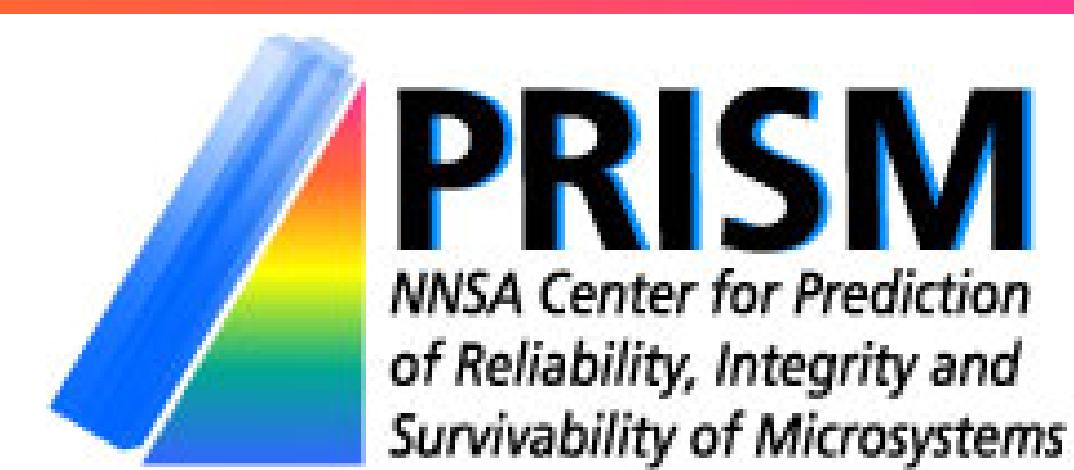
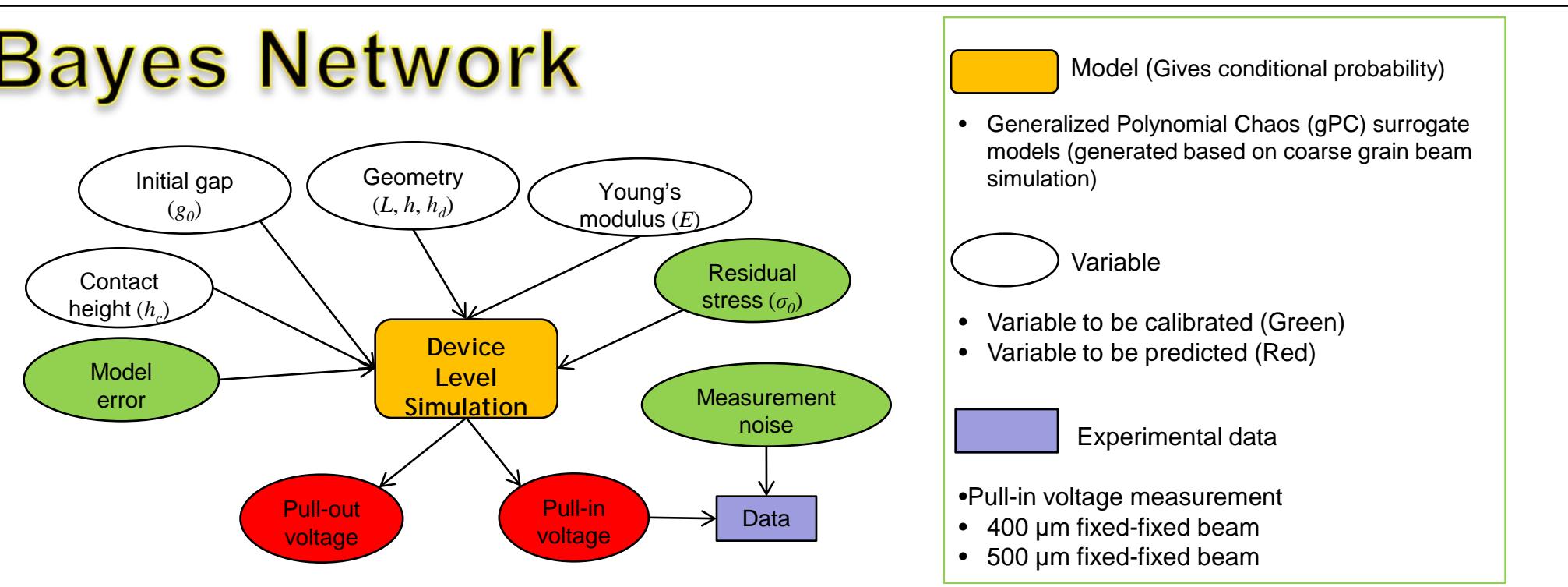


Integration of Calibration and Validation Results towards Prediction UQ

You Ling, Shankar Sankararaman and Sankaran Mahadevan, Vanderbilt University

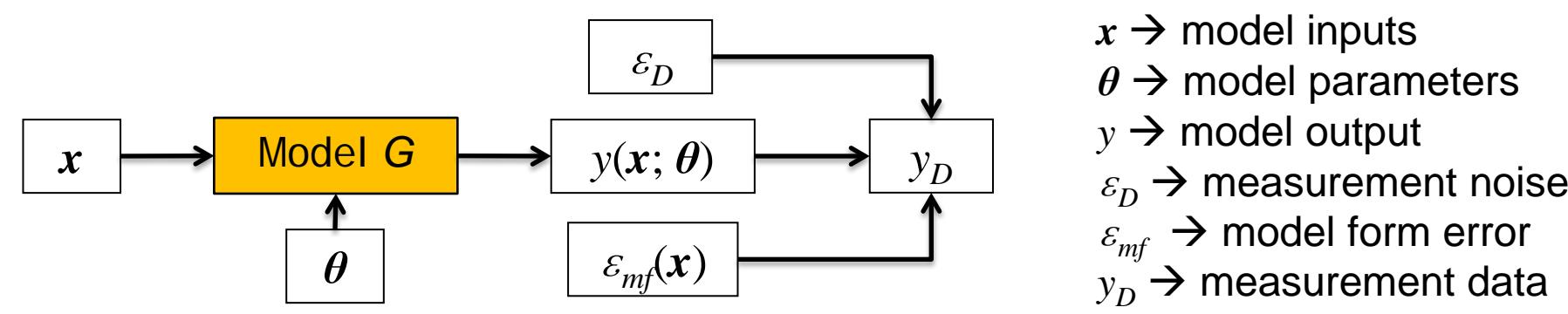


Bayes Network



Model Calibration with Bayes Network

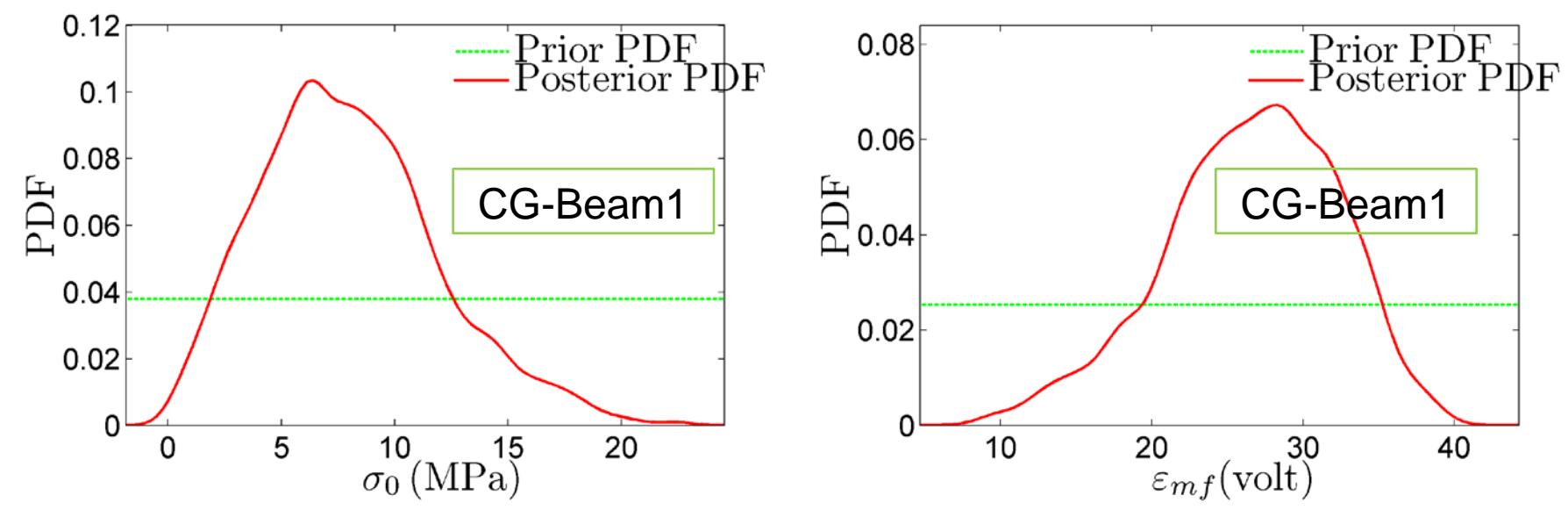
- Computational model $y = G(x; \theta)$



$x \rightarrow$ model inputs
 $\theta \rightarrow$ model parameters
 $y \rightarrow$ model output
 $\varepsilon_D \rightarrow$ measurement noise
 $\varepsilon_{mf}(x) \rightarrow$ model form error
 $y_D \rightarrow$ measurement data

$$\text{Bayesian calibration} \quad \pi(\theta | y_D) = \frac{\Pr(y_D | \theta) \pi(\theta)}{\int \Pr(y_D | \theta) \pi(\theta) d\theta}$$

- $\Pr(y_D | \theta)$: likelihood function of θ
- $\pi(\theta)$: prior probability density function of θ
- $\pi(\theta | y_D)$: updated probability density function of θ



Quantification of Model Errors

- Discretization error $\varepsilon_h \rightarrow$ Richardson extrapolation

$$\varepsilon_h = \frac{f_1 - f_2}{r^p - 1} \quad p = \frac{\log[(f_3 - f_2)/(f_2 - f_1)]}{\log(r)}$$

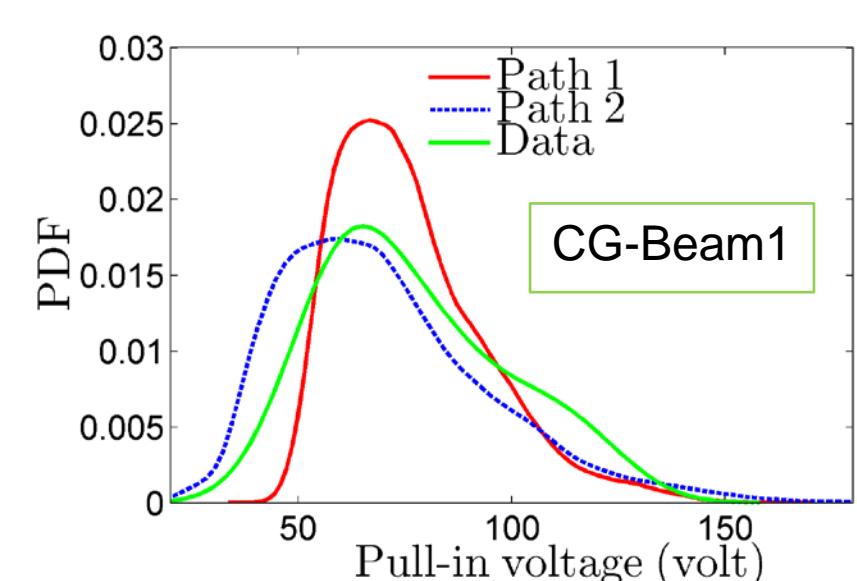
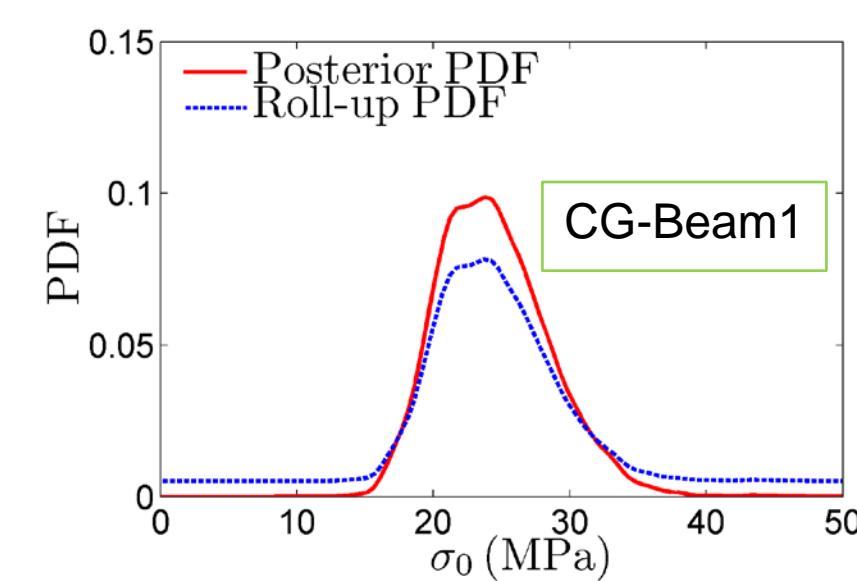
$f_1 \rightarrow$ Coarse mesh solution
 $f_2 \rightarrow$ Median mesh solution
 $f_3 \rightarrow$ Fine mesh solution
 $r \rightarrow$ Mesh refinement ratio (>1)

- Surrogate model fitting error $\varepsilon_f \rightarrow$ Gaussian process (GP) model

$$\begin{aligned} E[\varepsilon_f(x) | \varepsilon_f^*] &= \mathbf{h}^T(x)\beta + \mathbf{r}^T \mathbf{R}^{-1} (\varepsilon_f^* - \mathbf{H}\beta) \\ \text{Var}[\varepsilon_f(x) | \varepsilon_f^*] &= \sigma^2 (1 - \mathbf{r}^T \mathbf{R}^{-1} \mathbf{r}) \end{aligned}$$

- Model form error ε_{mf}

- Assumed as a random variable independent of model input x
- Calibrated using Bayesian method



$$\pi(\theta | y_{D1}, y_{D2}) = \pi(\theta | y_{D1}, G) \Pr(G | y_{D1}, y_{D2}) + \pi(\theta) (1 - \Pr(G | y_{D1}, y_{D2}))$$

$$B = \frac{\Pr(y_{D2} | G, y_{D1})}{\Pr(y_{D2} | \bar{G})}$$

$$\Pr(G | y_{D1}, y_{D2}) = \frac{B}{B+1}$$

