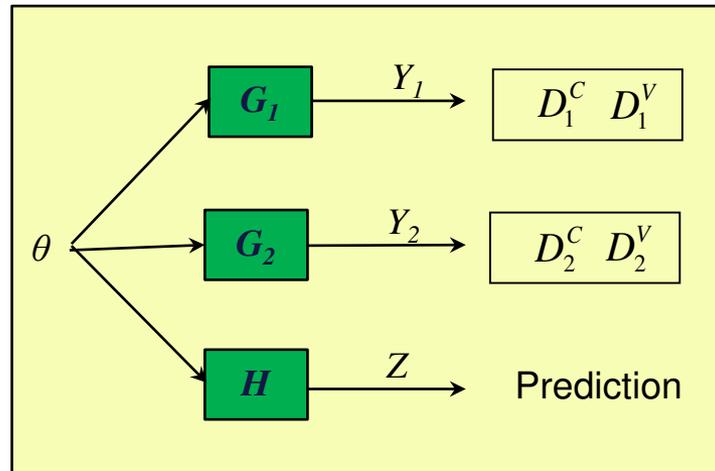


- Sequential  $\rightarrow$  model output
- $$\bar{\pi}(y) = \Pr(H_0 | D^V)\pi_0(y) + [1 - \Pr(H_0 | D^V)]\pi_1(y)$$

- Non-sequential  $\rightarrow$  model parameter
- $$\pi(\theta | D^C, D^V) = \pi(\theta | D^C, H_0)\Pr(H_0 | D^V) + \pi(\theta)[1 - \Pr(H_0 | D^V)]$$



# Tests at multiple levels of complexity

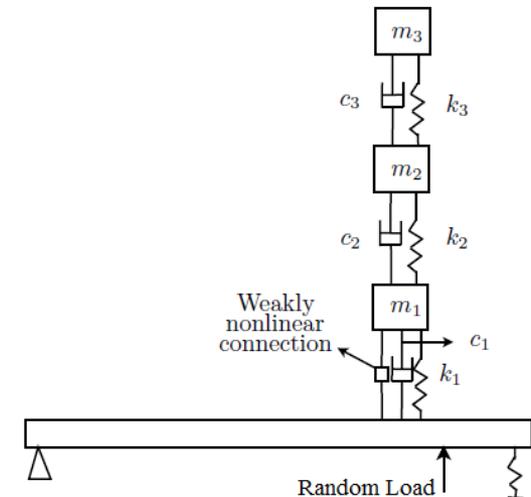
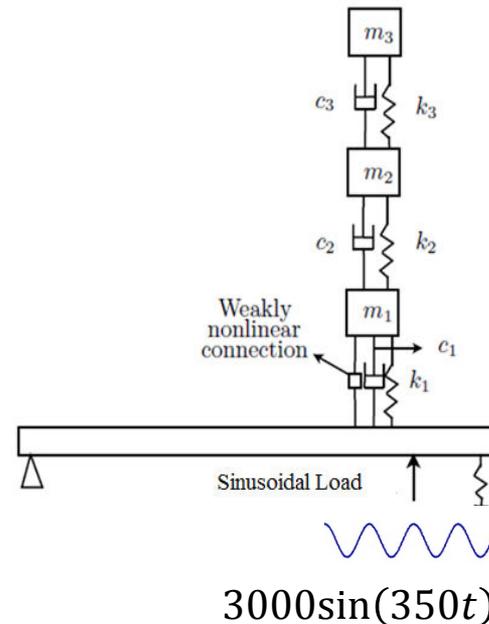
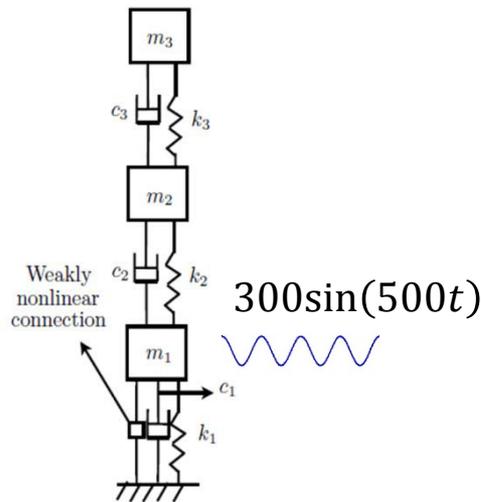


## Multi-level integration

$$\begin{aligned}
 - f(\theta | D_1^{C,V}, D_2^{C,V}) &= P(G_1)P(G_2)f(\theta | D_1^C, D_2^C) \\
 &+ P(G'_1)P(G_2)f(\theta | D_2^C) \\
 &+ P(G_1)P(G'_2)f(\theta | D_1^C) \\
 &+ P(G'_1)P(G'_2)f(\theta)
 \end{aligned}$$

Sankararaman & Mahadevan,  
RESS, 2015

# Sandia Dynamics Challenge Problem (2006)



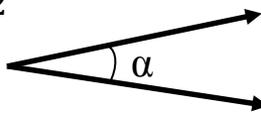
- Level 1
  - Subsystem of 3 mass-spring-damper components
  - Sinusoidal force input on  $m_1$
- Level 2
  - Subsystem mounted on a beam
  - Sinusoidal force input on the beam
- System Level
  - Random load input on the beam
  - Output to predict:  
**Maximum acceleration at  $m_3$**

# Inclusion of relevance of each level

- At each level
  - Global sensitivity analysis → vector of sensitivity indices
  - Sensitivity vector combines physics + uncertainty
  - Comparison with system-level sensitivity vector quantifies the relevance

## • Relevance

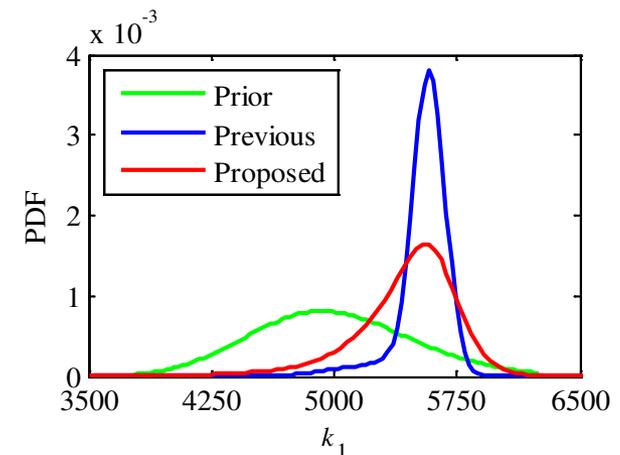
Li & Mahadevan, RESS, 2016

$$S_i = \left( \frac{V_{Li} \cdot V_s}{\|V_{Li}\| \|V_s\|} \right)^2$$


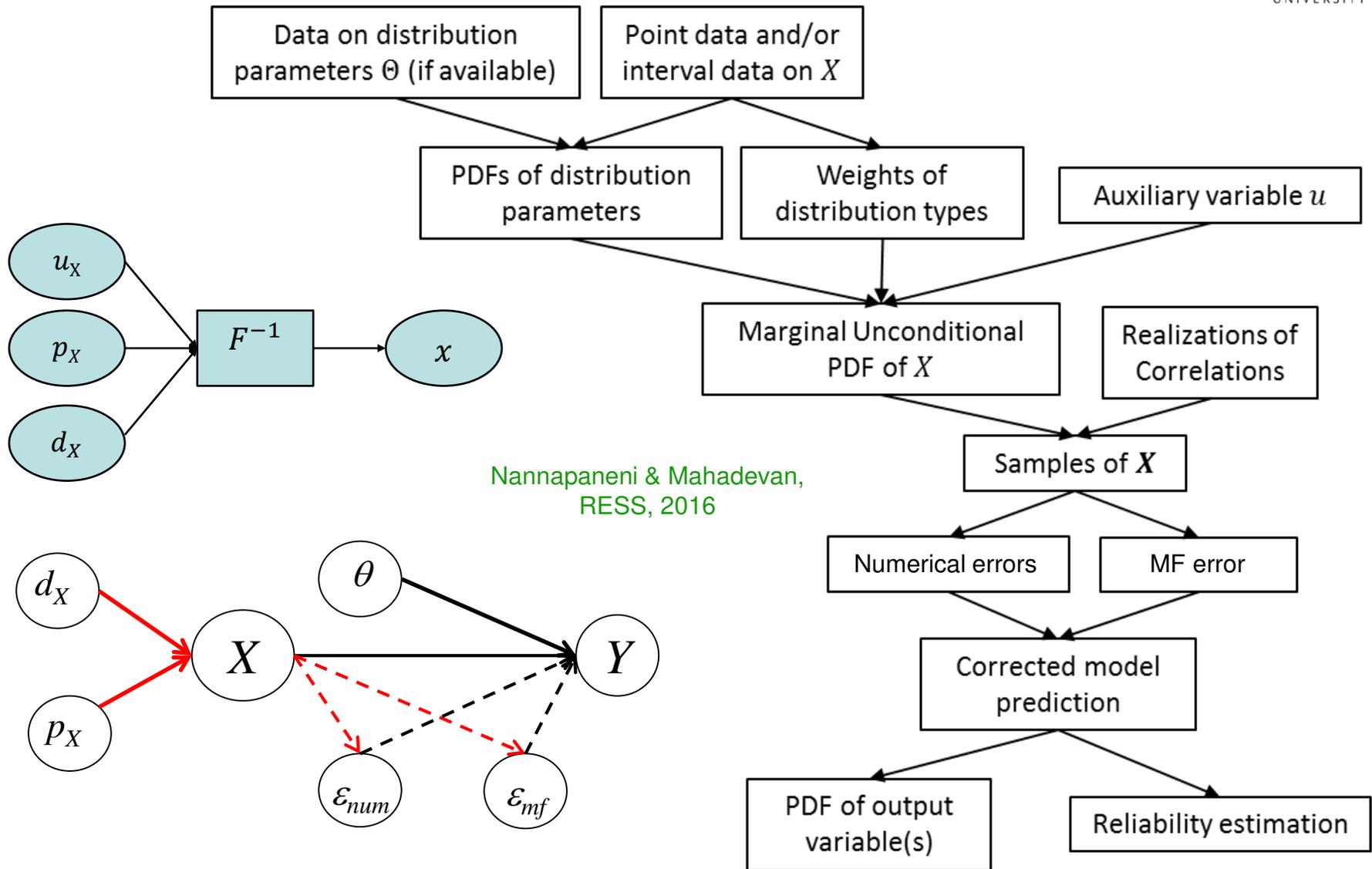
Relevance:  $\cos^2(\alpha)$   
Non-Relevance:  $\sin^2(\alpha)$

## • Integration

$$\begin{aligned} & f(\theta | D_1^{C,V}, D_2^{C,V}) \\ &= P(G_1 G_2 S_1 S_2) f(\theta | D_1^C, D_2^C) \\ &+ P(G_1 S_1 \cap (G_2' \cup S_2')) f(\theta | D_1^C) \\ &+ P(G_2 S_2 \cap (G_1' \cup S_1')) f(\theta | D_2^C) \\ &+ P((G_1' \cup S_1') \cap (G_2' \cup S_2')) f(\theta) \end{aligned}$$

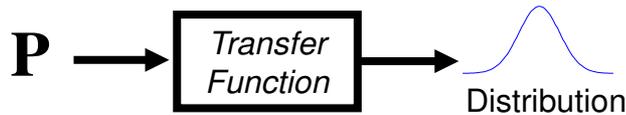


# Uncertainty Aggregation Flow



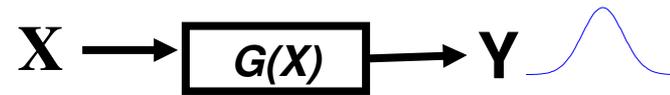
# Auxiliary Variable approach

- Data uncertainty



**Stochastic mapping**

- Model uncertainty

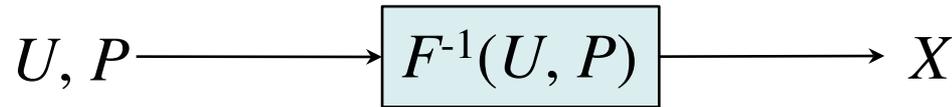


**Stochastic mapping**

- Introduce auxiliary variable  $U (0, 1)$

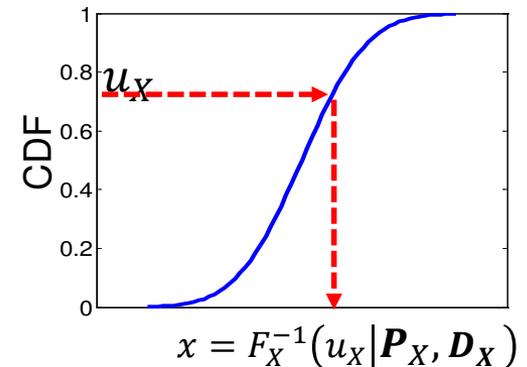
Sankararaman & Mahadevan, RESS, 2013

$$U = \int_{-\infty}^X f_X(x | P) dx$$

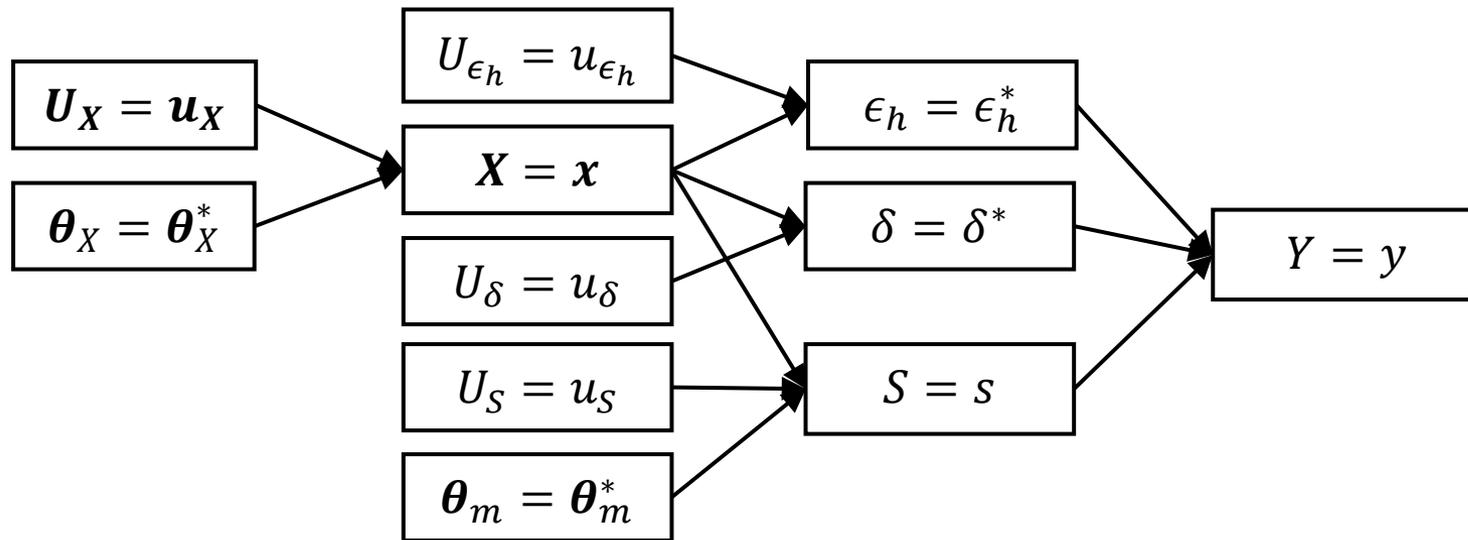


**One-to-one mapping**

- Prediction
  - Can include aleatory & epistemic sources at same level
- Uncertainty sensitivity analysis
  - Can include aleatory & epistemic sources at same level



# Global Sensitivity Analysis



- Deterministic function for GSA:
  - $Y = F(\boldsymbol{\theta}_X, \mathbf{U}_X, \boldsymbol{\theta}_m, U_S, U_{\epsilon_h}, U_\delta)$
- Auxiliary variables introduced for
  - Variability in input  $\mathbf{X}$
  - Model form error  $\delta(\mathbf{X})$
  - Discretization error  $\epsilon_h(\mathbf{X})$
  - Surrogate uncertainty in  $S(\boldsymbol{\theta}_m, \mathbf{X})$



## Sobol indices

$$S_i = \frac{V(E(Y|X_i))}{V(Y)}$$
$$S_i^T = 1 - \frac{V(E(Y|X_{-i}))}{V(Y)}$$

Li & Mahadevan, IJF, 2016

# Uncertainty aggregation scenarios

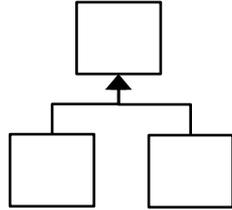


Single-component



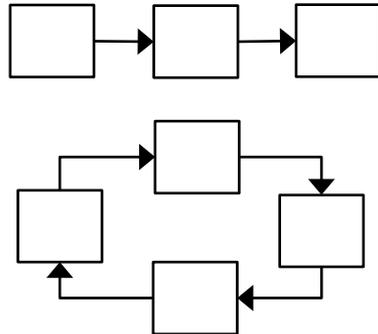
Aggregation of input variability,  
statistical uncertainty, and model  
uncertainty

Multi-level



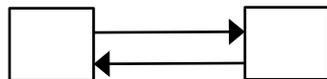
Multiple components organized in a  
hierarchical manner  
(components, subsystems, system)

Time-varying



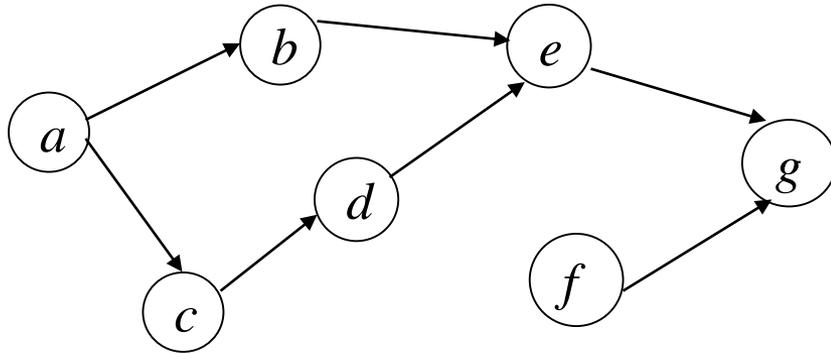
Multiple components occurring in a time  
sequence

Multi-physics



Multiple components with simultaneous  
interactions

# Bayesian network



$a, b, \dots$  component nodes (model inputs, outputs, parameters, errors)

$g$  – system-level output

$U$  - set of all nodes  $\{ a, b, \dots, g \}$

Joint PDF of all nodes

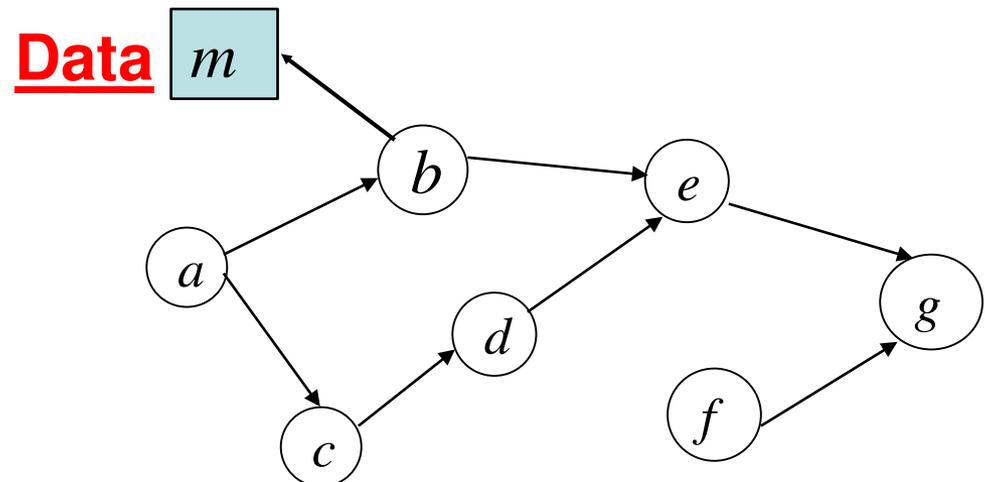
$$\pi(U) = \pi(a) \times \pi(b|a) \times \pi(c|a) \times \pi(d|c) \times \pi(e|b, d) \times \pi(f) \times \pi(g|e, f)$$

PDF of final output  $g$

$$\pi(g) = \int \pi(U) da db \dots df$$

With new observed data  $m$

$$\pi(U, m) = \pi(U) \times \pi(m|b)$$



# Bayesian network

## Construction of BN

- Physics-based
  - Structure based on system knowledge
  - Learn probabilities using models & data
- Data-based
  - Learn both structure and probabilities from data
- Hybrid approach

## Uses of BN

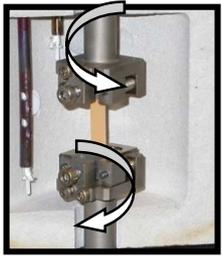
- Forward problem: UQ in overall system-level prediction
  - Integrate all available sources of information and results of modeling/testing activities
- Inverse problem: Decision-making at various stages of system life cycle
  - Model development
  - Test planning
  - System design
  - Health monitoring
  - Risk management

# Data at multiple levels of complexity

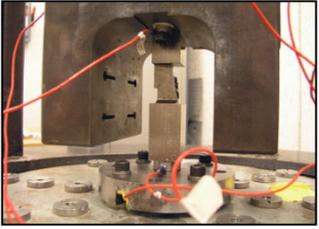
Foam

Joints

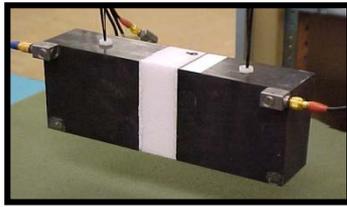
**Level 0**



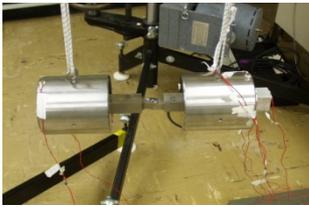
Material characterization



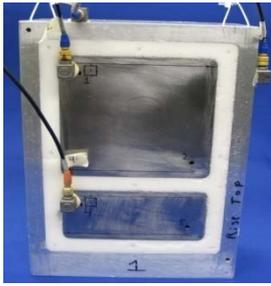
**Level 1**



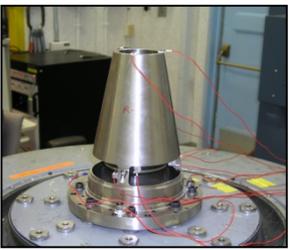
Component level



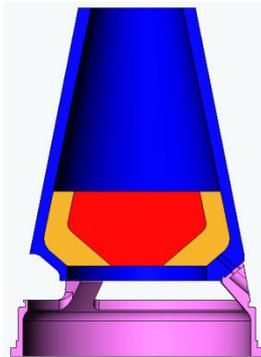
**Level 2**



Sub-system level



**System level**



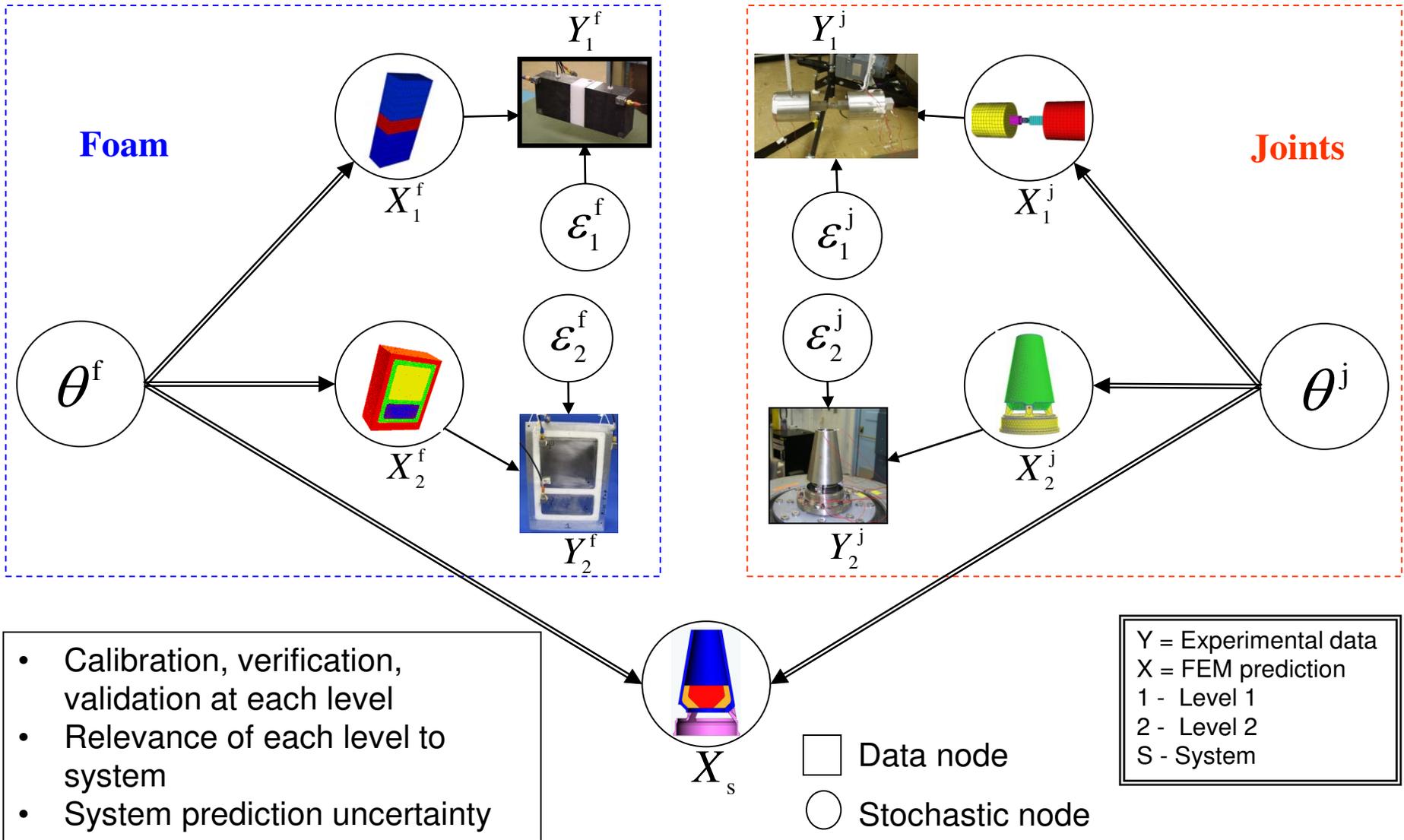
Predict peak acceleration of mass under impact load

Urbina et al, RESS, 2011

Hardware data and photos courtesy of Sandia National Laboratories



# Bayesian Network for Information Fusion (No system-level data)

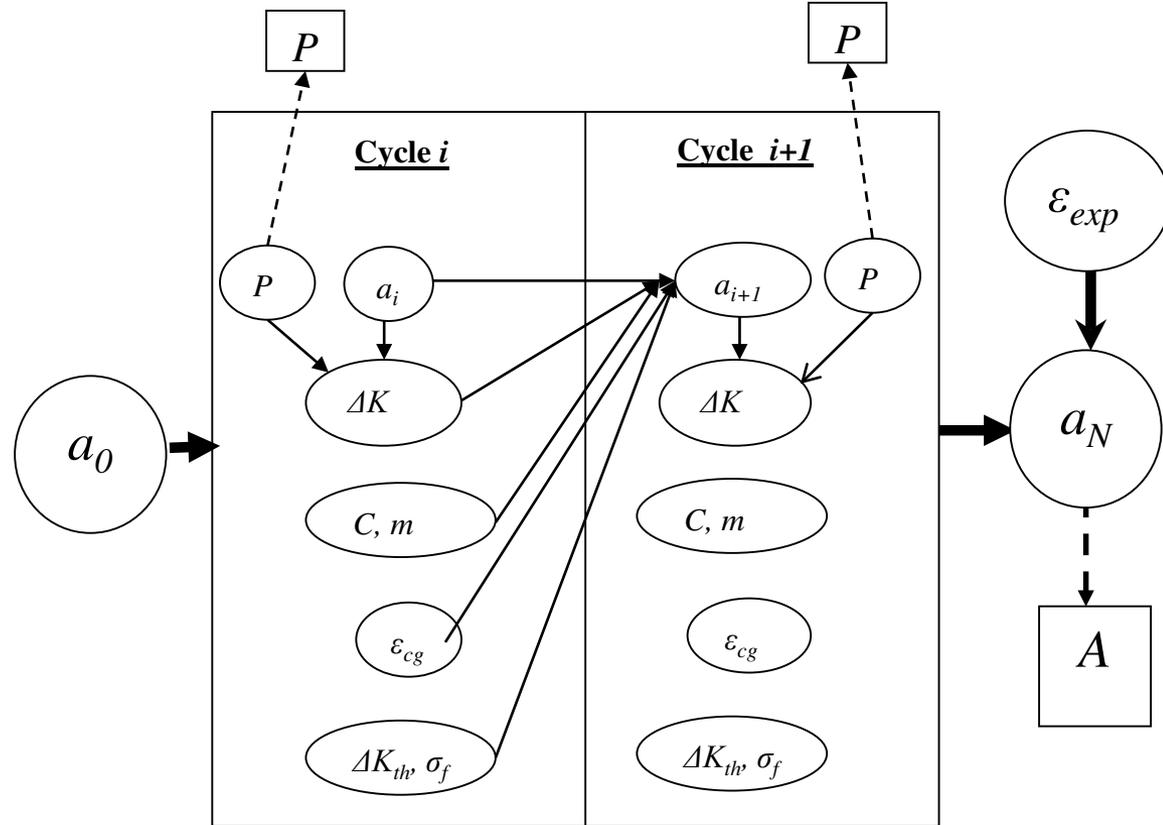
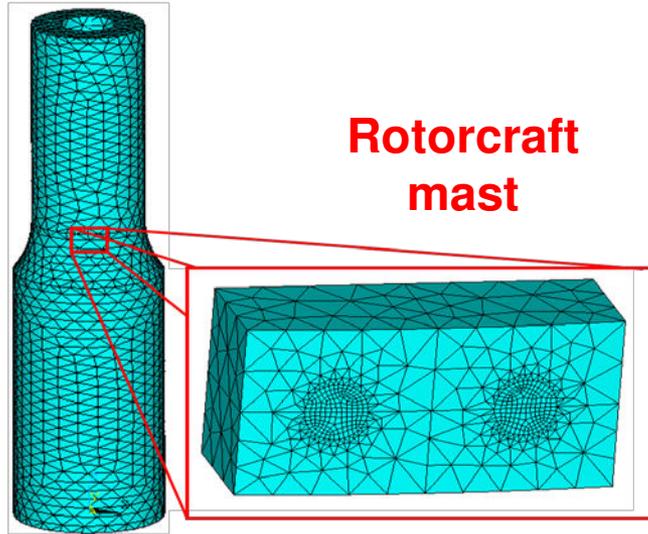


- Calibration, verification, validation at each level
- Relevance of each level to system
- System prediction uncertainty

Y = Experimental data  
X = FEM prediction  
1 - Level 1  
2 - Level 2  
S - System

# Crack growth prediction

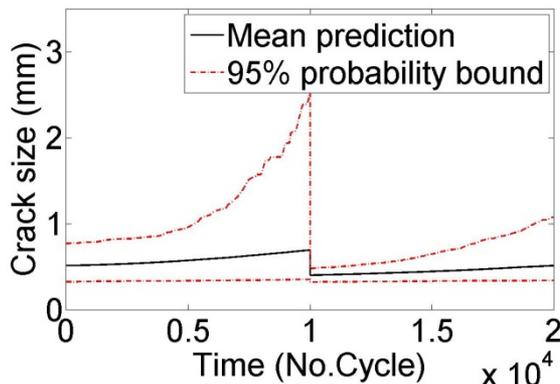
## -- Multiple models, time series data



**Dynamic  
Bayes Net**

**Include SHM data**

- Loads monitoring
- Inspection



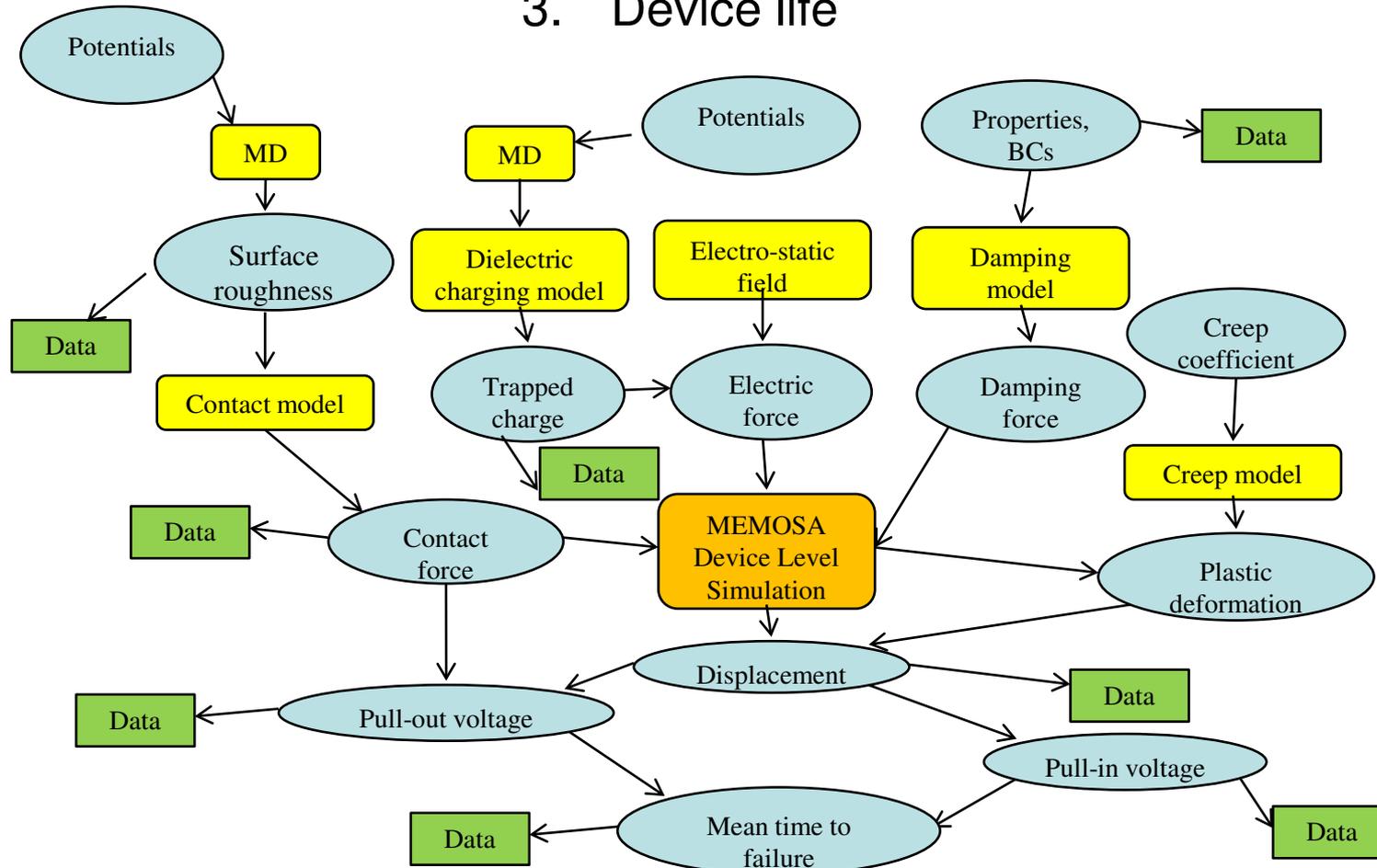
**Overall Crack Growth UQ**

Sankararaman et al, EFM, 2011  
Ling & Mahadevan, MSSP, 2012

# Bayesian Network for MEMS UQ

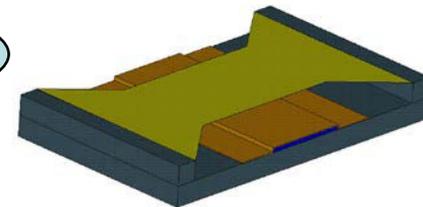
## Prediction goals

1. Gap vs. voltage
2. Pull-in and pull-out voltage
3. Device life



## Multiple Physics

1. Elasticity
2. Creep
3. Contact
4. Gas damping
5. Electrostatics

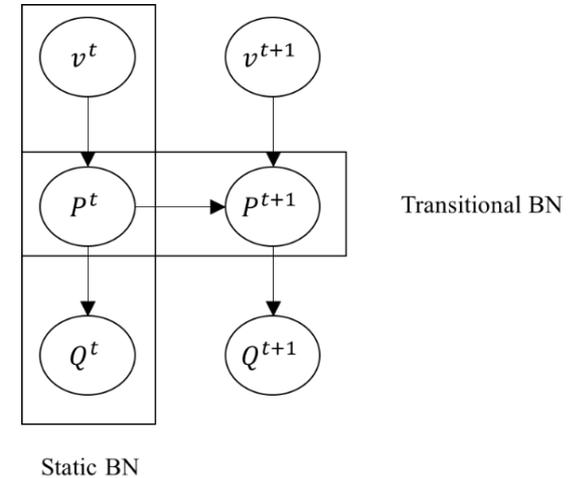


**RF MEMS Switch**  
**Purdue PSAAP**

# Dynamic Bayesian network

Extension of Bayesian network for modeling time-dependent systems

- Uncertainty aggregation over time
- Useful for probabilistic diagnosis and prognosis (SHM)



## DBN learning

Two stage learning

- Static BN learning: BN learning techniques (models, data, hybrid)
- Transitional BN learning: Models, Variable selection techniques (data)

## DBN Inference

MCMC methods: Expensive

Particle filter methods

- Sequential Importance Sampling (SIS)
- Sequential Importance Resampling (SIR)
- Rao-Blackwellized filter

Analytical approximations

- Gaussian inputs/outputs  $\rightarrow$  Kalman Filter, EKF, UKF

$$P^{t+1} = G(P^t, v^{t+1})$$

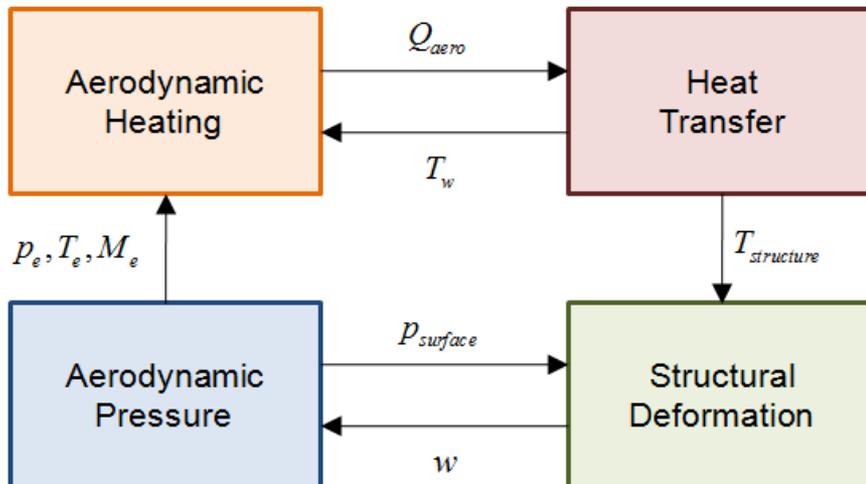
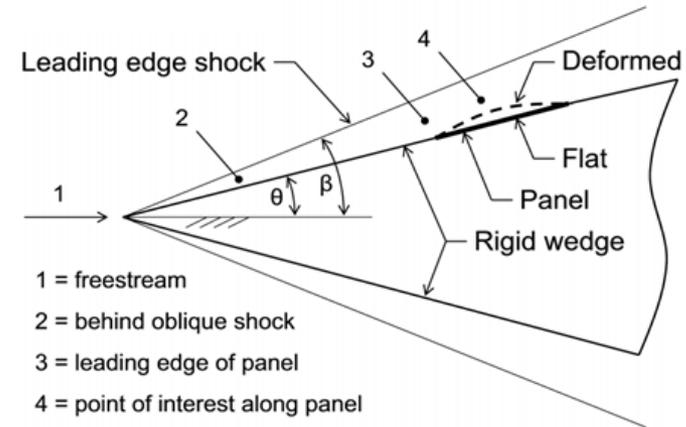
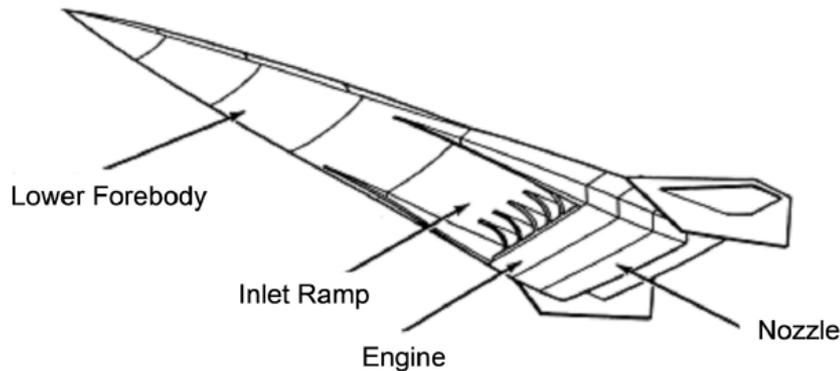
$$Q^t = H(P^t)$$

Bartram and Mahadevan, SCHM, 2014

# Multi-disciplinary analysis

## Hypersonic aircraft panel

- Coupled fluid-thermal-structural analysis



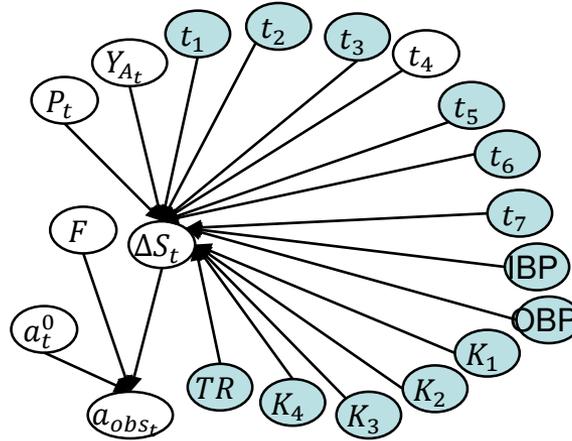
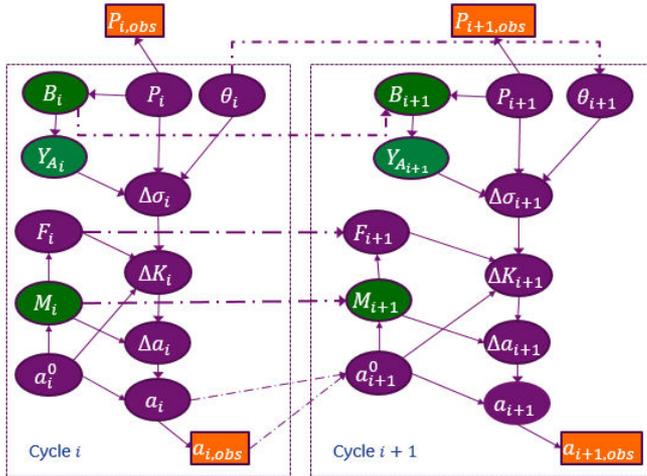
## Transient analysis

- Model error estimation in different disciplines
- Error accumulates across disciplinary models and over time
- Dynamic Bayesian network (DeCarlo et al, 2014)

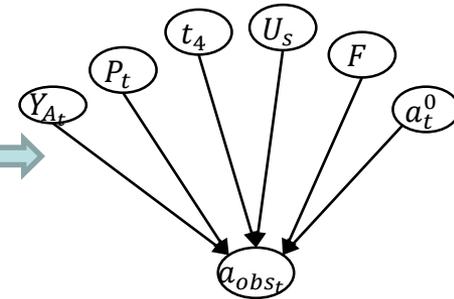
# Airframe Digital Twin

## Dynamic Bayesian Network

→ Fusion of multiple models and data sources



## Two-layer BN + UKF

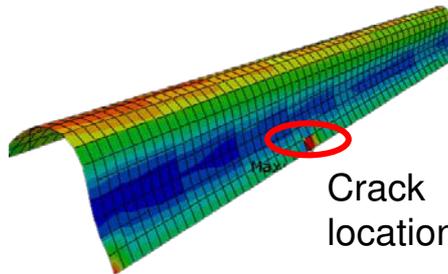
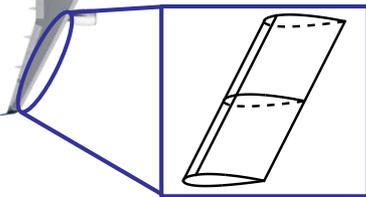


10 hrs → 2 hrs → 1 sec

Scalability → GSA → auxiliary variable, stratified sampling  
→ Collapse the BN and apply UKF

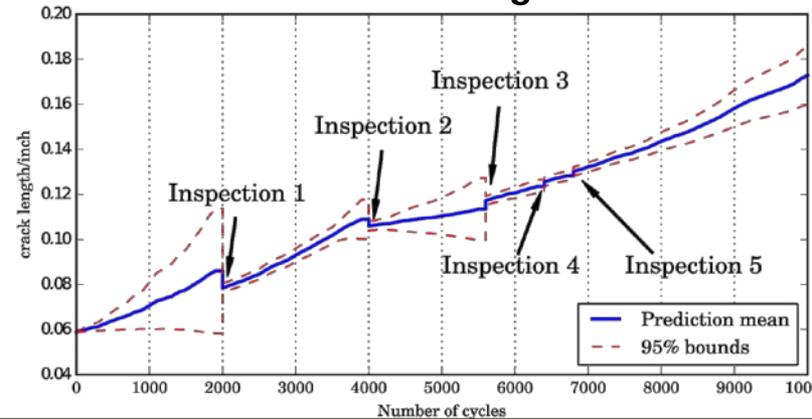


Aircraft wing



Crack location

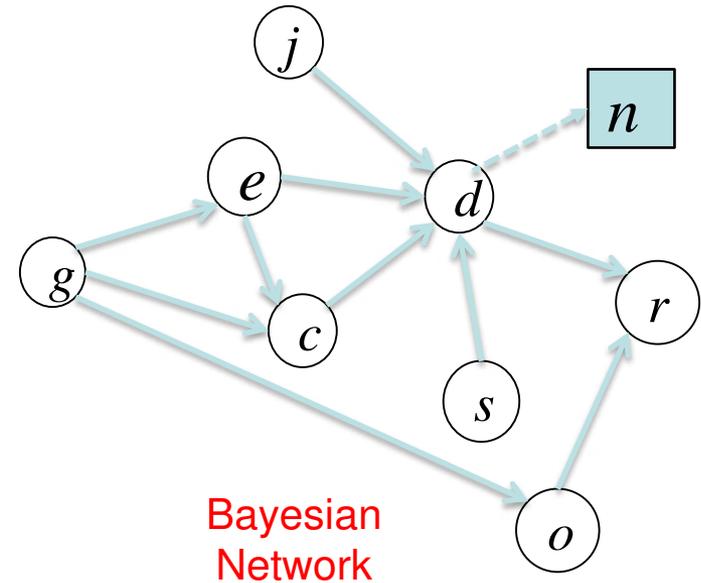
## Crack Growth Prognosis UQ



# Comprehensive framework for uncertainty aggregation and management

## Information fusion

- Heterogeneous data of varying precision and cost
- Models of varying complexity, accuracy, cost
- Include calibration, verification and validation results at multiple levels



## Facilitates

- Forward problem: Uncertainty aggregation in model prediction
  - Integrate all available sources of information and results of modeling/testing activities
- Inverse problem: Resource allocation for uncertainty reduction
  - Model development, test planning, simulation orchestration, system design, manufacturing, operations, health monitoring, inspection/maintenance/repair

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