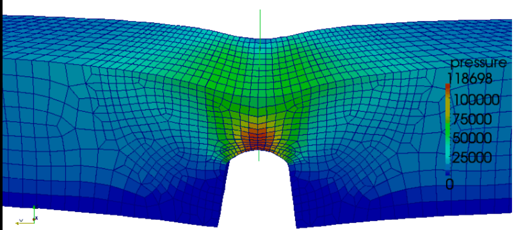
SAND2014-0214C

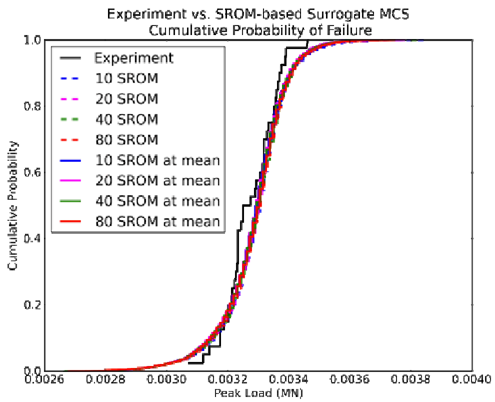
L2 Laser Weld Milestone

August 26, 2013

Revised for PPM Summit

January 16, 2014





Jay Foulk, John Emery, Rich Field, Kyle Karlson, Mircea Grigoriu (Cornell University)

Sandia National Laboratories

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SAND 2013-7167 P

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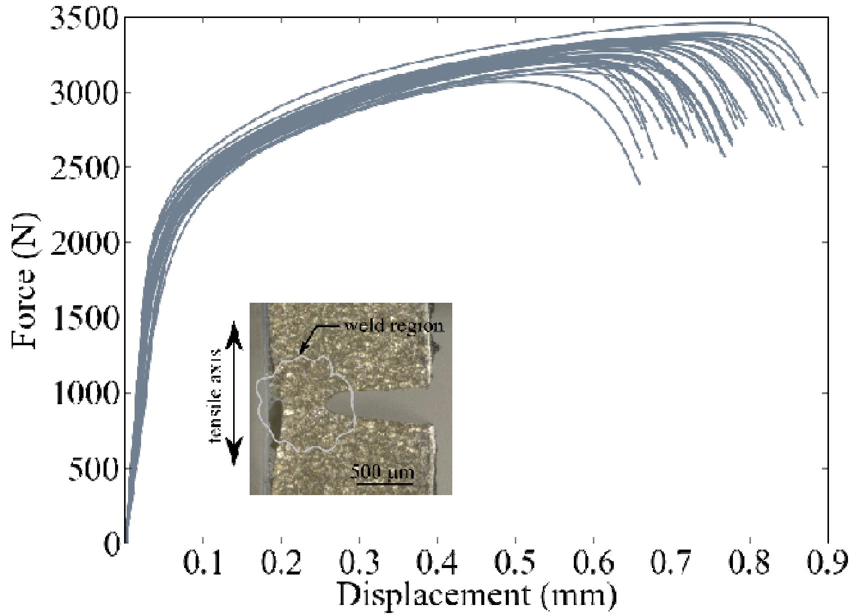
At 10,000 feet (3000 m)

We care about 304L laser welds: 304L laser welds are pervasive throughout the stockpile. Understanding the performance of 304L laser welds enables designers to be better stewards of the stockpile.

We observe variability: The ductility of 304L laser welds varies from specimen to specimen. We observe both material and geometric variability.



We care about the impact of variability on performance: We need to develop methods that capture and propagate variability in a mathematically rigorous manner. The tail of the distribution matters.

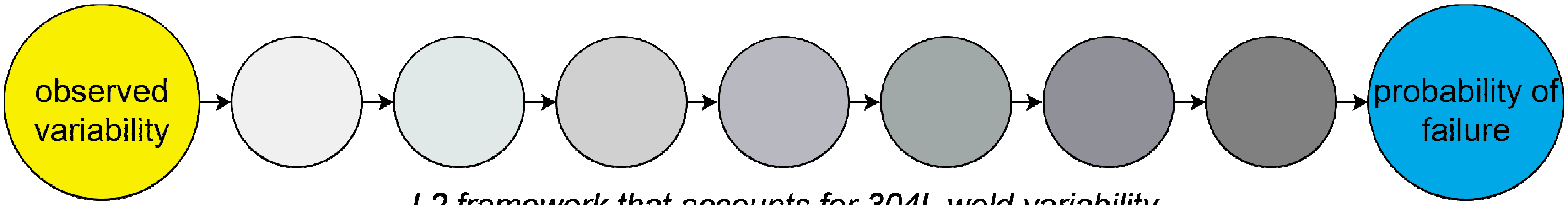
We seek the tail with limited computational resources: The only general approach to determine the tails of the output distribution is through repeated random sampling, Monte Carlo Simulation (MCS). We do not, however, have the computational resources to repeatedly sample component or system level finite element models. We need to be smarter in how we apply MCS.

We need a framework that is flexible and extensible: We need to have the ability to incorporate new experiments and consider new physics. The analyst, not the framework, should dictate the path forward.

Go write a milestone

Description: Thousands of feet of 304L stainless steel laser welds reside in numerous weapon components, including first-order nuclear safety systems, that serve a wide variety of functions. These welds must remain structurally sound in both normal and abnormal environments. Variability in weld geometry and material properties can have a critical impact on performance margins and uncertainties in both current and future designs. Historically, component analysis models have incorporated variability through a statistically limited set of experimental data. This milestone will deliver a *capability* for constructing component-scale models from a statistically significant population of the weld response obtained from both experiments and higher fidelity simulations.

Completion Criteria: *Demonstration* of a *framework* that accounts for 304L weld variability through the construction of component level models for quasi-static mechanical environments.



L2 framework that accounts for 304L weld variability

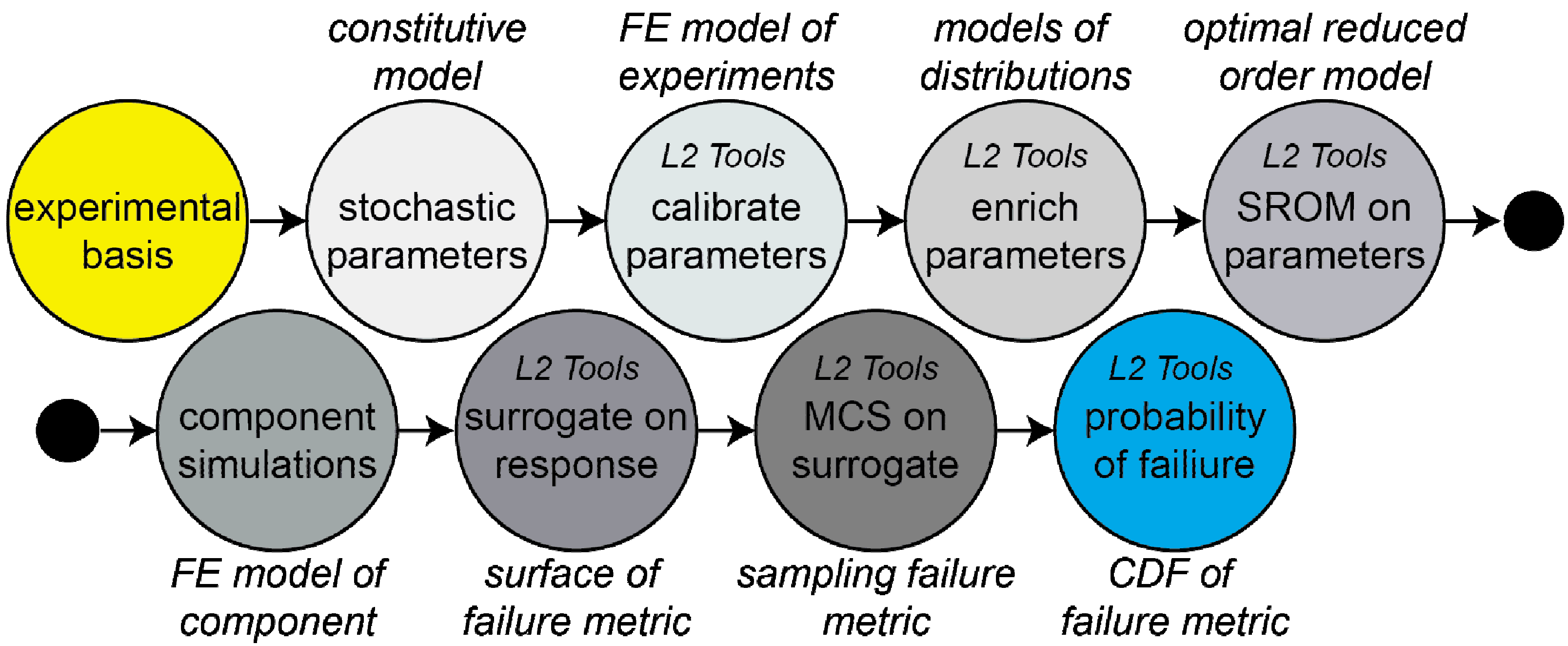
Committee chair: John Pott

Committee members: Jay Dike (Analysis), Frank Dempsy (Analysis), Sharlotte Kramer (Experiments), Jake Ostien (Mechanics), Brian Adams (Optimization/Uncertainty), Mike Maguire (Welding)

Executive summary

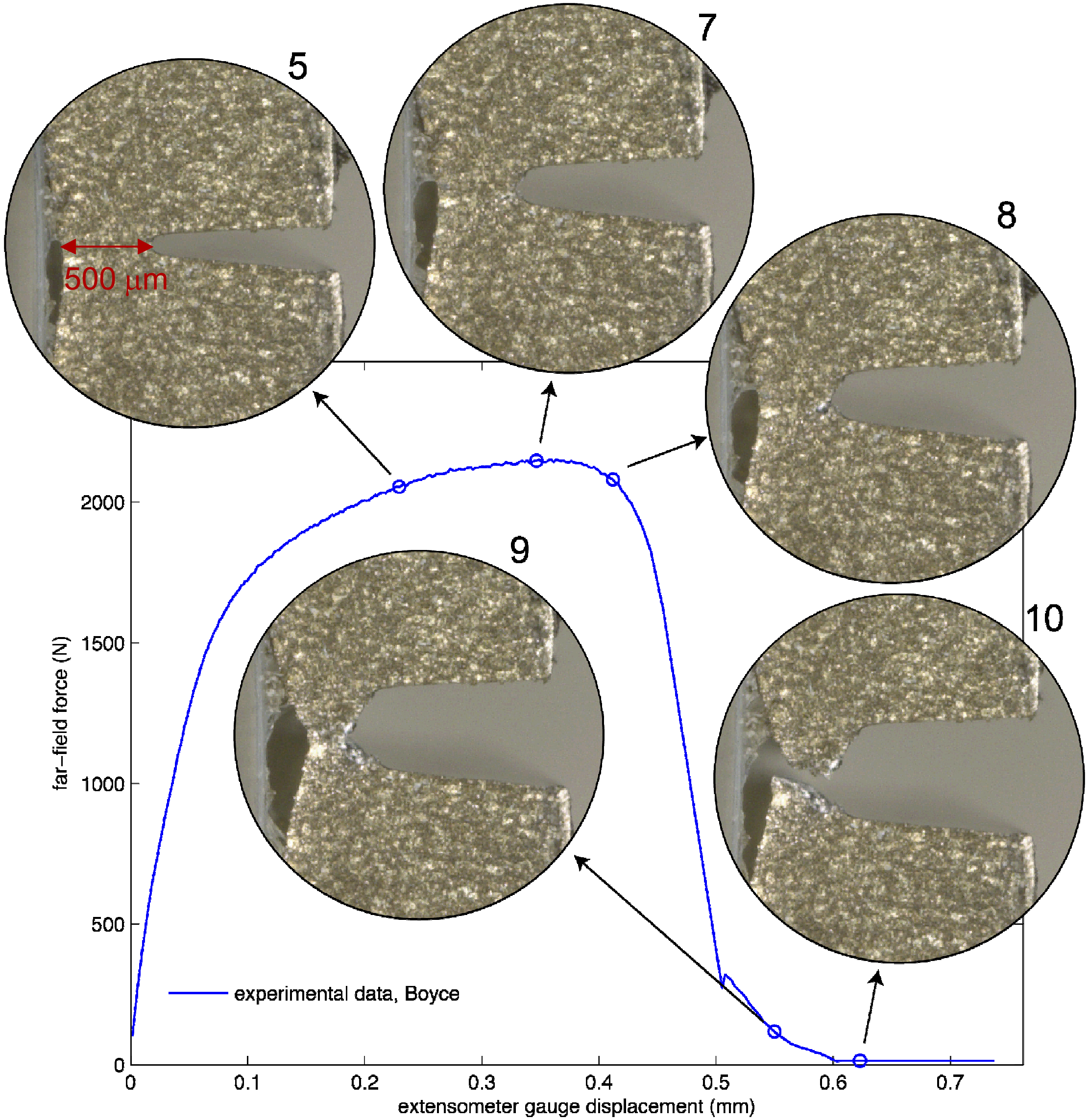
Our work illustrates a framework for *constructing* stochastic reduced order models (SROMs) to capture geometric/material variability in 304L laser welds.

- Developed tools for calibration, enrichment, and the construction of SROMs
- Applied “brute force” Monte Carlo with 5000 finite element (FE) calculations to obtain the character of the output failure metric
- SROM-based surrogate accurately computed the cumulative distribution function, capturing the lower tail, at 0.8% of the computational cost (40 vs 5000 FEA)
- On an equal computational footing, we compared the SROM surrogate to sets of “brute force” Monte Carlo based on 40 FE calculations. The SROM-based surrogate is far more accurate.



Motivation – mechanics

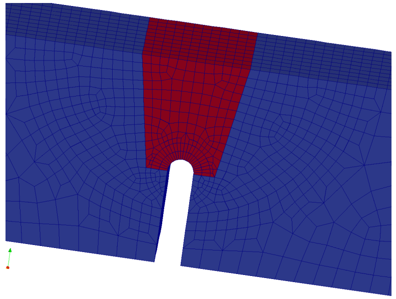
Modeling the failure process is beyond the scope of the L2 milestone. We *attempt* to capture global necking through the calibration of a rate and temperature independent J_2 plasticity model.

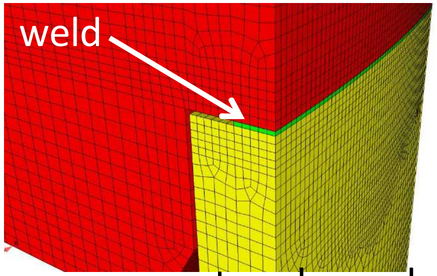


Because necking is the dominant mechanism prior to failure, we can employ unloading as a failure metric.

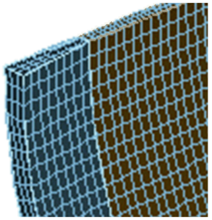
Motivation – QMU

- We often deal with physical systems involving multiple physics and spanning many length / time scales
- The FE models of such systems are very large and complex
- Uncertainty is always present; QMU analyses are often desirable
- Monte Carlo Simulation (MCS) is the only general approach for uncertainty propagation and QMU studies
- How do we make MCS feasible with large complex FE models?
- Move to a Stochastic Reduced Order Model
  - Idea – approximate random function on infinite sample space with a new random function on a finite sample space
  - "Smart Monte Carlo"



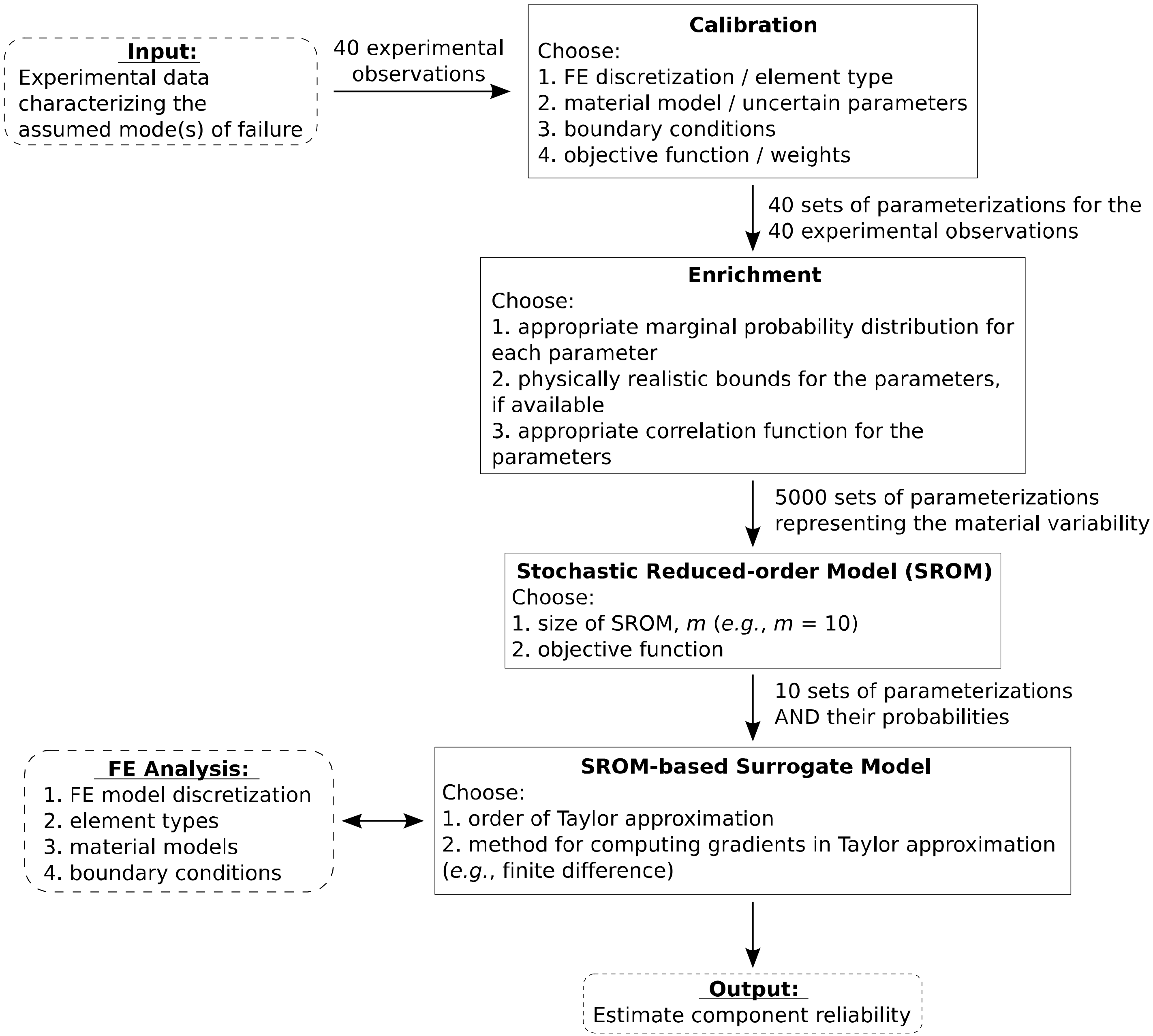


component-scale model
(~12 elements in ligament)

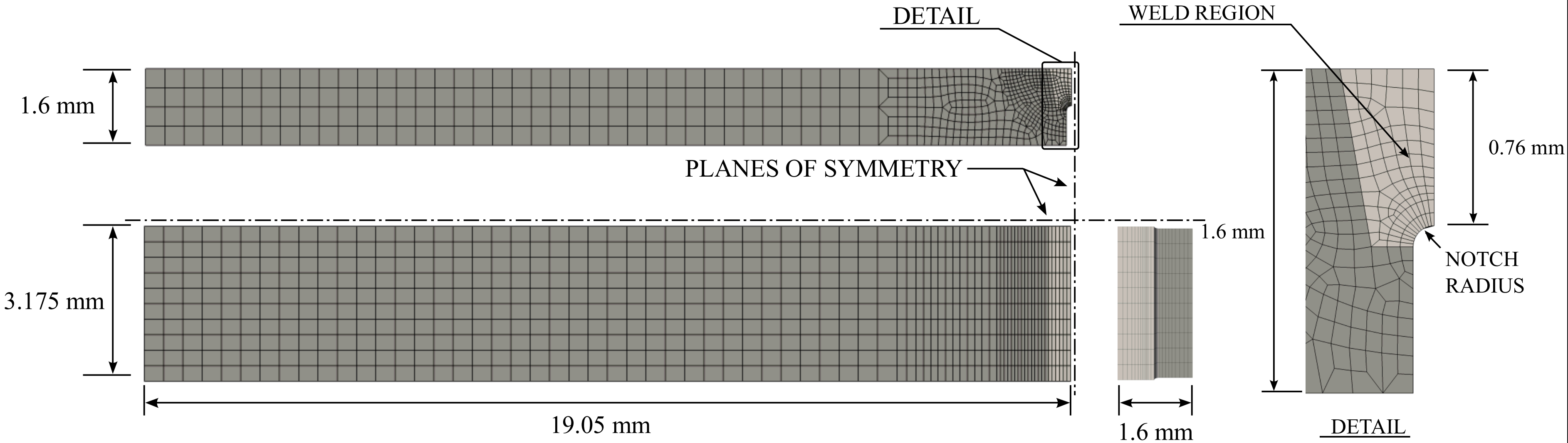


~4 elements through thickness

FE model of system (o(e7) DOF)


Input:
Experimental data characterizing the assumed mode(s) of failure
40 experimental observations
Calibration
Choose:
1. FE discretization / element type
2. material model / uncertain parameters
3. boundary conditions
4. objective function / weights
40 sets of parameterizations for the 40 experimental observations
Enrichment
Choose:
1. appropriate marginal probability distribution for each parameter
2. physically realistic bounds for the parameters, if available
3. appropriate correlation function for the parameters
5000 sets of parameterizations representing the material variability
Stochastic Reduced-order Model (SROM)
Choose:
1. size of SROM, m (e.g., m = 10)
2. objective function
10 sets of parameterizations AND their probabilities
FE Analysis:
1. FE model discretization
2. element types
3. material models
4. boundary conditions
SROM-based Surrogate Model
Choose:
1. order of Taylor approximation
2. method for computing gradients in Taylor approximation (e.g., finite difference)
Output:
Estimate component reliability

Minimize variables, modify geometry



base sheet: deterministic
weld region: stochastic

$$\sigma_y = Y + \kappa \qquad \dot{\kappa} = [H - R\kappa]\,\dot{\epsilon}_p$$

$$\kappa(\epsilon_p) = \frac{H}{R}\left[1 - \exp(-R\epsilon_p)\right]$$

Simplifications

1. *Explore BCJ_mem for flexibility (rate, temperature)*
2. *Assume weld is rate/temperature independent*
3. *Assume the weld is homogeneous*
4. *Transition from a sharp crack to a smooth notch*

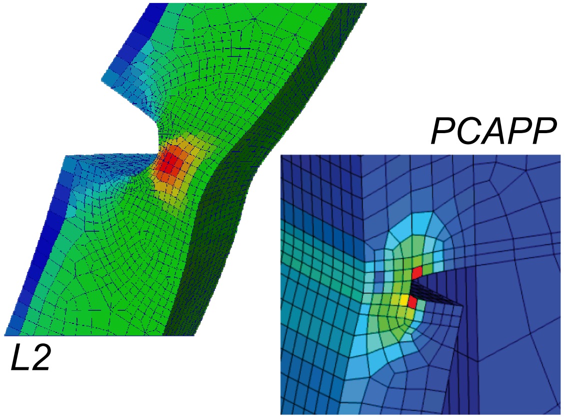
Y	initial yield stress
H	hardening (linear)
R	recovery coefficient

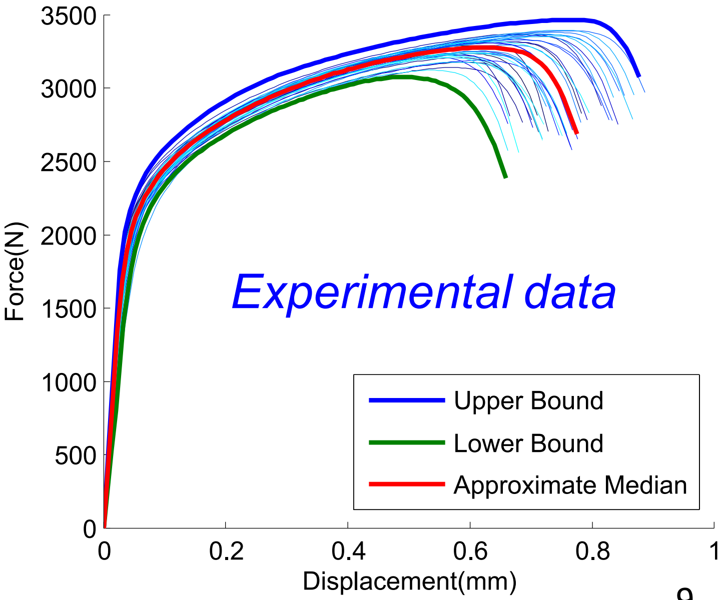
Current work: 3 material constants, dimensionality = 3

MatCal wraps Dakota

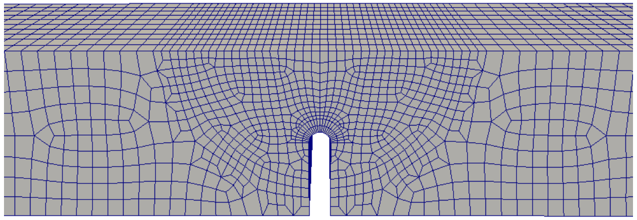
Move calibration from Matlab to Dakota. Develop a robust tool for analysts.

- Developed a wrapper for Dakota – MatCal - https://snl-wiki.sandia.gov/display/solids/MatCal+-+Material+Model+Calibration+Tool
- Initially, the simulation was calibrated to the upper bound, approximate median and lower bound of the experimental data sets using the global optimization routine *ncsu_direct* from DAKOTA.
  - The calibrations were weighted to favor data points between the elastic region and peak load on the force displacement curve.
  - Large parameter bounds chosen for the optimizations.
- The results from these initial calibrations were further improved using the least squares calibration algorithm *nl2sol* from DAKOTA.
- The calibration bounds were tightened using the results from global optimizations and an initial point near the upper bound was chosen for the remaining 37 calibrations employing *nl2sol*.

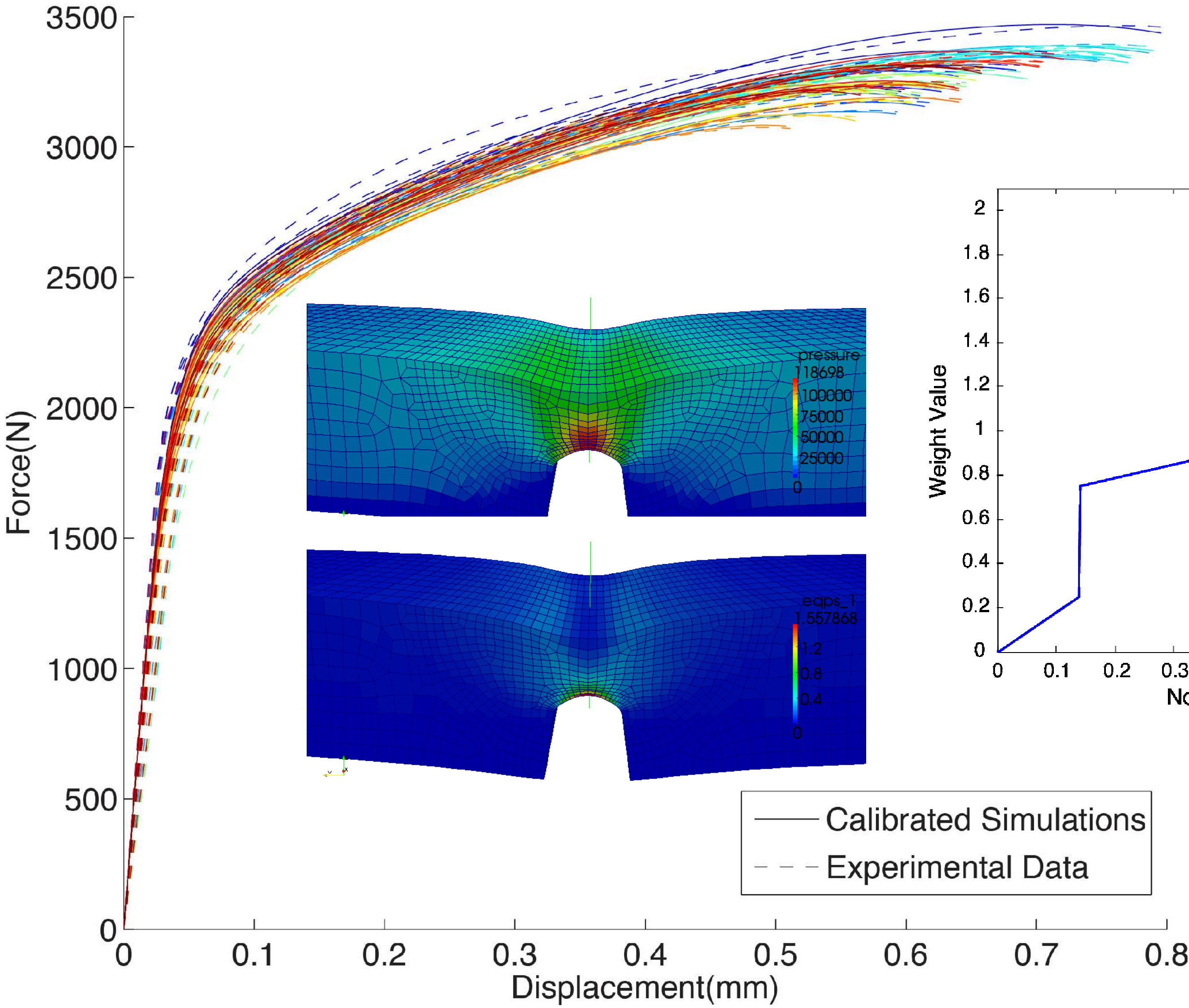




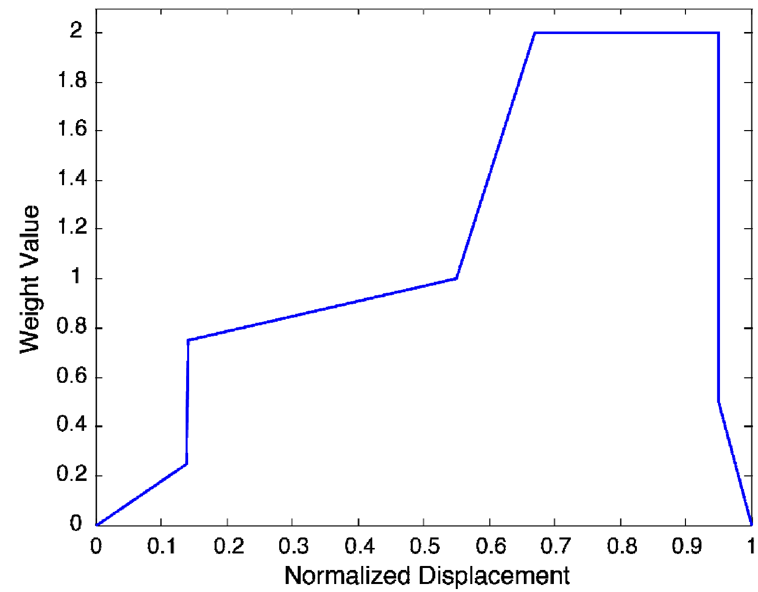
proposed discretization ~ component discretization



Reasonable fits to experiments



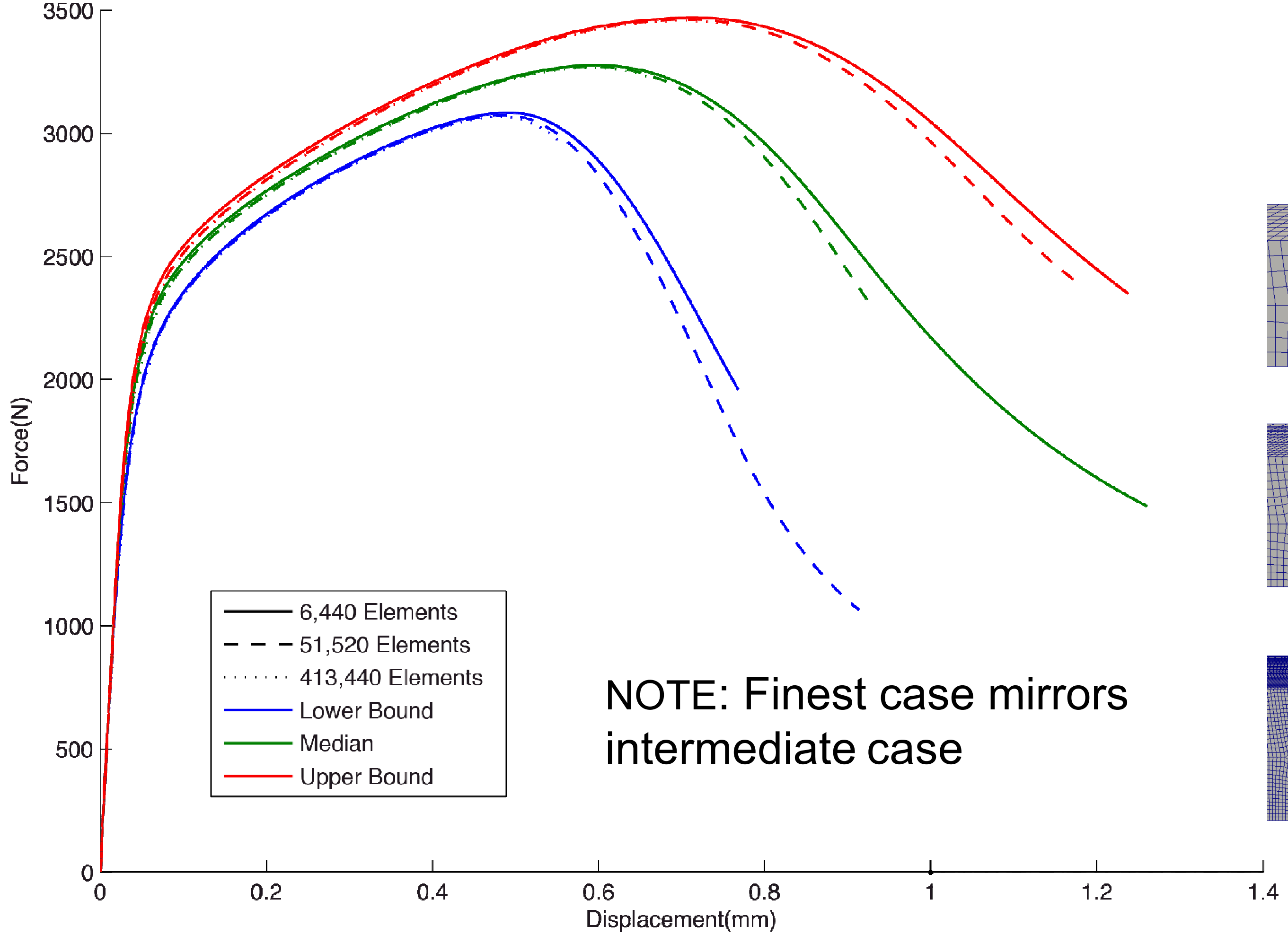
weight function



focus on necking

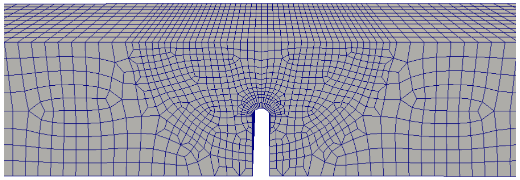
Small changes under refinement

Although we are convoluting material and geometric variability, we are relatively independent of the discretization. We have less to worry about – for far-field tension

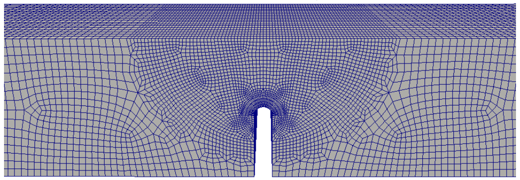


NOTE: Finest case mirrors intermediate case

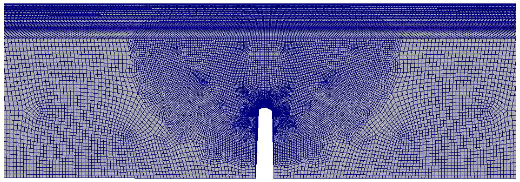
6,440 elements



51,520 elements



413,440 elements

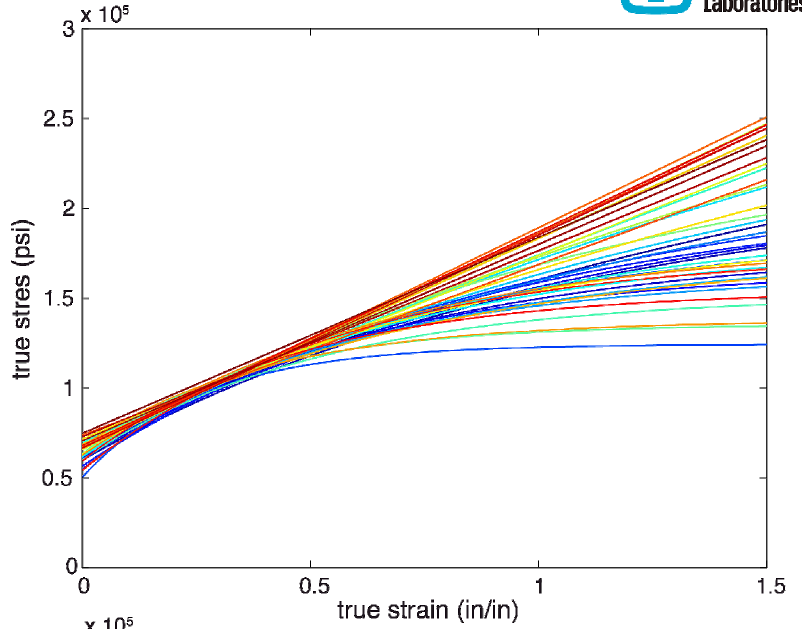


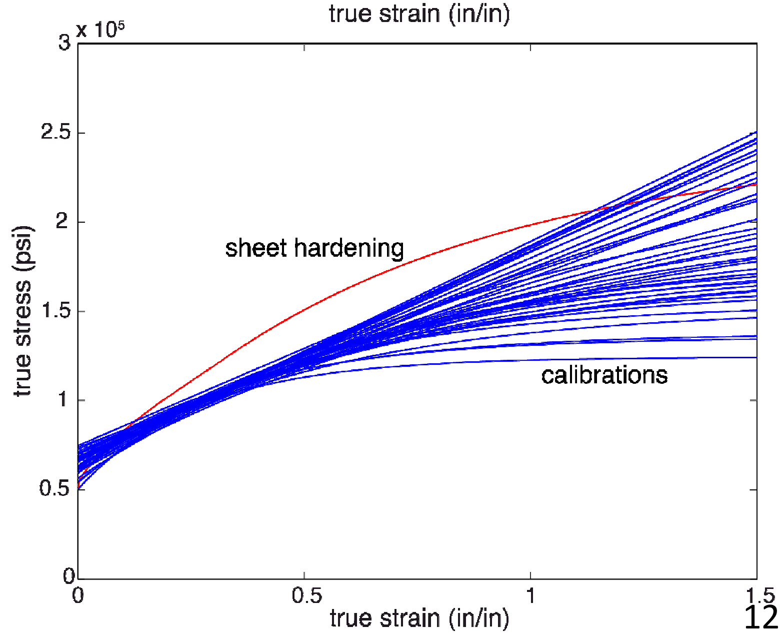
Results of calibration

	Yield Stress	Recovery Constant	Hardening Constant	Norm of Error (To peak load)
Data Set 5	6.740E+04	5.393E-01	1.202E+05	**18.89**
Data Set 10	5.988E+04	9.108E-01	1.444E+05	**19.45**
Data Set 9	6.153E+04	1.393E+00	1.634E+05	**20.56**
Data Set 8	6.089E+04	9.225E-01	1.460E+05	**22.21**
Data Set 25	5.455E+04	1.797E+00	2.005E+05	**22.49**
Data Set 31	5.650E+04	1.093E+00	1.681E+05	**22.94**
Data Set 19	6.327E+04	8.896E-01	1.467E+05	**25.60**
Data Set 30	5.026E+04	3.762E+00	2.789E+05	**26.80**
Data Set 32	5.955E+04	1.352E+00	1.738E+05	**27.74**
Data Set 7	6.984E+04	6.550E-01	1.225E+05	**27.95**
Data Set 21	6.125E+04	1.727E+00	1.776E+05	**29.15**
Data Set 1	6.650E+04	1.307E+00	1.451E+05	**29.79**
Data Set 23	6.763E+04	5.850E-01	1.262E+05	**30.52**
Data Set 18	6.598E+04	3.533E-01	1.252E+05	**30.52**
Data Set 22	6.156E+04	1.393E+00	1.680E+05	**31.15**
Data Set 26	6.220E+04	1.200E+00	1.604E+05	**31.18**
Data Set 6	6.977E+04	9.873E-02	1.095E+05	**33.11**
Data Set 27	5.984E+04	1.895E+00	1.742E+05	**33.65**
Data Set 38	6.310E+04	2.801E+00	2.029E+05	**35.19**
Data Set 33	6.324E+04	8.190E-01	1.543E+05	**36.91**
Data Set 11	6.680E+04	3.131E-02	1.185E+05	**37.55**
Data Set 34	6.750E+04	3.570E-01	1.254E+05	**37.62**
Data Set 15	6.565E+04	4.650E-05	1.209E+05	**38.04**
Data Set 4	7.142E+04	0.000E+00	1.023E+05	**38.33**
Data Set 36	6.298E+04	1.257E+00	1.602E+05	**39.04**
Data Set 28	7.133E+04	3.672E-01	1.130E+05	**39.86**
Data Set 13	6.854E+04	0.000E+00	1.147E+05	**43.00**
Data Set 24	6.603E+04	1.307E+00	1.447E+05	**43.47**
Data Set 29	6.718E+04	2.500E+00	1.765E+05	**43.48**
Data Set 39	6.236E+04	1.476E+00	1.775E+05	**43.49**
Data Set 16	6.609E+04	0.000E+00	1.231E+05	**44.37**
Data Set 40	7.375E+04	8.557E-03	9.537E+04	**44.75**
Data Set 17	6.682E+04	2.622E-02	1.208E+05	**45.97**
Data Set 20	5.415E+04	1.706E+00	2.071E+05	**46.46**
Data Set 37	5.933E+04	2.109E+00	2.009E+05	**48.16**
Data Set 12	6.782E+04	0.000E+00	1.191E+05	**48.52**
Data Set 14	6.643E+04	0.000E+00	1.187E+05	**55.21**
Data Set 2	7.283E+04	0.000E+00	1.036E+05	**57.55**
Data Set 35	7.046E+04	0.000E+00	1.095E+05	**60.95**
Data Set 3	7.475E+04	0.000E+00	1.090E+05	**94.89**

Average	6.467E+04	9.160E-01	1.467E+05	37.66
Median	6.600E+04	8.543E-01	1.446E+05	37.23
Standard Deviation	5.452E+03	9.055E-01	3.780E+04	13.97

$$\sigma_y = Y + \frac{H}{R}\left[1 - \exp\left(-R\epsilon_p\right)\right]$$





Data “Enrichment”

- Motivation
  - For optimal results, SROM construction requires abundant data
  - Experimental data is often very limited
  - We need a method to enrich the existing experimental data set
- One approach – translation random vectors
  - A probabilistic model with functional form based on physical arguments, calibrated to available data
  - Able to match second-moment properties (mean, covariance) and marginal distributions; these are quantities we can easily estimate from data
  - Straightforward to produce large numbers of samples for SROM construction
  - This approach is widely used at Sandia and elsewhere

How to choose probability distribution

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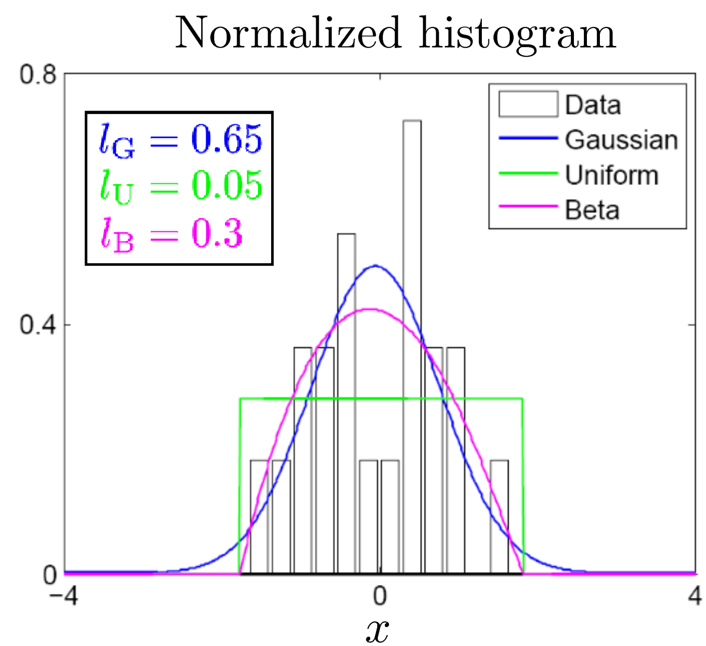
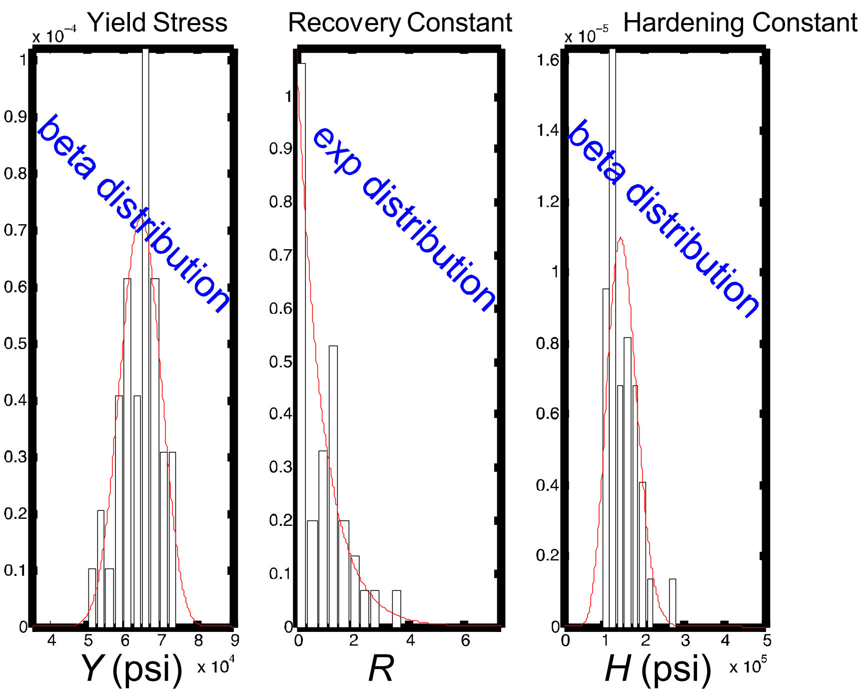
- 20 independent samples of X
  - $x_1, x_2, \ldots, x_{20}$
- Statistical considerations
  - Method of moments
  - Method of maximum likelihood
- Physical considerations
  - What are the underlying physics?
  - Is X continuous or discrete?
  - Is X bounded?
  - Is PDF symmetric about mean?
- Other considerations
  - Conservatism / ease of use
  - What are the consequences / tradeoffs between the different models?

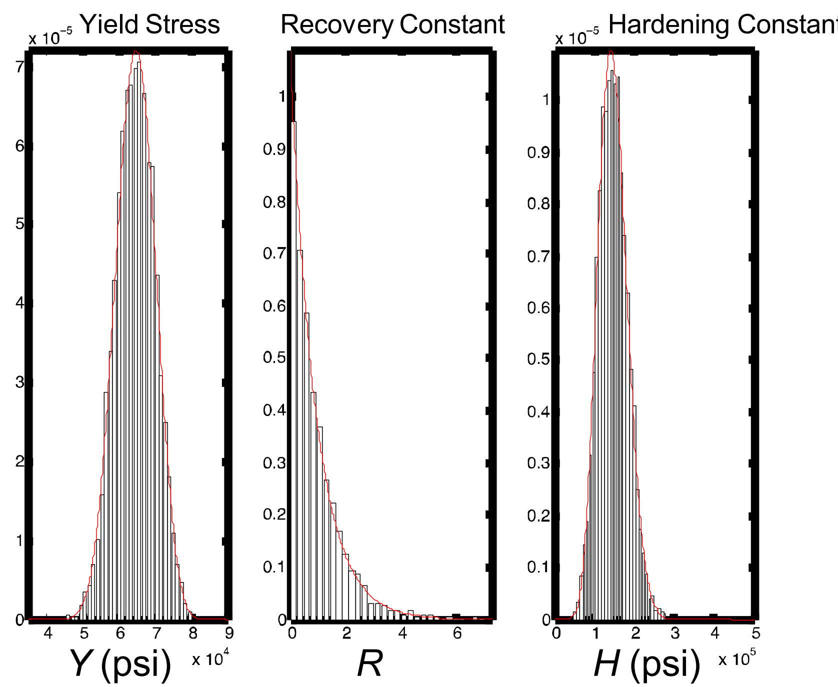


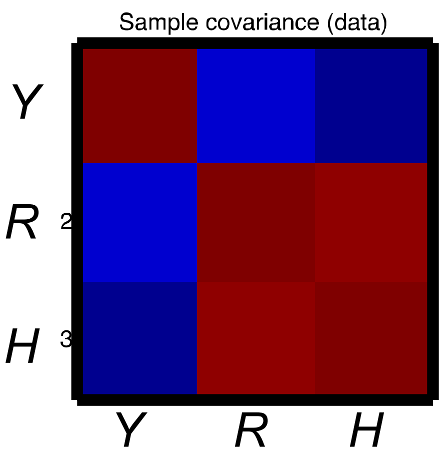
Application to weld data

- Available information
  - 40 experimental measurements of weld geometry
  - Mapped to 3 constitutive model parameters via detailed FE analysis and optimization routine
    - Yield stress (Y), recovery constant (R), hardening constant (H)
  - Lower and upper bounds on each model parameter
    - Expert judgment, FE analysis to determine onset of unrealistic material behavior
  - Estimate covariance matrix based on 40 samples of model parameters
- Modeling assumptions
  - Yield stress and hardening constant follow a beta distribution
  - Recovery constant follows an exponential distribution
  - Consistent with bound information and some literature
  - Alternative distributions can be studied at a later date

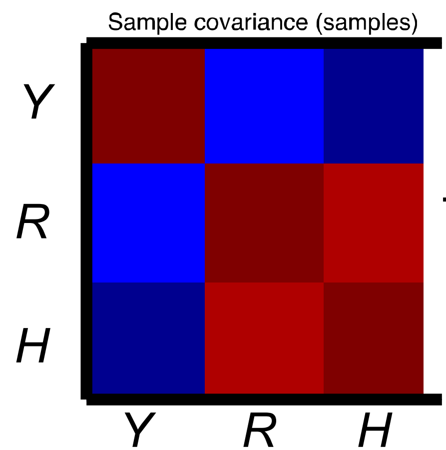
Results





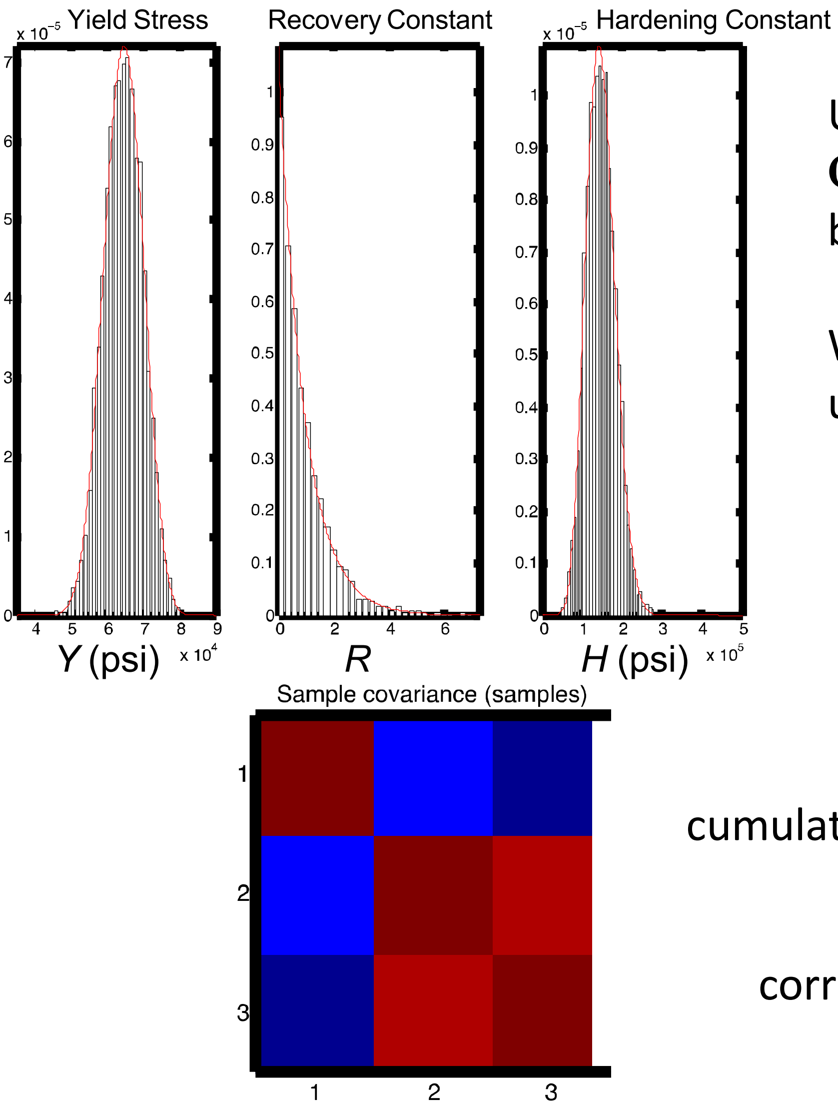


Experimental Data



Translation Model

Uncertain input data



Uncertain data:
$\boldsymbol{\Theta} \in \mathbb{R}^3$ = vector describing weld constitutive behavior (yield *Y*, recovery *R*, hardening *H*).

What are the some measures to quantify these uncertain data?

Estimators of important properties

moments: $$\hat{\mu}_s(r) = \sum_{i=1}^{n} (1/n)\,(\theta_{i,s})^r,$$

cumulative distribution: $$\hat{F}_s(x) = \sum_{i=1}^{n} (1/n)\,1(\theta_{i,s} \leq x)$$

correlation function: $$\hat{c}(s,t) = \sum_{i=1}^{n} (1/n)\,\theta_{i,s}\,\theta_{i,t}$$

NOTE: If other properties are deemed important, include them.

Reduced-order model for uncertainty

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To develop a model that optimally represents the uncertainty in the input we choose a discrete random variable $\tilde{\boldsymbol{\Theta}}$. The SROM is then defined by the collection $\left(\tilde{\boldsymbol{\theta}}_k, \tilde{p}_k\right)$ k = 1, ..., m that minimizes an objective function of the form:

$$\underbrace{\max_{1\le r\le \bar{r}} \max_{1\le s\le d} \alpha_{s,r}|\tilde{\mu}_s(r) - \hat{\mu}_s(r)|}_{\text{moments}} + \underbrace{\max_{1\le s\le d} \beta_s|\tilde{F}_s(x) - \hat{F}_s(x)|}_{\text{cumulative distribution}} + \underbrace{\zeta_{s,t} \max_{s,t} |\tilde{c}(s,t) - \hat{c}(s,t)|}_{\text{correlation}}$$

SROM (solve for $\tilde{p}_k$ given a set of m randomly chosen samples from V)

$$\tilde{\mu}_s(r) = \mathrm{E}[\tilde{\Theta}_s^r] = \sum_{k=1}^{m} p_k\,(\tilde{\theta}_{k,s})^r$$

$$\tilde{F}_s(x) = \Pr(\tilde{\Theta}_s \le x) = \sum_{k=1}^{m} p_k\,1(\tilde{\theta}_{k,s} \le x)$$

$$\tilde{c}(s,t) = \mathrm{E}[\tilde{\Theta}_s\,\tilde{\Theta}_t] = \sum_{k=1}^{m} p_k\,\tilde{\theta}_{k,s}\,\tilde{\theta}_{k,t}$$

Estimates of uncertainty

$$\hat{\mu}_s(r) = \sum_{i=1}^{n}(1/n)\,(\theta_{i,s})^r,$$

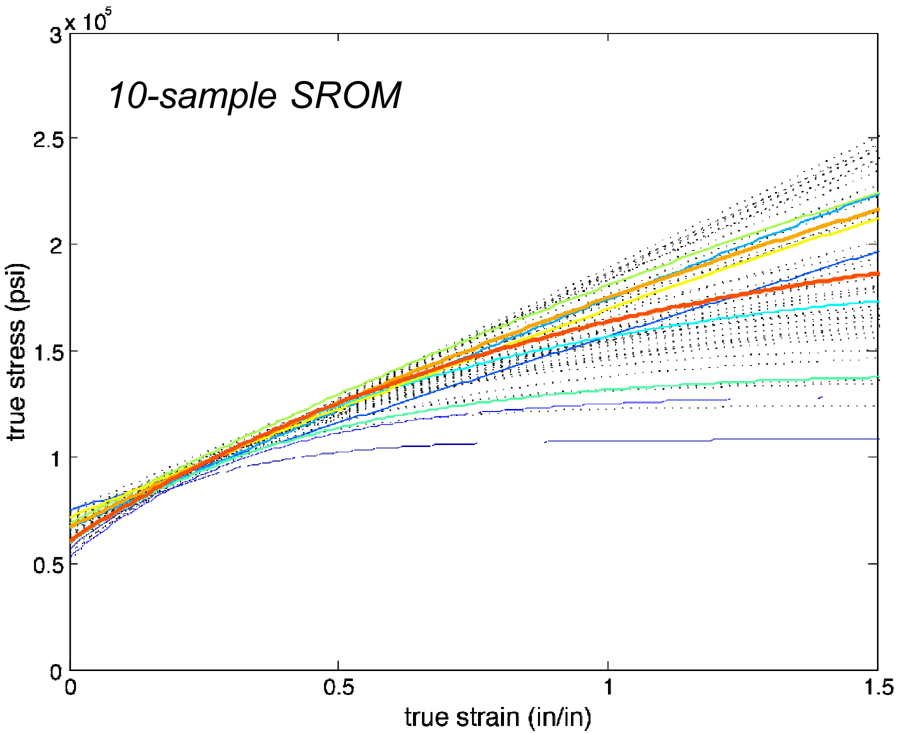
$$\hat{F}_s(x) = \sum_{i=1}^{n}(1/n)\,1(\theta_{i,s} \le x)$$

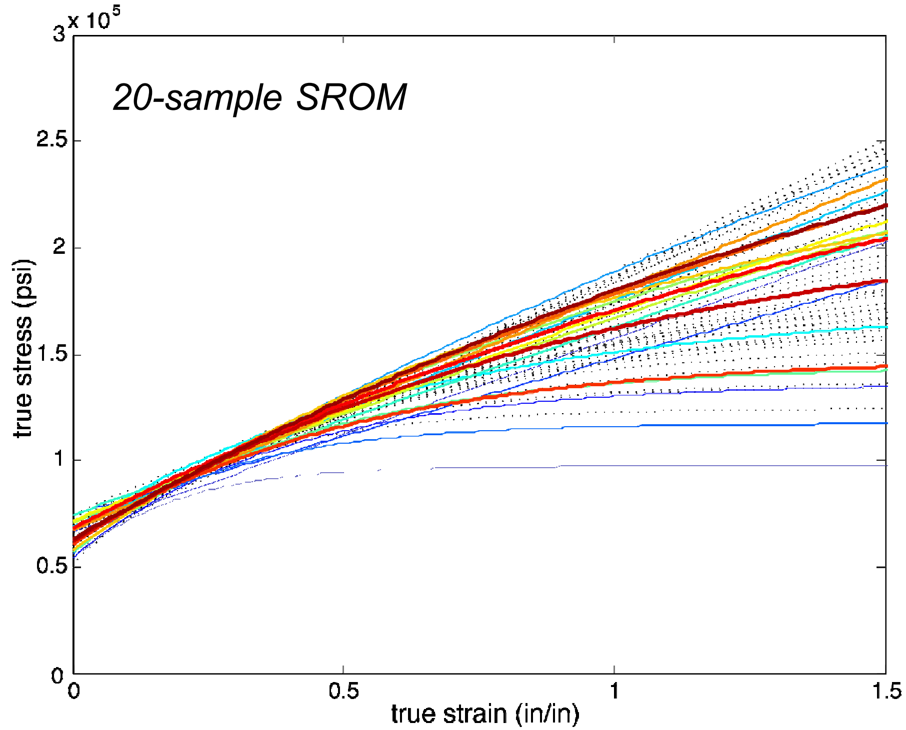
$$\hat{c}(s,t) = \sum_{i=1}^{n}(1/n)\,\theta_{i,s}\,\theta_{i,t}$$

with m << n and $\alpha,\ \beta,\ \zeta > 0$ are weights and subject to probabilities $\tilde{p}_k \ge 0$ and $\sum_k \tilde{p}_k = 1$.

Graphical representation of SROMs

These figures compare the SROMs to the calibrated fits. NOTE: The SROMS are derived from the enriched, 5000 samples. The calibrated fits are the dotted lines and the SROMs are painted from least probable (blue, thin) to most probable (red, thick).

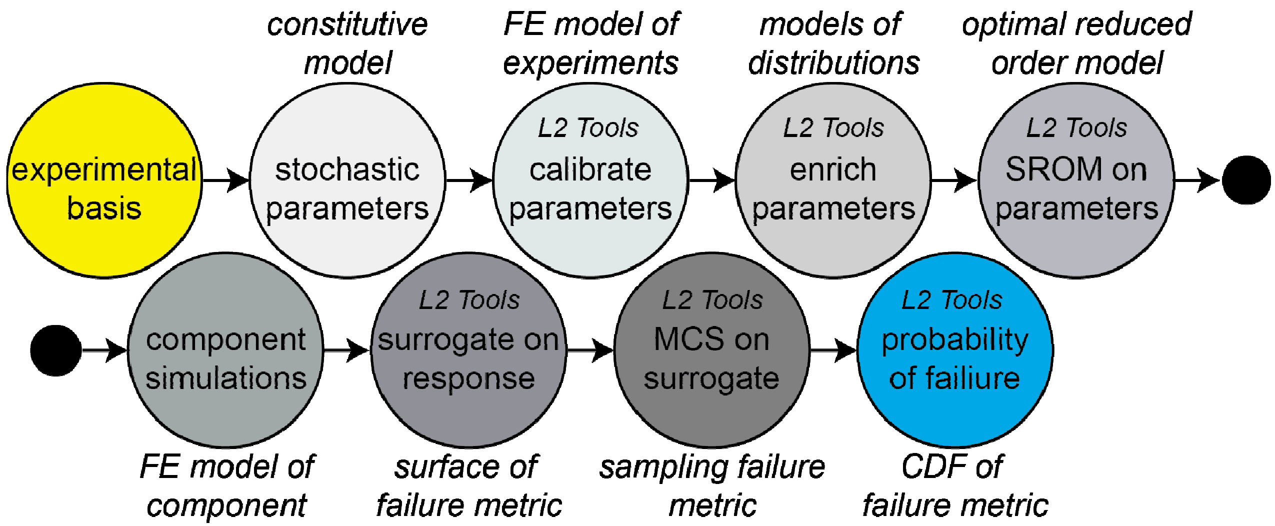




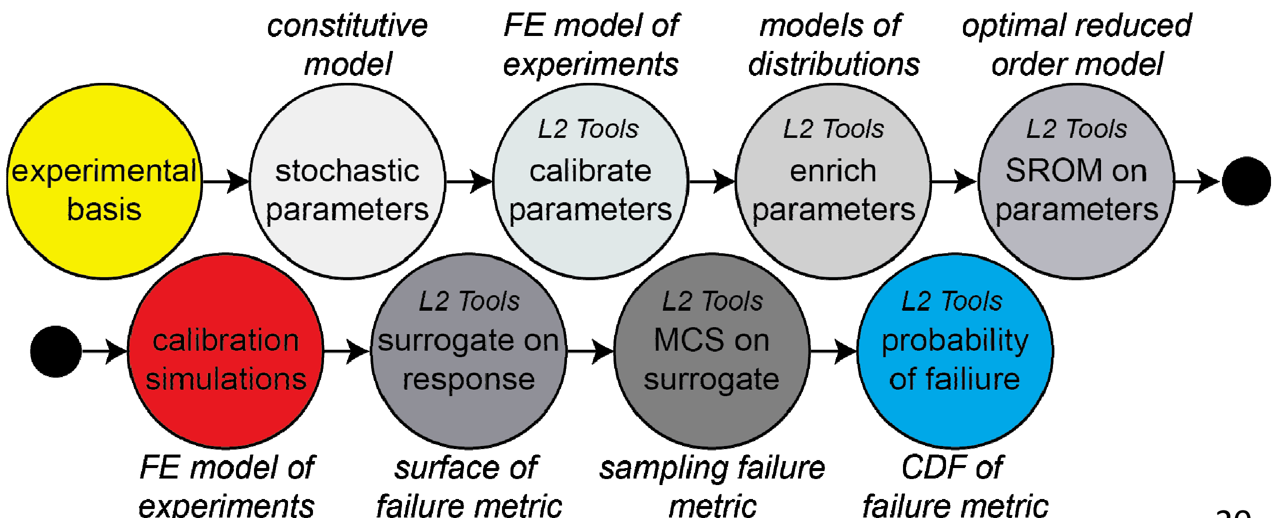
NOTE: Exponential distribution (no upper bound) for R lowers plateau in response

Whoa! L2 finished. Consistent?

We generated multiple SROMs and established a framework for the stochastic, input parameters.

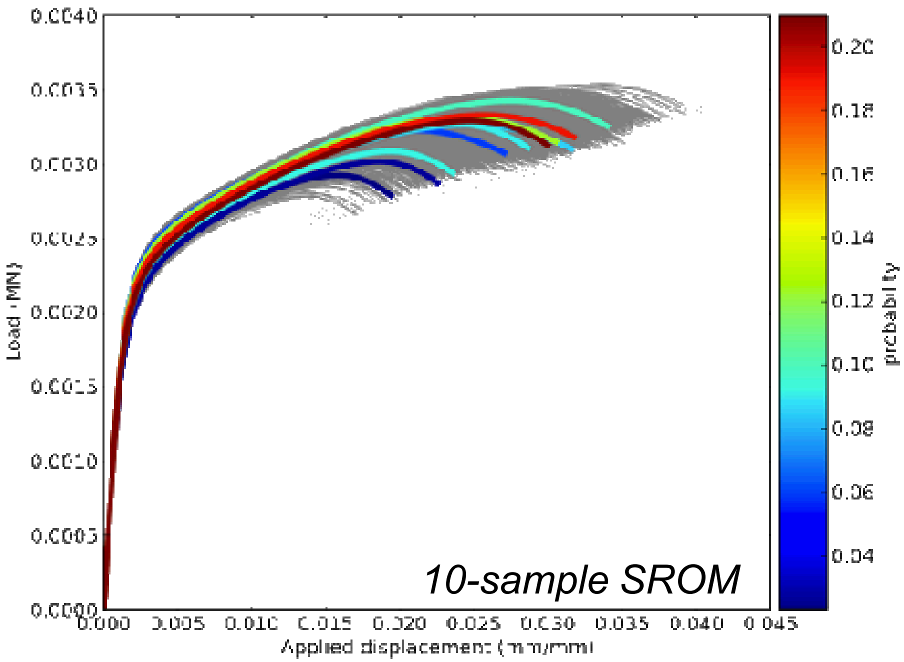


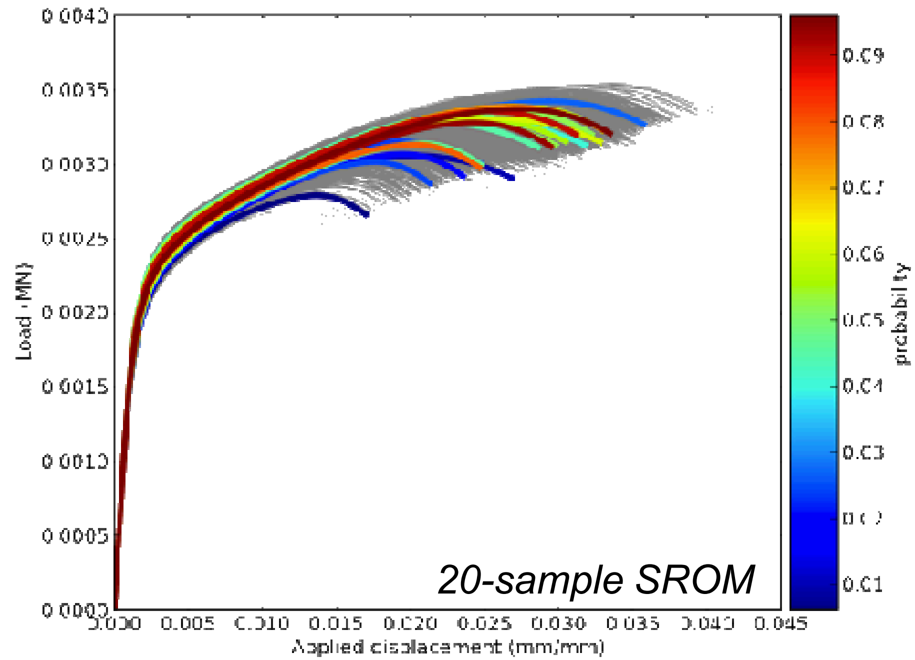
Given the SROM input, we seek to show consistency by comparing SROM output to all 5000 enriched samples.



SROM output to enriched data

These figures compare the load versus displacement curves. The colored lines are the FE-computed results using the 10- and 20-sample SROMs (color indicates probability). The fine gray lines are the FE-computed results using the 5000 enriched samples used to construct the SROMs.

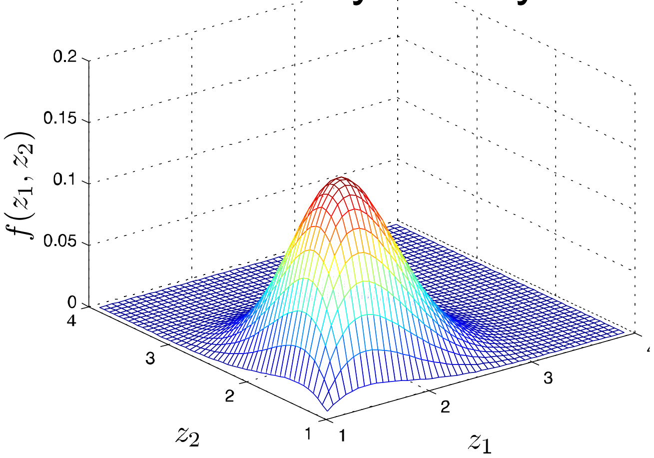




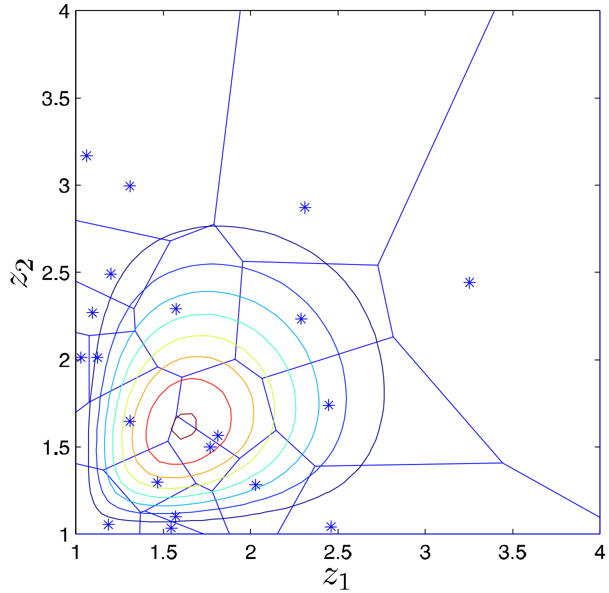
NOTE: SROM output lie within the 5000 samples used to construct the SROM

Construction of SROM surrogate

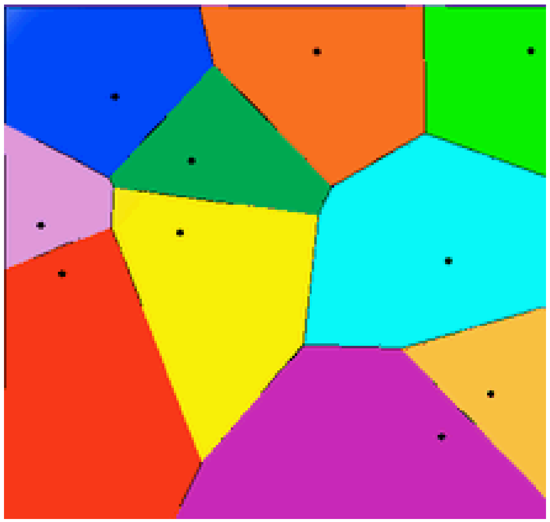
Probability density



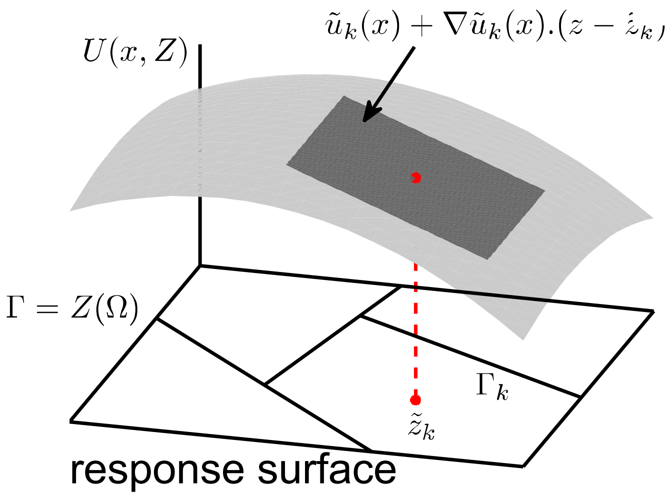
SROM surrogate



Simplicity of Voronoi



ttp://en.wikipedia.org/wiki/Voronoi_diagram



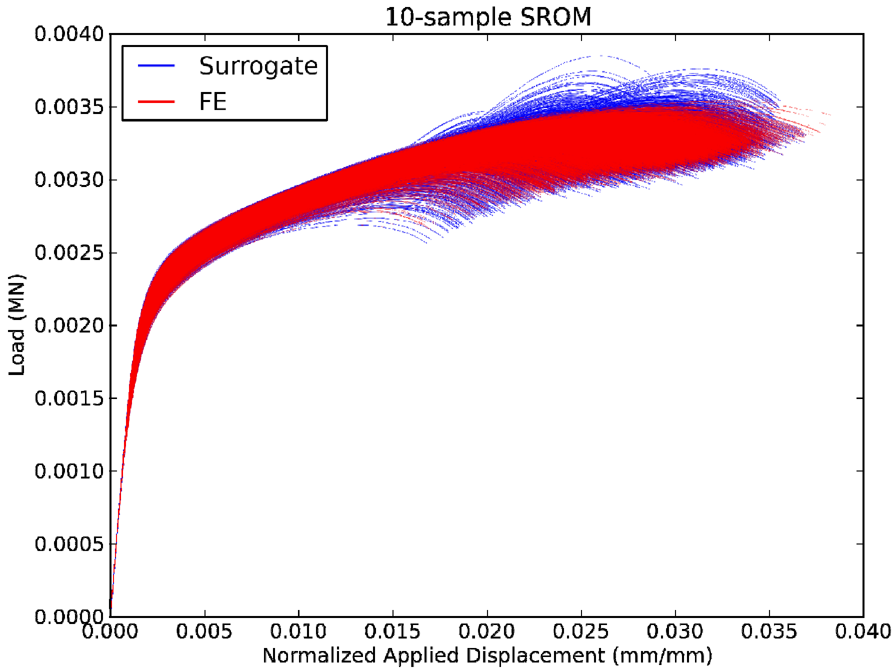
A Voronoi tessellation is constructed around a set of seed points (black dots). In our work, these seed points are the SROM samples. In general, the seed point is not located at the cell's centroid. Instead, we determine an expansion point that is consistent with our 5000 random samples to minimize the error.

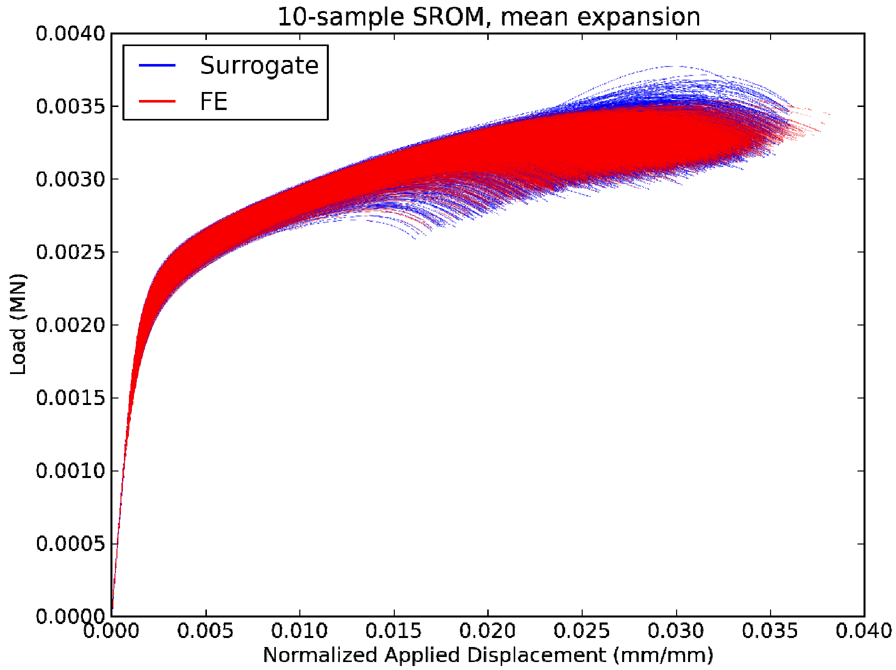
Assumption: The response surface is differentiable

Results of surrogate

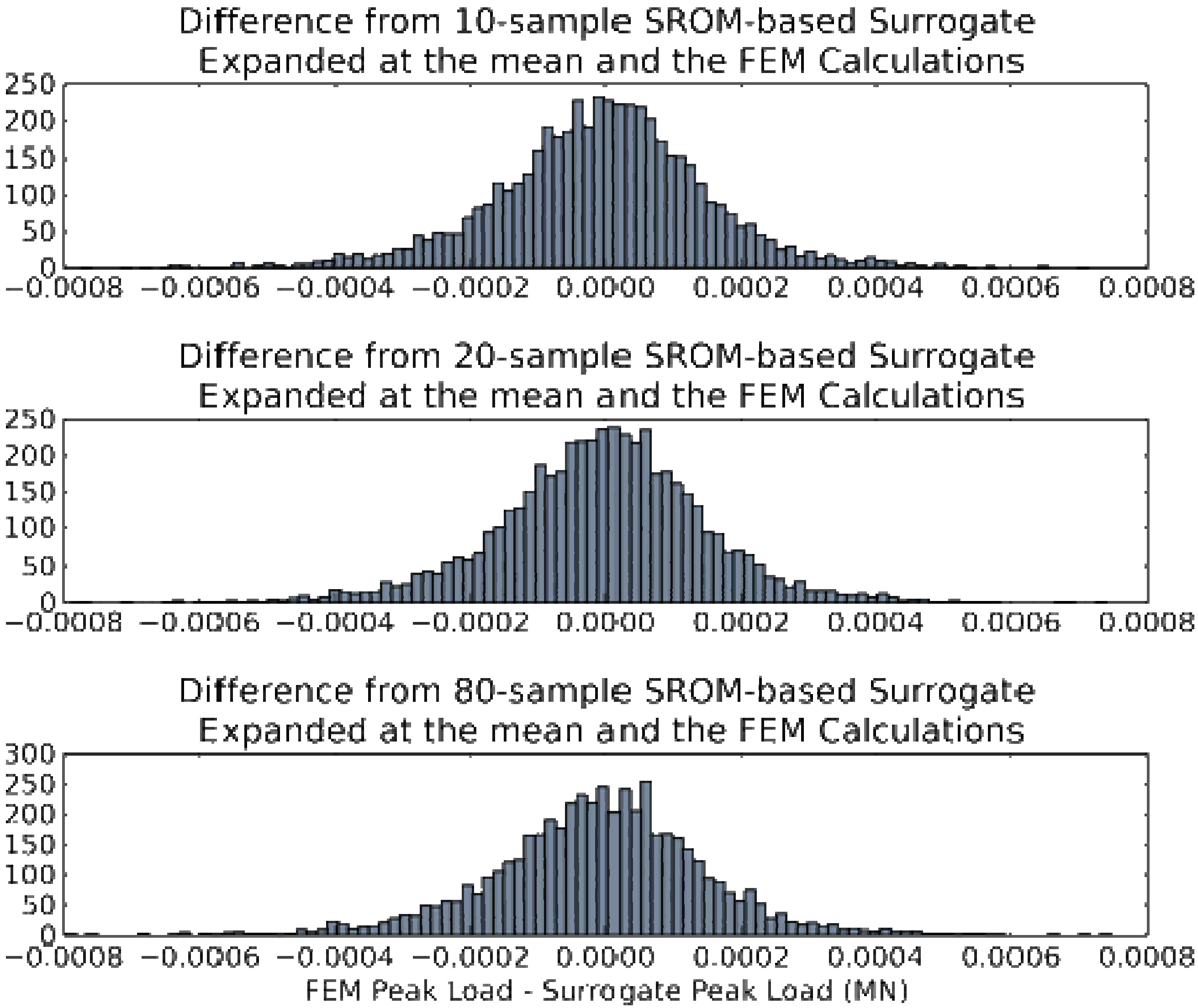
Using an expansion about the mean of the data within a cell leads to more consistent sampling and increases the accuracy of the Taylor Series Expansion.

REMINDER: 10 SROM samples are being compared to 5000 FE simulations





The mean error is nearly zero



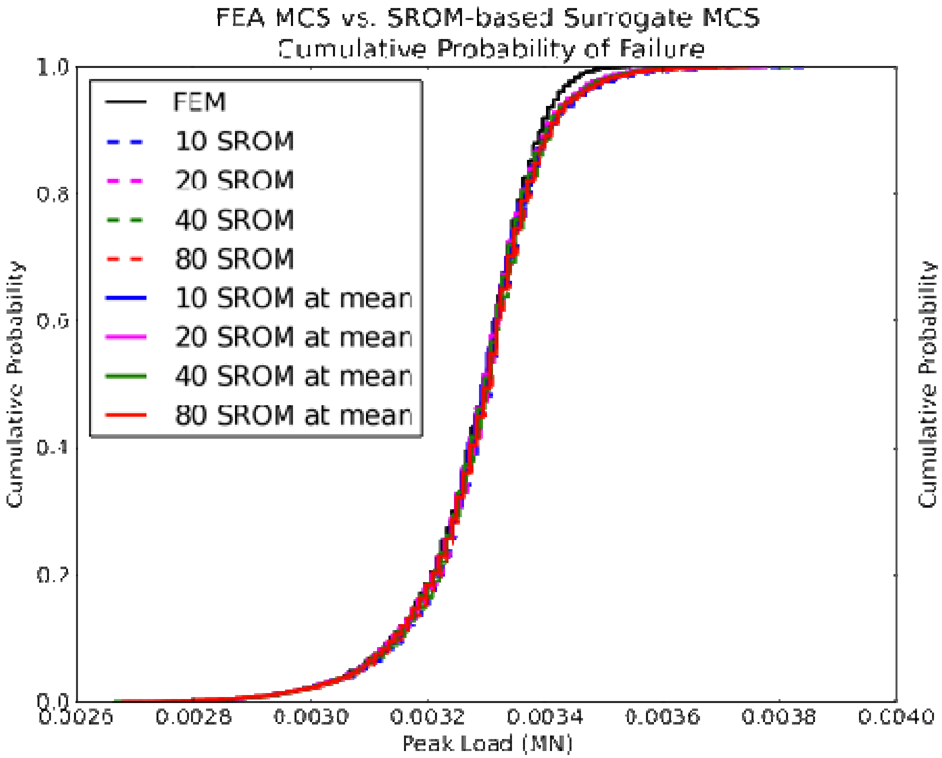
Histograms of the error $h(Y) - h(\tilde{g}(\tilde{X}))$ with $h(Y) = Y$.

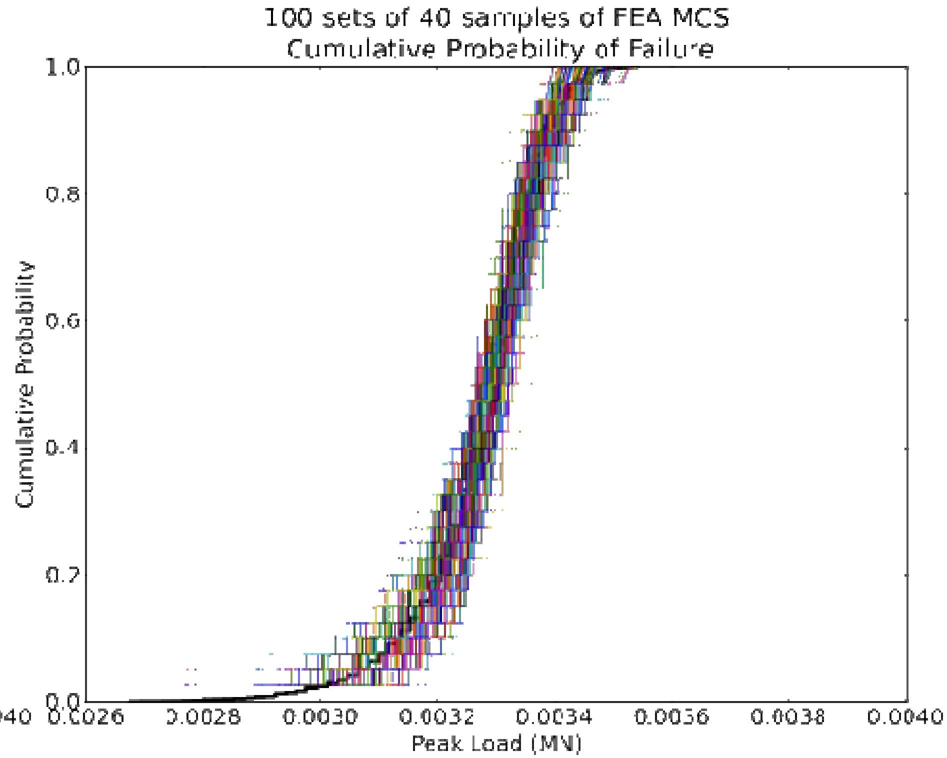
We note that $\mathrm{E}[Y - \tilde{g}(\tilde{X})] \approx 0$ as guaranteed by slide 53.

NOTE: The error has a distribution and the mean is nearly zero.

SROM versus Monte Carlo

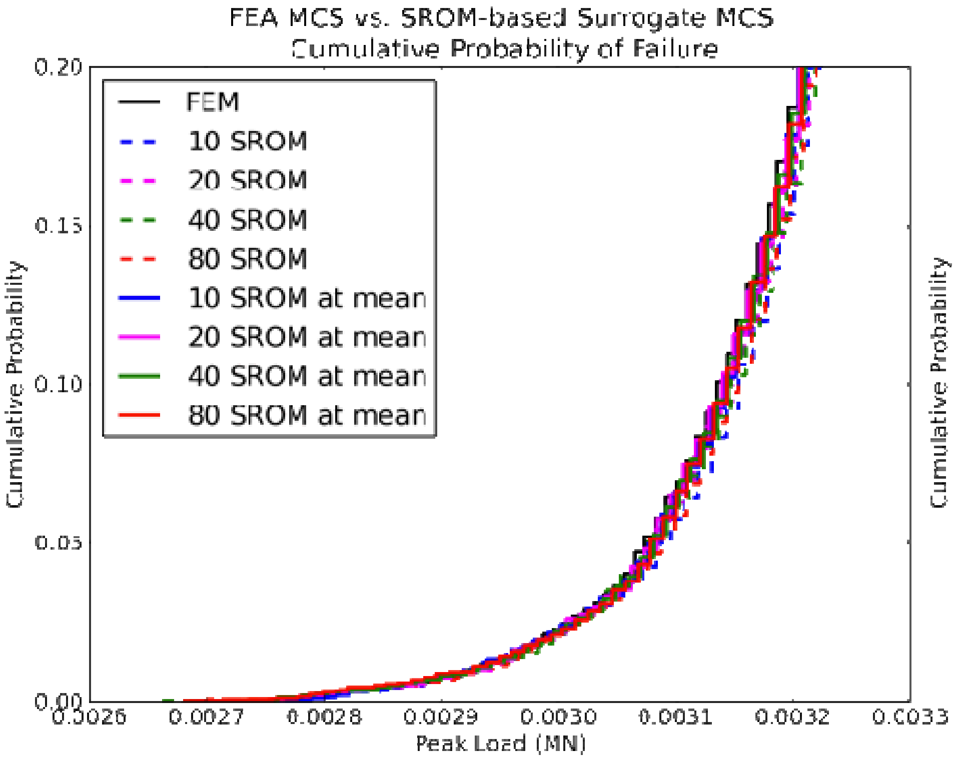
Comparing the cumulative probability of failure between multiple SROM samples and 100 sets of 40 FE simulations employing Monte Carlo. The piecewise linear 10 sample *SROM has the same computational cost as 40 Monte Carlo samples.*

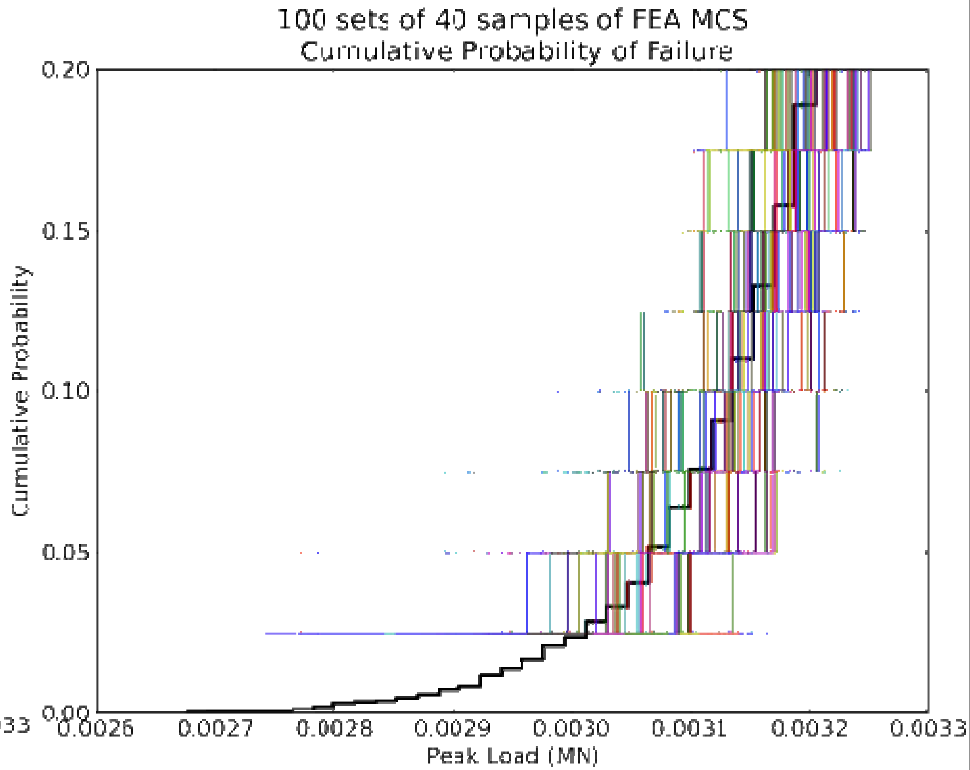




SROM captures the tail in the CDF

For this particular geometry and loading, we may consider peak load to define failure and derive margins from the tail of the distribution. *If you can only afford 40 calculations, the SROM-based surrogate is superior.*

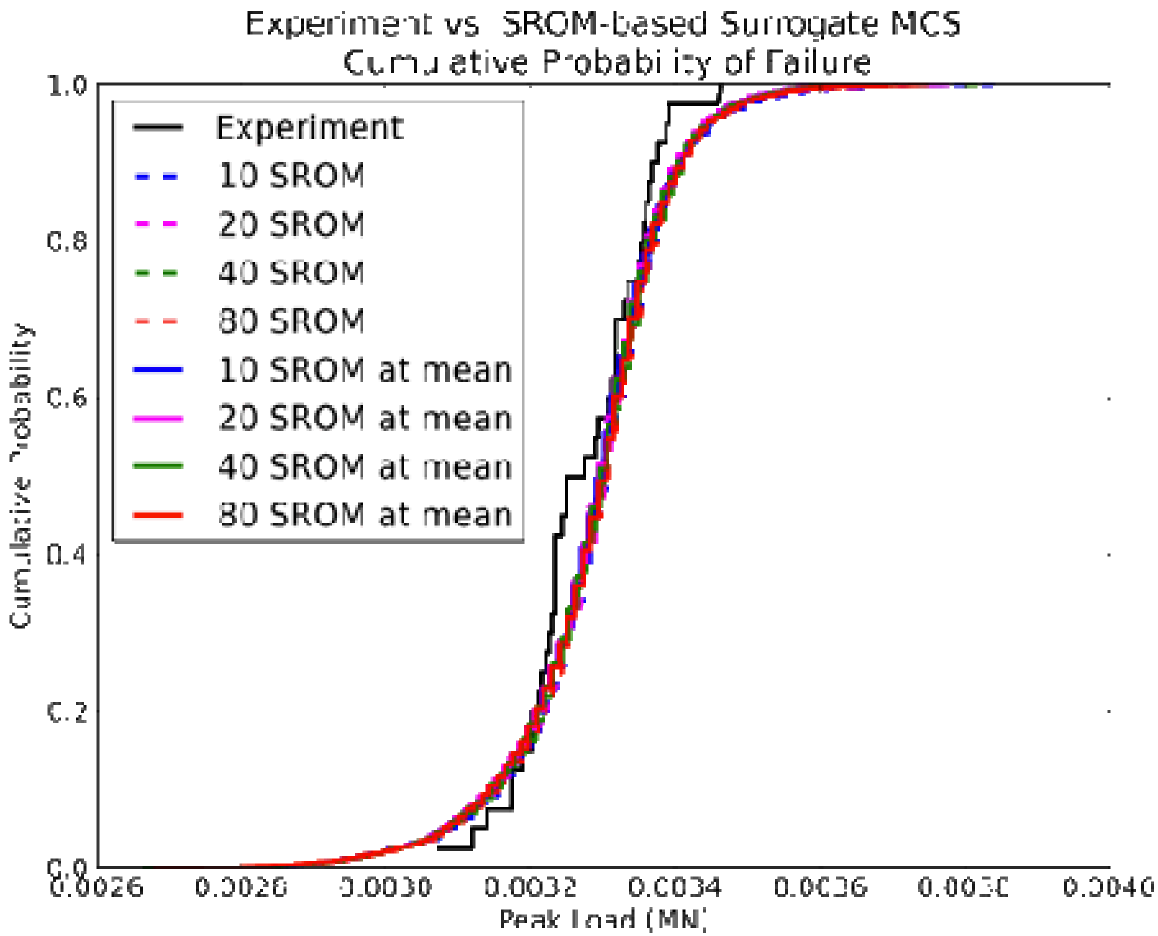


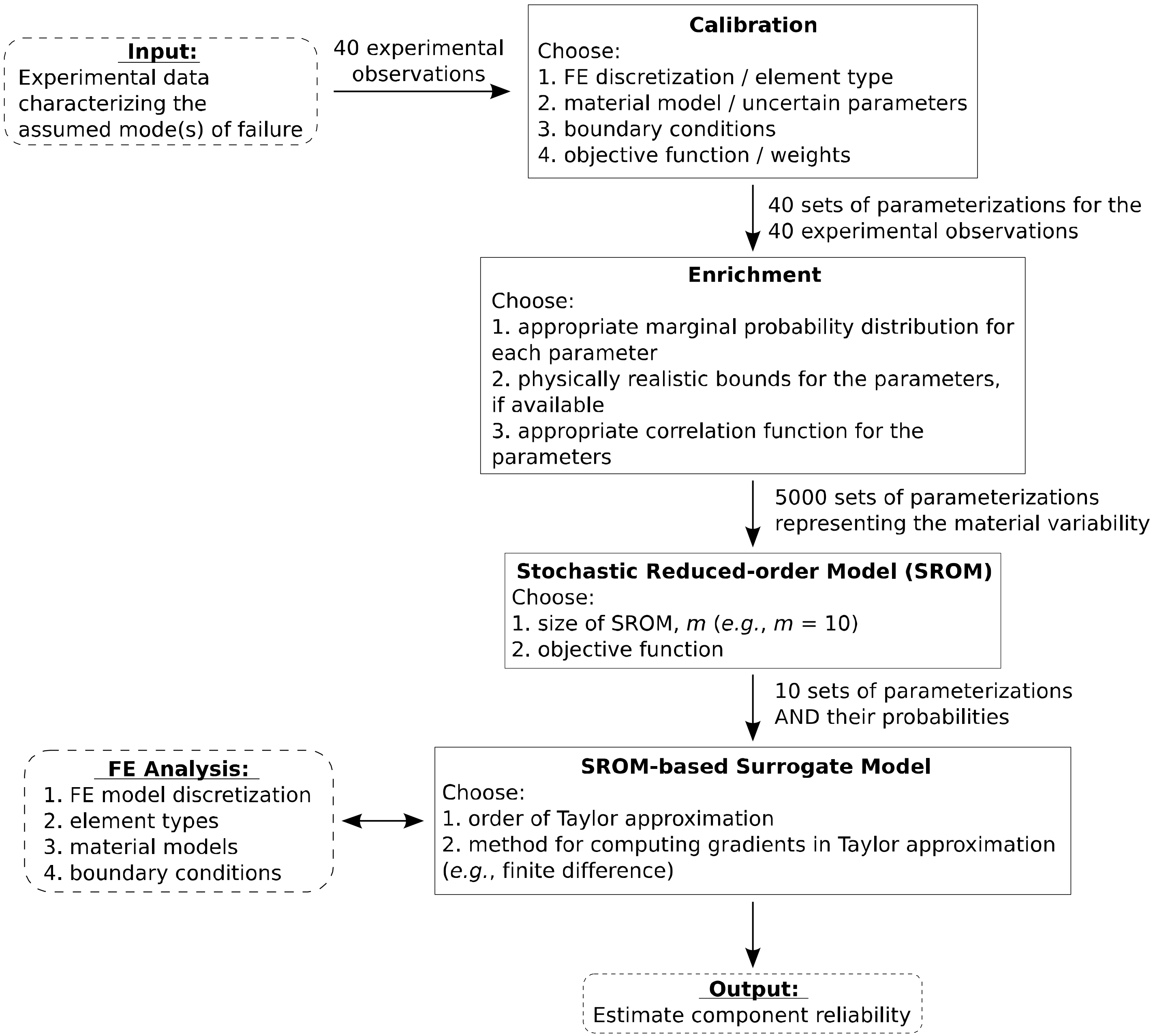


NOTE: 10-sample SROM has the same computational cost as 40 Monte Carlo samples.

Reflecting again on experiments

Although we have illustrated the framework with enriched data, we can always reflect on the 40 sets of data that initiated this work. Encouraging.




Input:
Experimental data characterizing the assumed mode(s) of failure
40 experimental observations
Calibration
Choose:
1. FE discretization / element type
2. material model / uncertain parameters
3. boundary conditions
4. objective function / weights
40 sets of parameterizations for the 40 experimental observations
Enrichment
Choose:
1. appropriate marginal probability distribution for each parameter
2. physically realistic bounds for the parameters, if available
3. appropriate correlation function for the parameters
5000 sets of parameterizations representing the material variability
Stochastic Reduced-order Model (SROM)
Choose:
1. size of SROM, m (e.g., m = 10)
2. objective function
10 sets of parameterizations AND their probabilities
FE Analysis:
1. FE model discretization
2. element types
3. material models
4. boundary conditions
SROM-based Surrogate Model
Choose:
1. order of Taylor approximation
2. method for computing gradients in Taylor approximation (e.g., finite difference)
Output:
Estimate component reliability

Summary

- Laser welds are pervasive and dictate issues of nuclear safety
- Developed a stochastic framework that maps variability to performance
- Constitutive, finite-element, and statistical models incorporate physics
- Illustrated that the methodology is superior to standard MCS