SAND2019-4637PE

Sandia National Laboratories

Multiscale Uncertainty Propagation for Fasteners

PRESENTED BY

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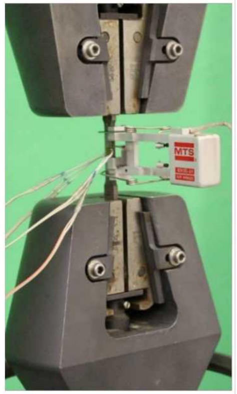
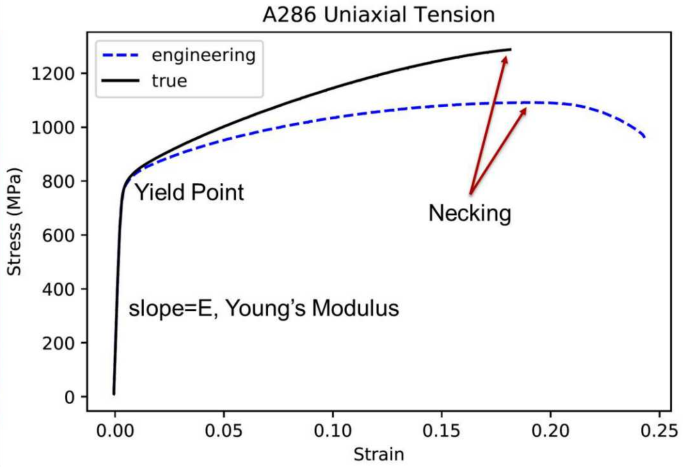
Outline

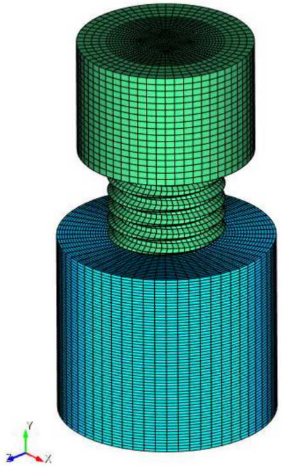
Part 1: Nonlinear Model Calibration

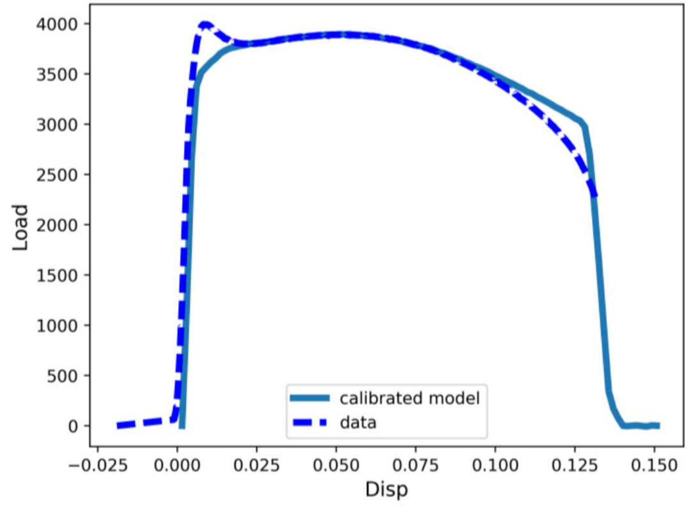
Background





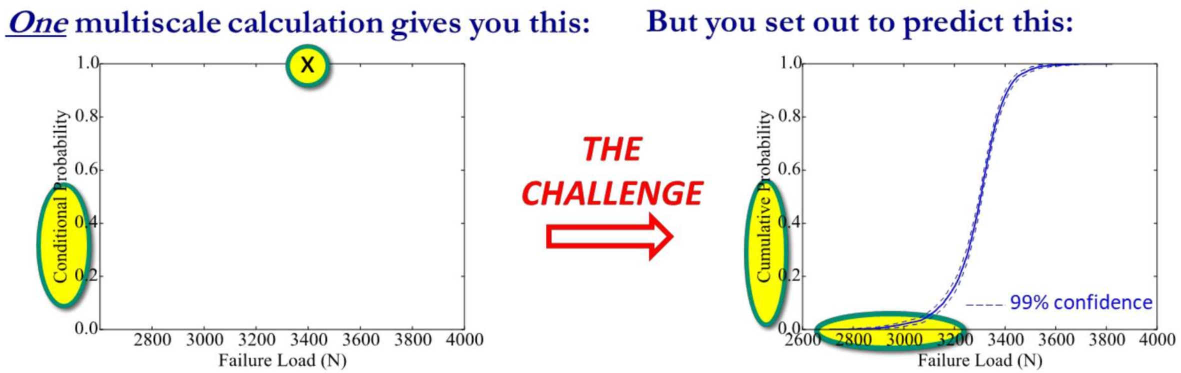
Plasticity Model Calibration Tool



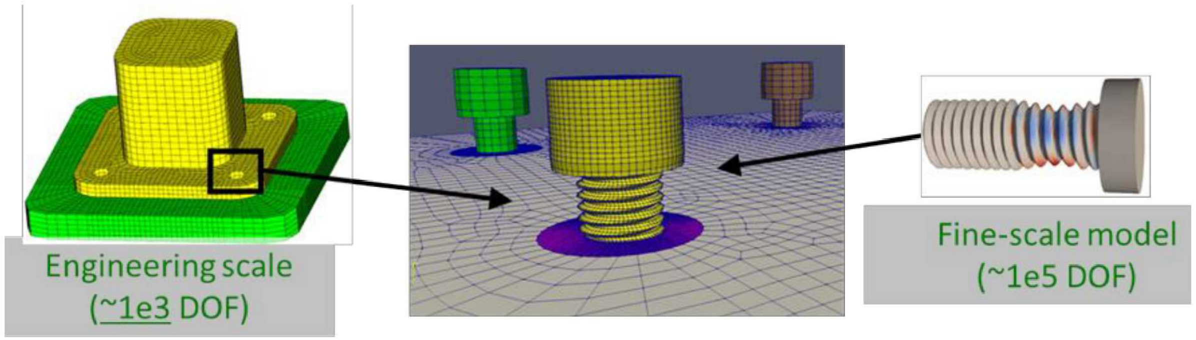


Part 2: Multiscale Uncertainty Propagation

Background

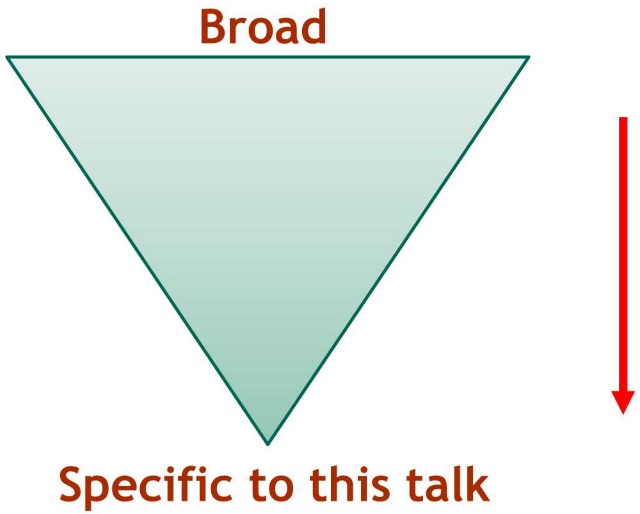


Bolted Joint Example



Nonlinear Material Model Calibration

Background: what is being calibrated?



Nonlinear solid mechanics

Material modeling

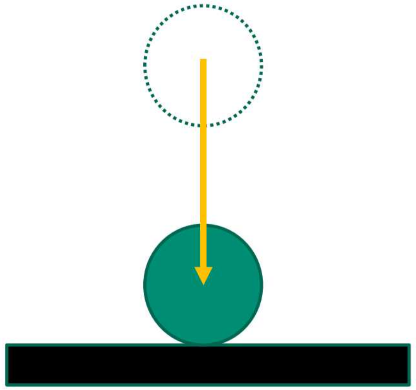
J2 Metal Plasticity

Strain Hardening

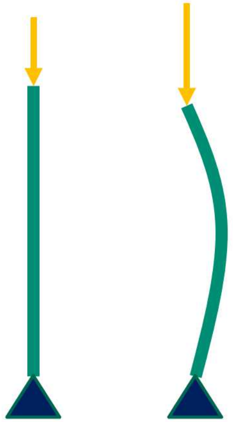
Nonlinear Solid Mechanics

- At Sandia we perform nonlinear solid mechanics simulations of various systems
- *Nonlinear* : the solution doesn't scale proportionally to the applied loading
  - In general the solution must be solved incrementally
    - Implicit time integration
    - Explicit time integration
  - Types of nonlinearity in solid mechanics simulations
    - Contact
    - Geometric (large deformations)
    - **Material**
      - This is the aspect that usually needs to be calibrated

Contact: initially, the two bodies do note exert force on each other, but after some displacement they abruptly do



Geometric: the initially straight beam buckles after some loading, leading to a reduction in load carrying capacity

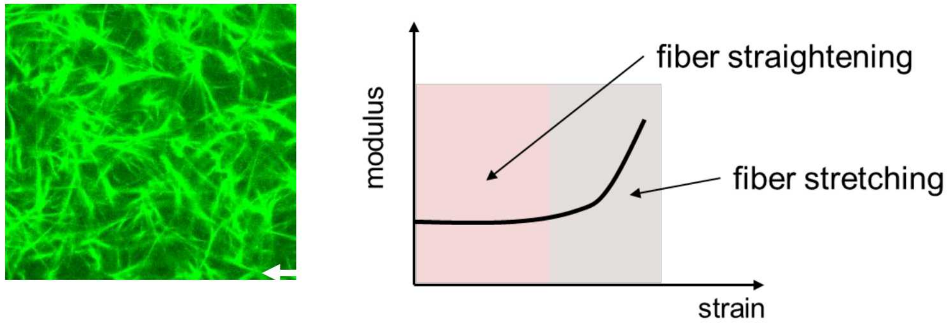


While we rely on our FEA codes to accurately simulate contact and geometric nonlinearities, material nonlinearity is largely modeled phenomenologically, dictated by user-defined parameters

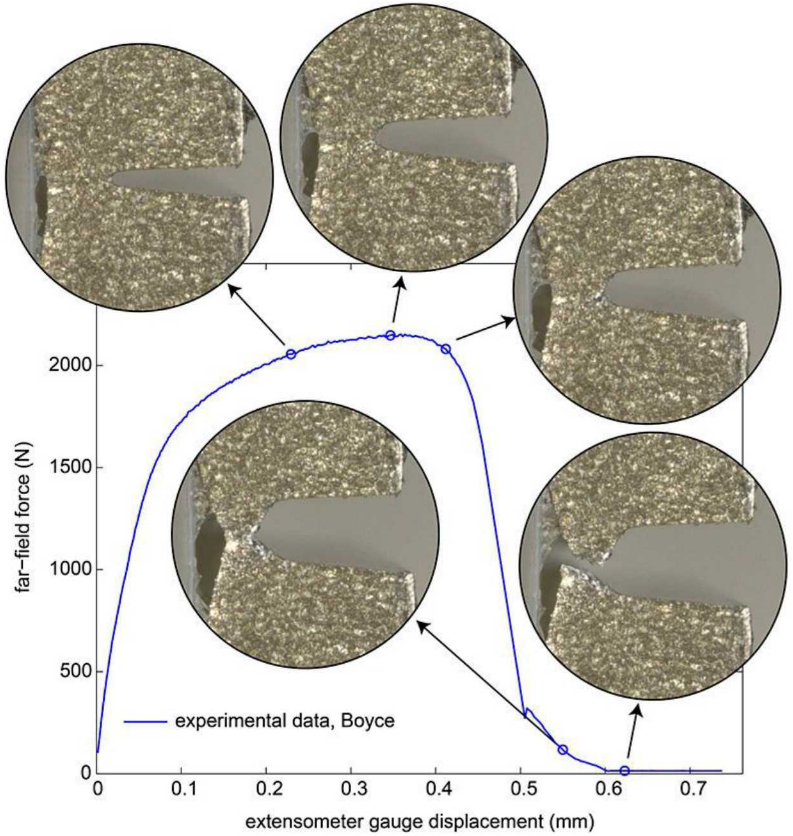
Material Modeling

- For solid mechanics, materials are often classified according to their:
  - Homogeneity: spatial variation
  - Anisotropy: directional dependence
  - Nonlinearity: how does stiffness change with strain?
  - Inelasticity: if unloaded, does material return to original state?
- Whether a material can be considered homogeneous or isotropic depends on the length-scales of interest.
  - For most practical engineering calculations for metal structures, we assume isotropic and homogeneous materials.
- Beyond very small strains, metals yield and have **inelastic, nonlinear** deformations (plasticity).
  - FEA of components for design evaluation can assume linear elasticity and still be extremely valuable
  - However, if you want to accurately simulate the response of metal components under large deformations, must account for their plasticity
    - If extreme loading is involved, material failure may also need to be modeled

Collagen is a hydrogel on macroscale, but it exhibits nonlinear elastic behavior due to its microstructural response

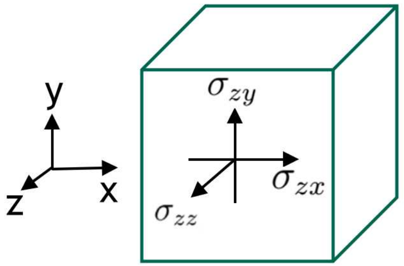


Tension test of a notched stainless steel 304L specimen [1]



[1] Emery et. al., 2015 (https://doi.org/10.1002/nme.4935)

J2 Metal Plasticity



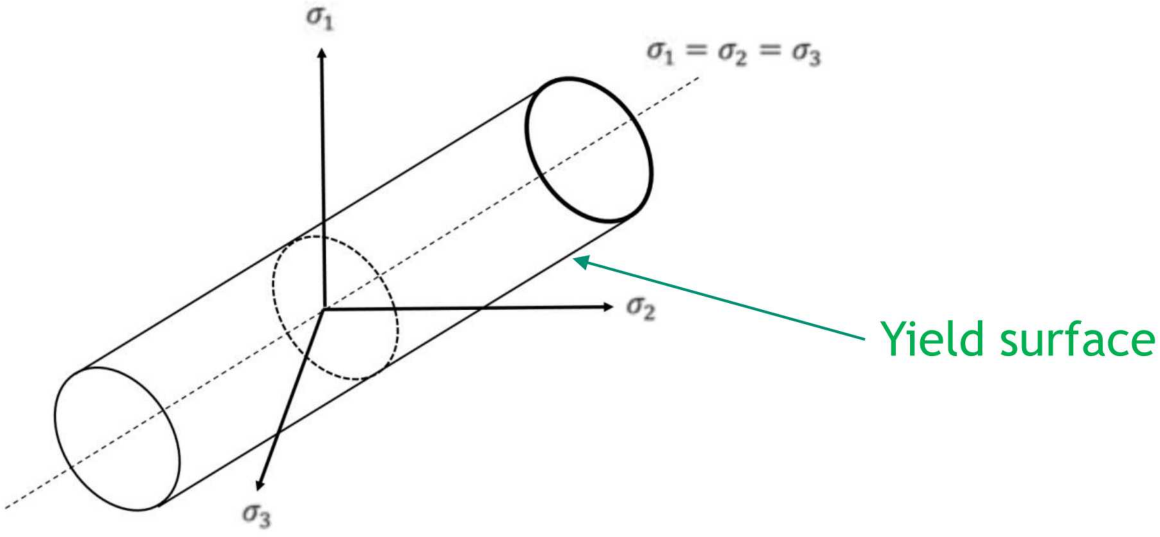
$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \sigma_{ij}$$

- Stress tensor can be decomposed into:
  - Volume changing (volumetric) deformation
    - Related to normal stresses
  - Shape changing (deviatoric) portion
    - Related to shear stresses

$$\sigma_{ij} = S_{ij} + \tfrac{1}{3}\sigma_{kk}\delta_{ij}$$
$$J_2 = \tfrac{1}{2}S_{ij}S_{ij}$$
$$\sigma_{vm} = \sqrt{3J_2}$$

- Metals generally plastically deform due to deviatoric stresses **S**
  - The "second invariant" of the deviatoric stress tensor is called J2.
  - Von Mises stress comes from J2
    - Conveniently, Von Mises stress is equal to applied stress in uniaxial tension
  - Von Mises is a common "yield criterion" for metals
    - Von Mises stress defines a cylindrical 3D **yield surface** in "principal stress space", with its axis along hydrostatic stress states
    - If a given material element's principal stresses give a Von Mises stress that is higher than the yield stress, the element will deform plastically

$$\sigma_{vm} = \sqrt{\tfrac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]}$$

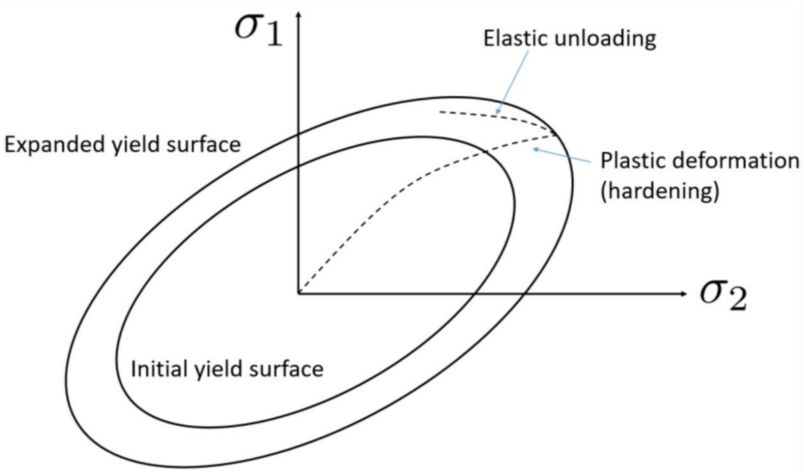


Strain Hardening

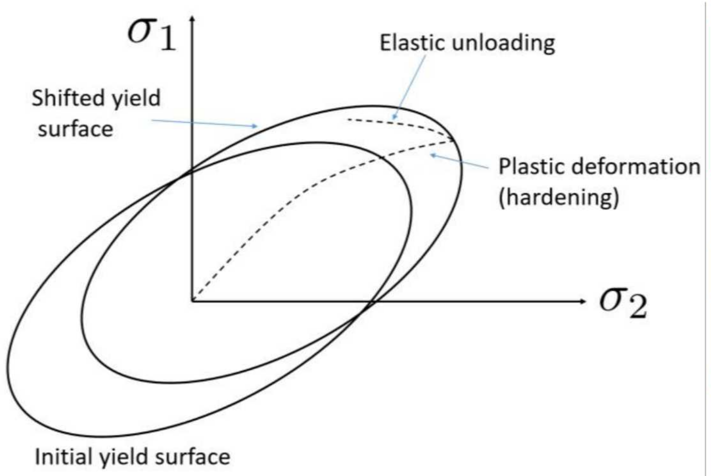
- If a metal continues to be loaded past yield, it begins "hardening"
  - Complicated microstructural causes that can't be practically modeled, so phenomenological models are used
- This can be understood as the yield surface expanding (isotropic hardening) or translating (kinematic hardening) to accommodate the increasing Von Mises stress
- Very ductile alloys (e.g. 304L stainless steel) can accommodate a lot of plastic strain/hardening before fracture
- For J2 plasticity, the hardening behavior can be described with a "hardening curve"
  - This can be obtained from a uniaxial tension test, up until necking
- In general, a hardening curve can only be directly obtained from a test if the test has a uniform state of strain (or if one can reasonably be assumed)
  - If not, an inverse calibration procedure must be used

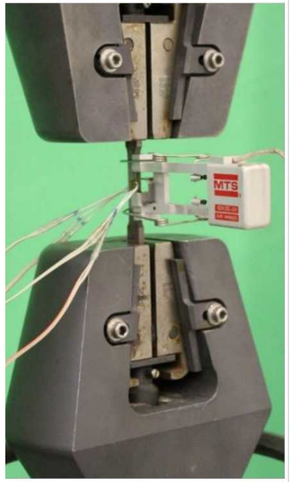
We often need to calibrate the hardening curve for a given material model so that it gives the correct response in a system model

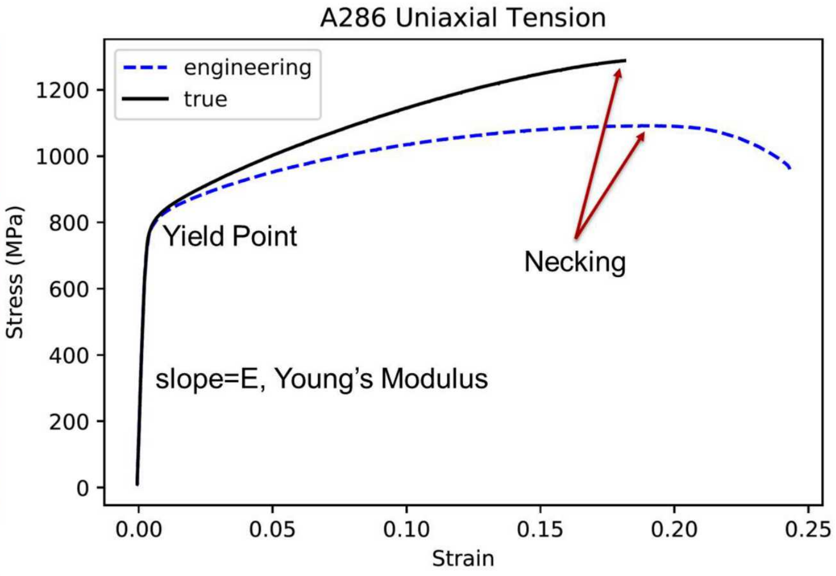
Isotropic Hardening



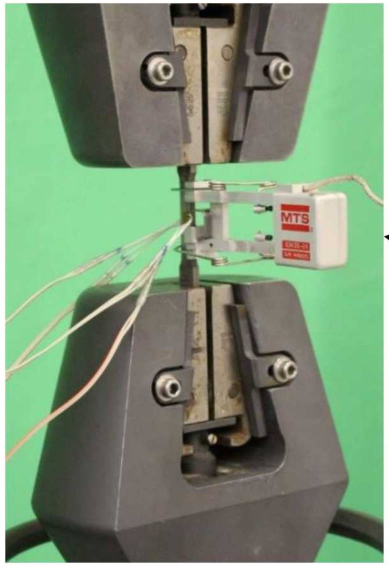
Kinematic Hardening







Hardening Curve Calibration: Conventional Methods



General Inverse FEA Optimization Approach

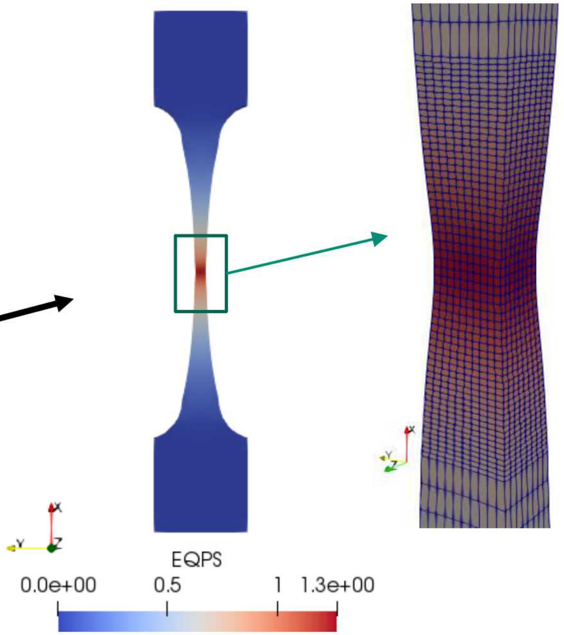
TEST
Measured response (load vs displacement)

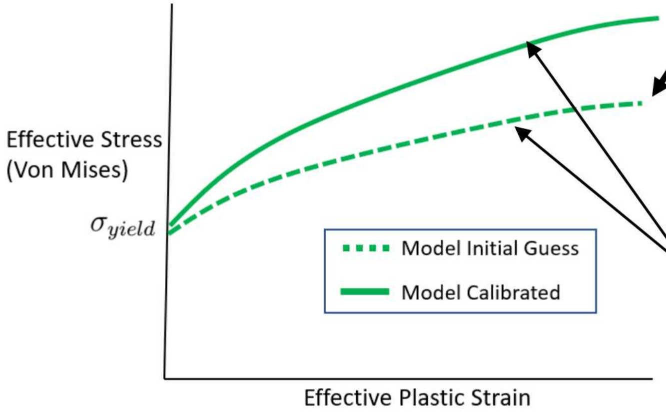
FINITE ELEMENT MODEL
Simulate the test measurements

GUESS DESIGN VARIABLES
(hardening curve)

MODEL CALIBRATION
Repeatedly simulate FE model, optimizing design variables so that the model output better matches the test data.

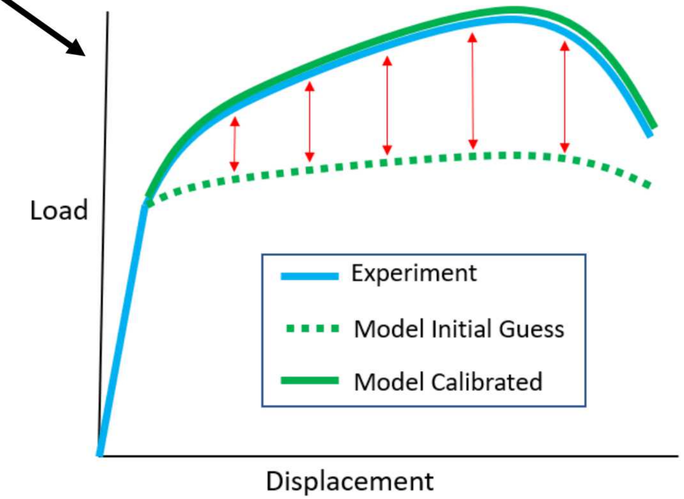
Calibrated Design Variables





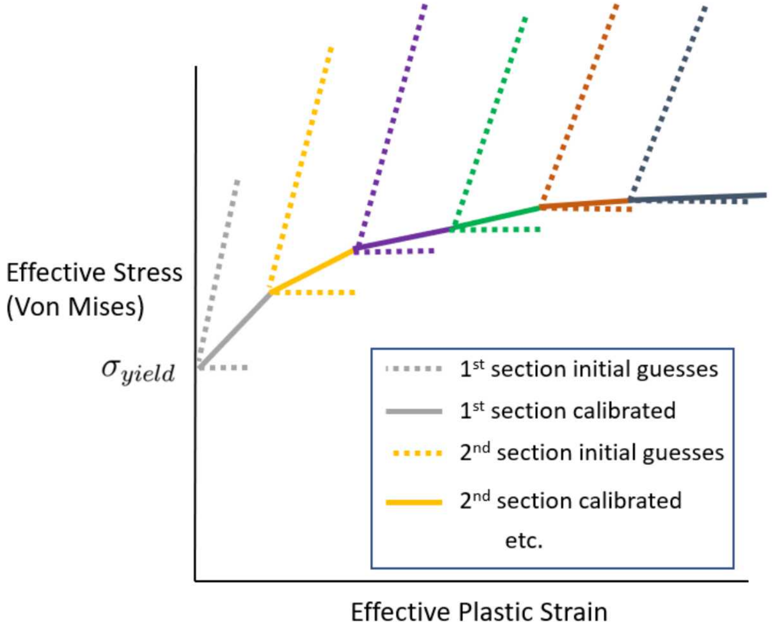
Typically described by analytical function,

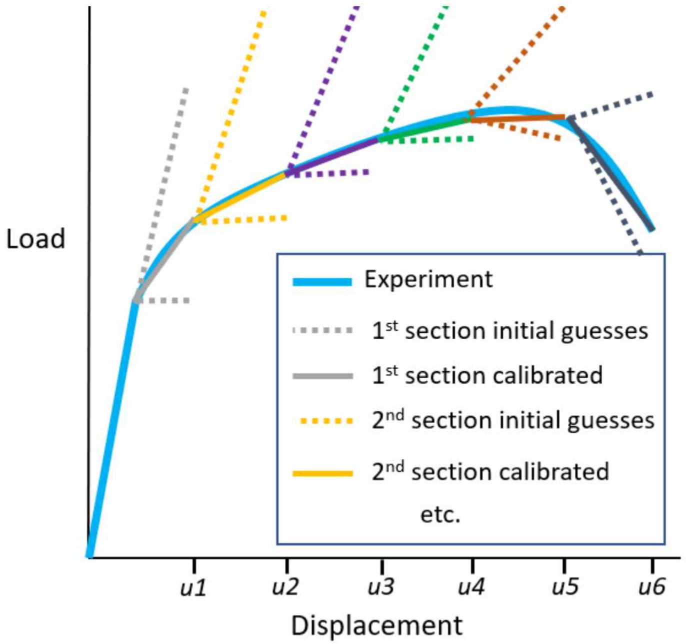
e.g. $\sigma = \sigma_{y0} + A\epsilon_p^B$



Hardening Curve Calibration: Incremental Method

- Typically, the hardening curve would be described by an analytical function for the previous method
  - This limits how well you can match arbitrary load vs displacement curves
- An alternative approach would be to use a piecewise linear hardening curve for more flexibility
  - This is very difficult to calibrate using conventional methods if a lot of segments are used in the piecewise curve
    - The number of design variables gets big, and the load-displacement isn't that sensitive to any one segment
- Novel approach is to use an incremental solution strategy, calibrating each individual segment of the piecewise linear hardening curve
  - Now can use a root finding algorithm rather than cost function minimization





With this method, structural models can be more effectively calibrated to arbitrary load-displacement response

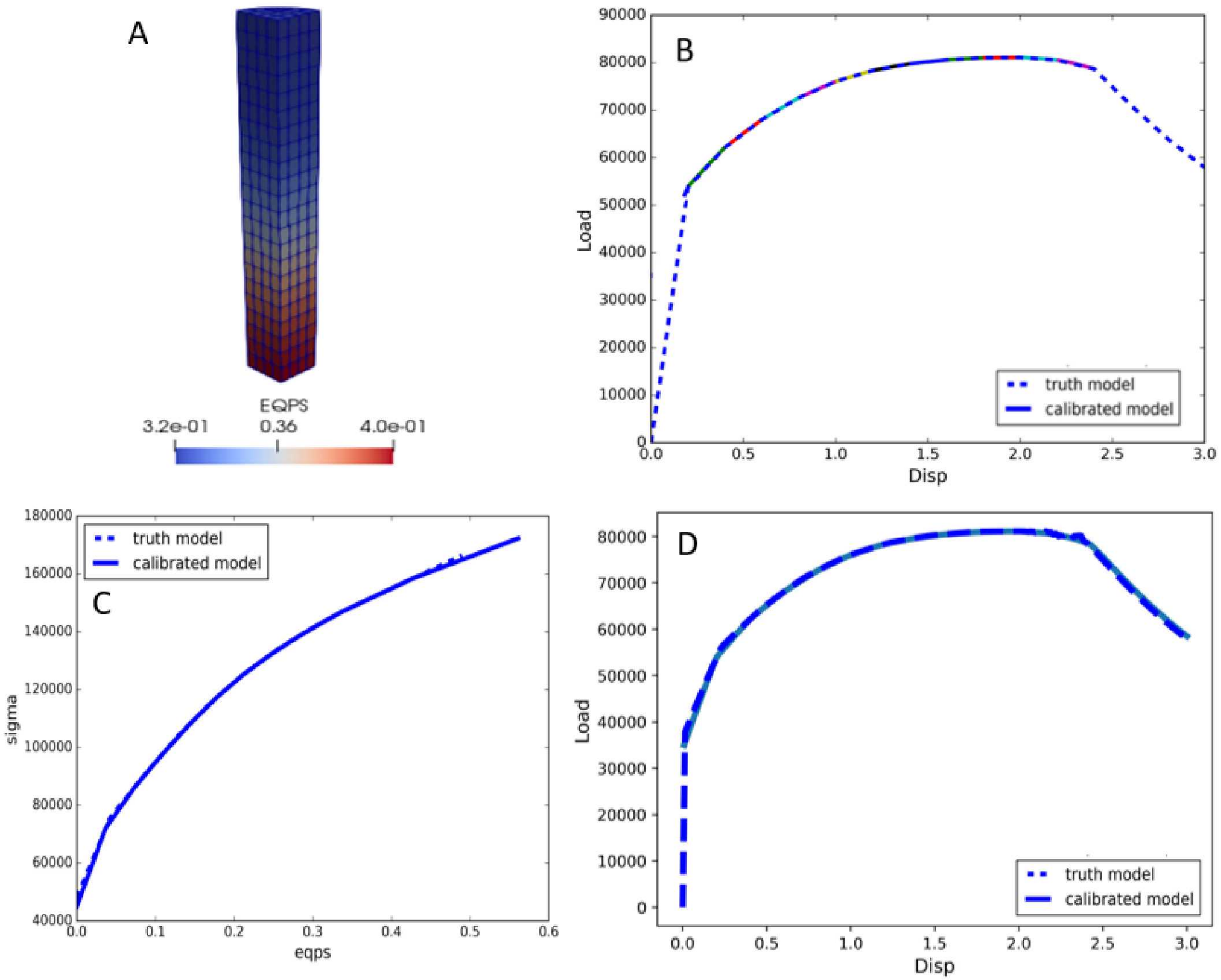
Example: Uniaxial Tension

A.) FE model--symmetry BC's used to represent full cylinder.

B.) Load vs Displacement Incremental Calibration Results

C.) "Truth" hardening curve compared to the calibrated hardening curve

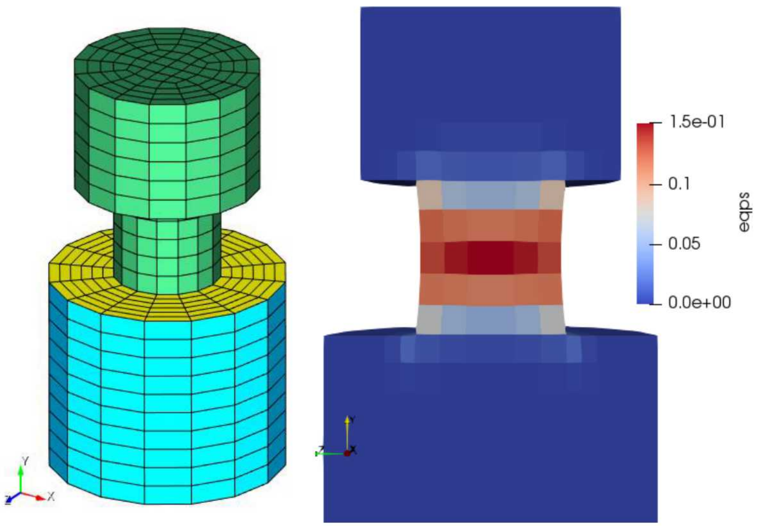
D.) Model re-ran once with calibrated hardening curve to verify the incremental approach matches the final model



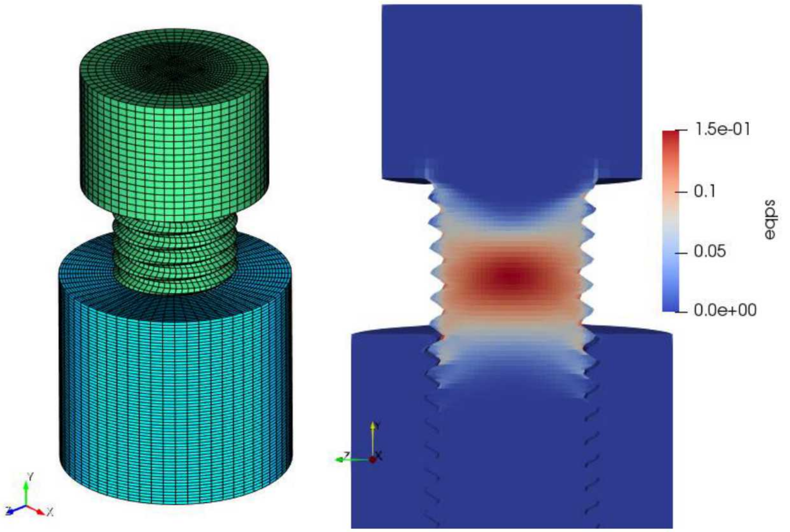
Example: Fastener Models

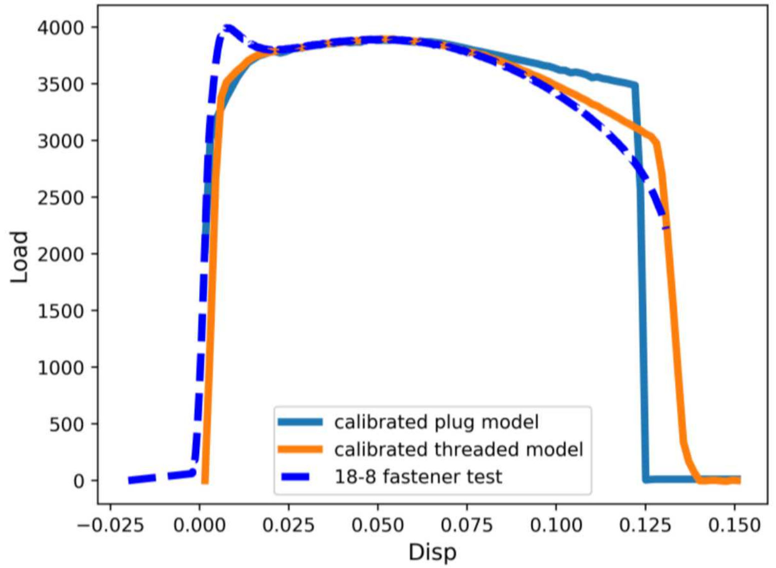
- Calibrate fastener models of varying fidelity to tension tests of a given screw

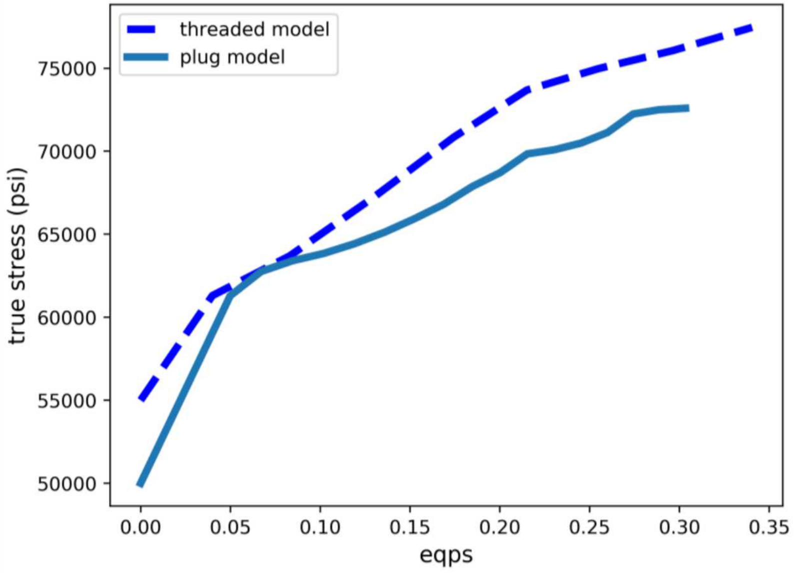
Plug model



Threaded model







Outline

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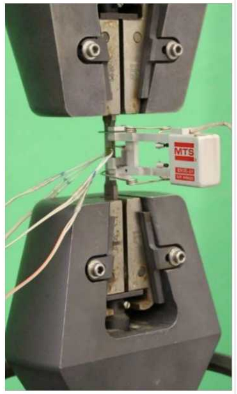
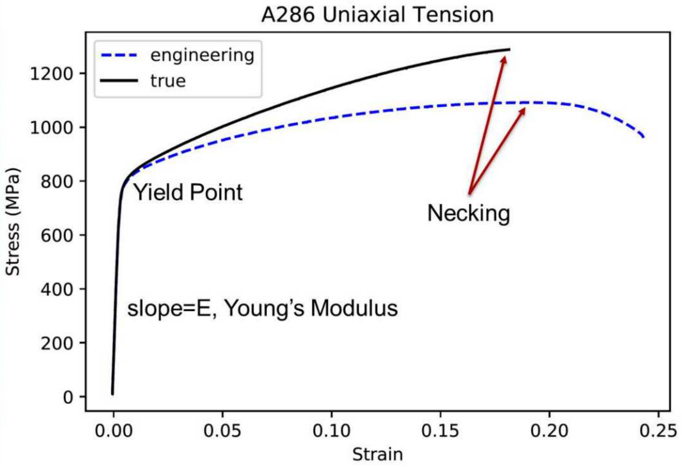
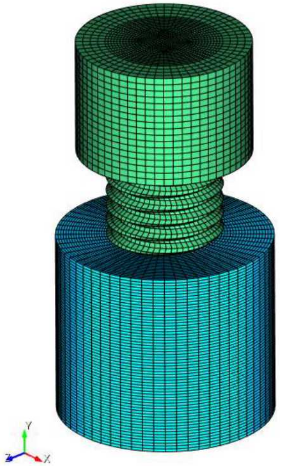
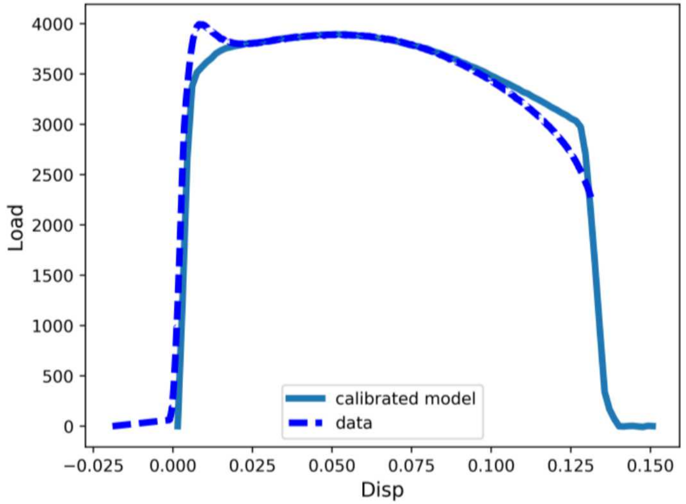
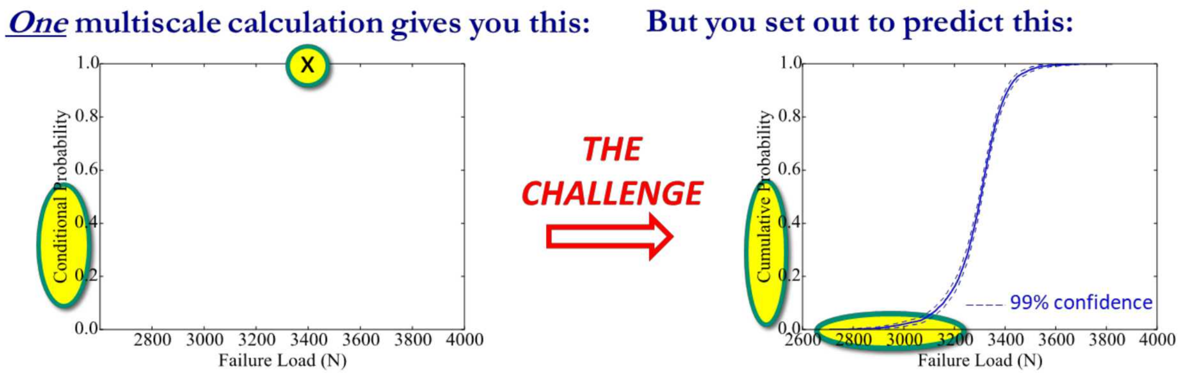



Plasticity Model Calibration Tool

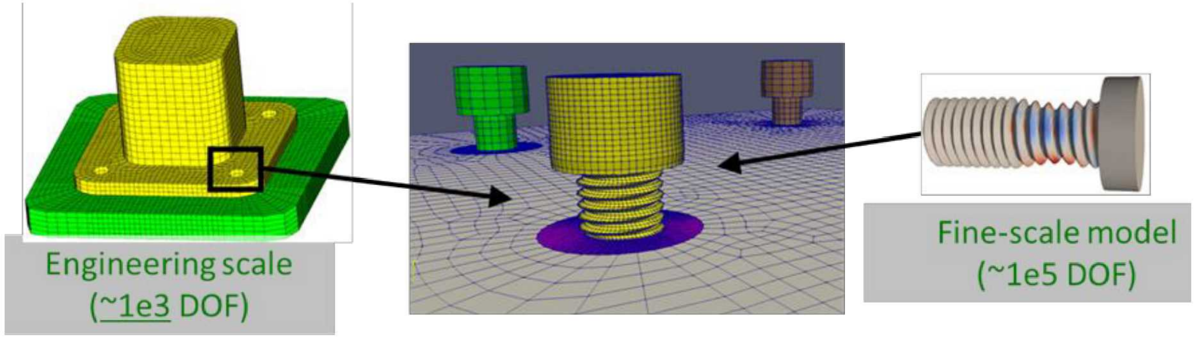



Part 2: Multiscale Uncertainty Propagation

Background



Bolted Joint Example



Outline: Multiscale Uncertainty Propagation

Motivation

Hierarchical model for multiscale (multifidelity) uncertainty propagation

FE models used in the hierarchy

Deterministic calculations

Pretend probability and model

Another model – stochastic reduced-order model (SROM)

Low-fidelity predictions of failure

High-fidelity predictions, followed by chaos

Higher-fidelity sanity

Summary

Motivation

$$f : x \mapsto y$$

If x is random, so is y (even when f is deterministic).

x might be random due to measurement errors, manufacturing defects, and materials microstructure, etc. f might be random due to, *e.g.*, random boundary conditions.

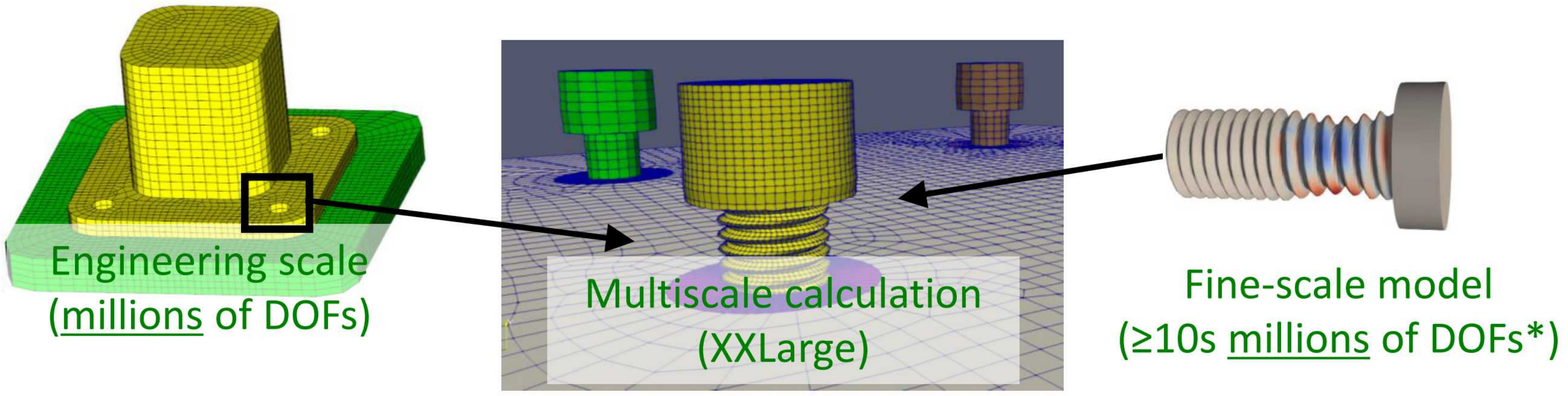
The most general way to compute statistics for and predict tail behavior of y is to generate samples of x and evaluate f(x) = y. We call this Monte Carlo (MC) simulation.

For large systems, f is expensive.

For failure, we may want to include a lot of detail in f, which exacerbates our situation and introduces multiple length scales of concern.

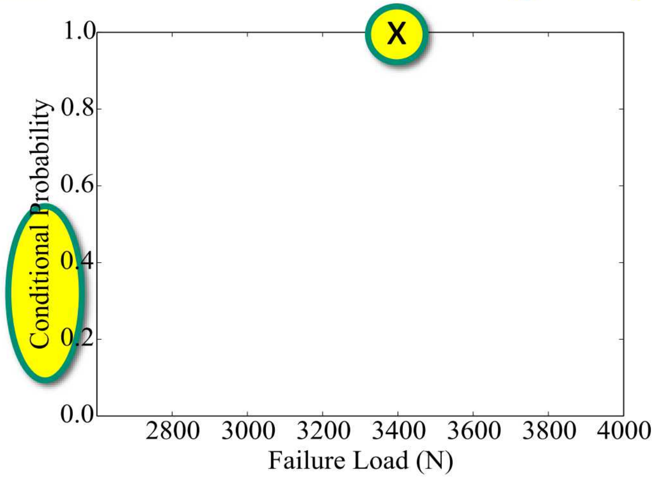
So, maybe we develop a multiscale numerical method for concurrent multiscale simulation.

One multiscale calculation is necessary but not sufficient



(*admittedly a bit gratuitous for the present example)

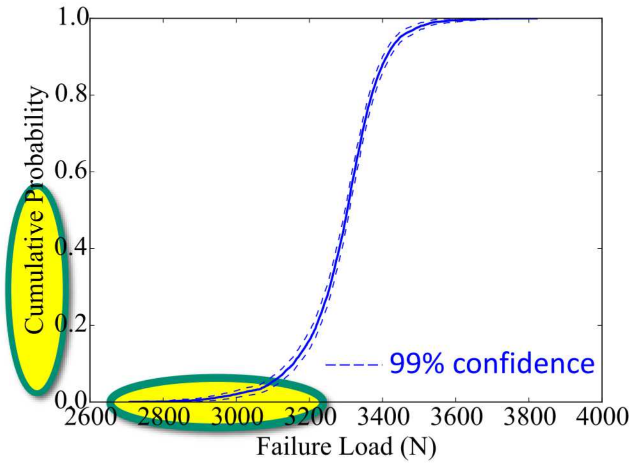
One multiscale calculation gives you this:



One point for *conditional* probability of failure $\Pr(t_f \le t | B_i)$, conditioned on choice of bolt B_i.

THE CHALLENGE

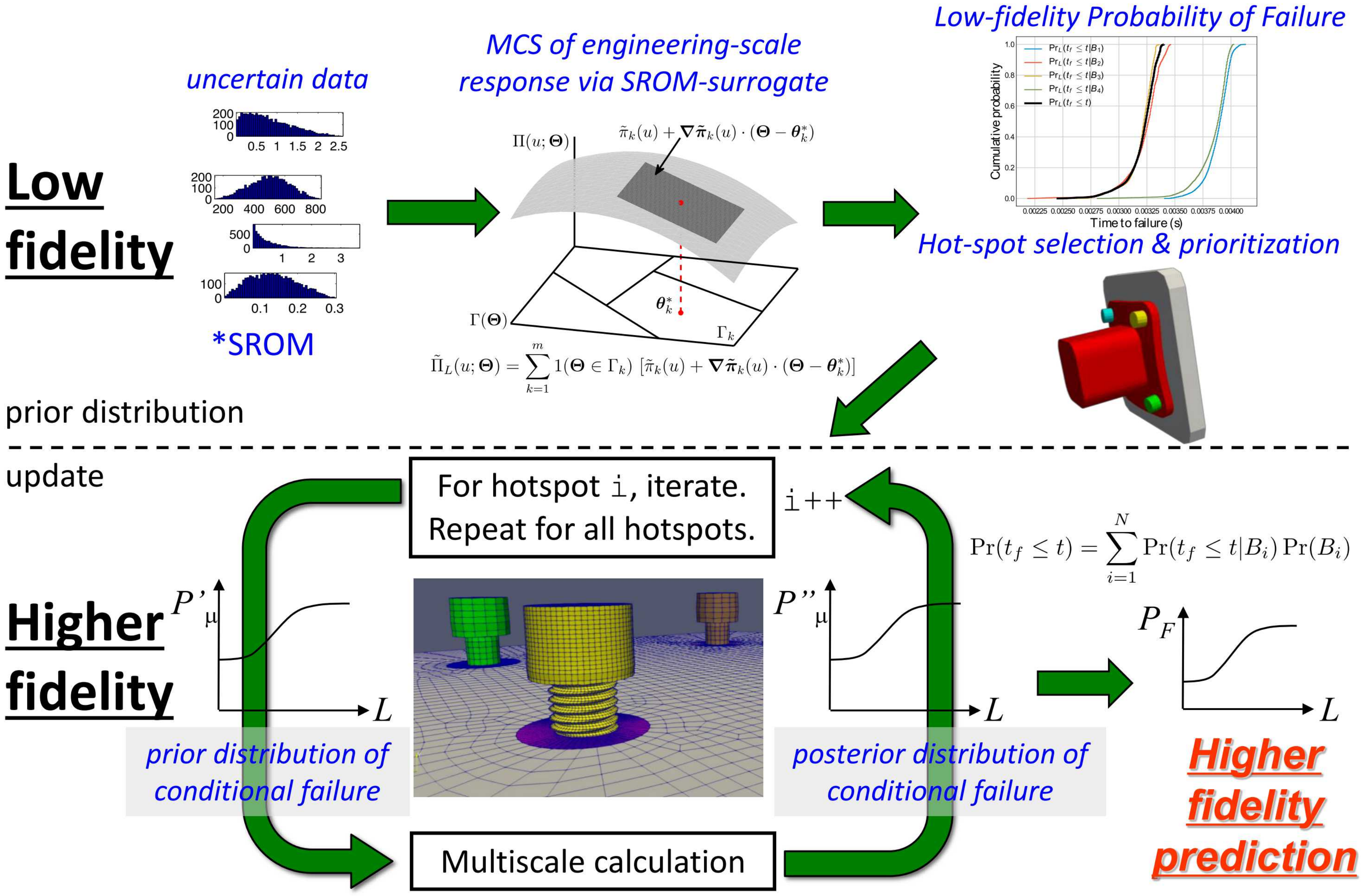
But you set out to predict this:



The tail of the *cumulative* failure, which requires many MC samples.

$$\Pr(t_f \le t) = \sum_{i=1}^{N} \Pr(t_f \le t | B_i) \Pr(B_i)$$

Schematic of our hierarchical approach

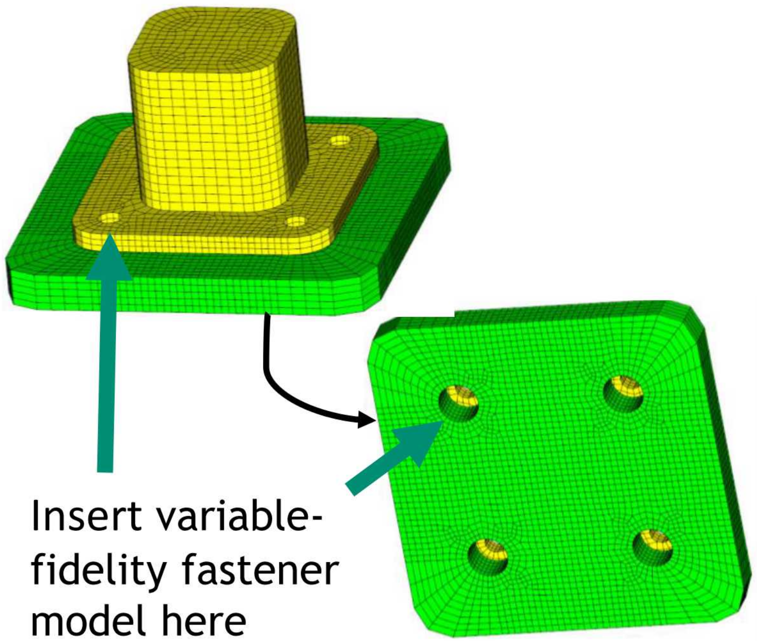


In the following, we use a lot of “models.” Here we provide a high-level overview to help keep things straight:

- Low fidelity finite element model (lofi FE) – a finite element model containing lower-fidelity geometric representation.
- High fidelity finite element model (hifi FE) – a finite element model with improved (relative to lofi FE) geometric fidelity.
- Truth finite element model – a finite element model used in lieu of experimental data as a truth solution.
- Stochastic reduced-order model (SROM) – a surrogate model to expedite uncertainty propagation.
- Lofi SROM and hifi SROM – SROMs built with the lofi FE and hifh FE models, respectively.

Finite element model(s)

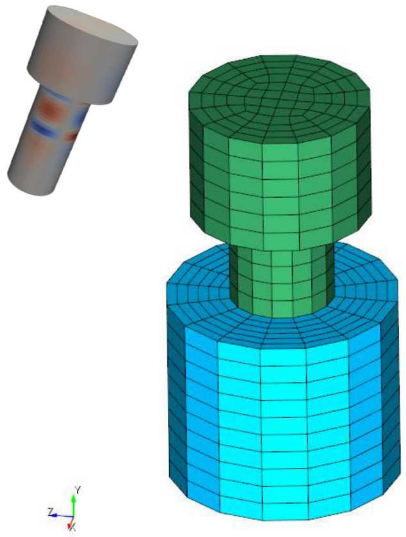
Bolted component



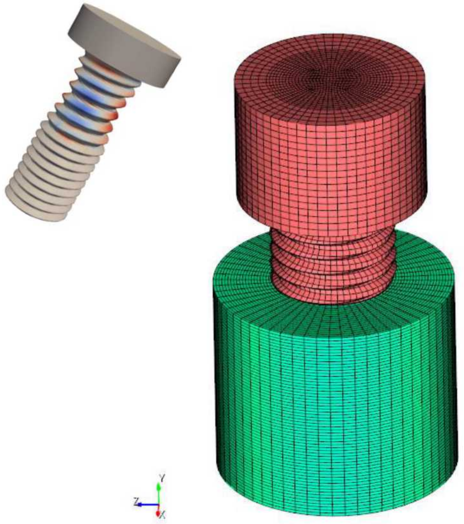
Insert variable-fidelity fastener model here

Bottom view

Component model
- 16,000 elements
- Minimum element edge: 0.036” – time step ~ 2e-07 s
- BC’s: hold outside of (green) plate fixed, apply δx, δy, δz at upper surface of component (yellow)



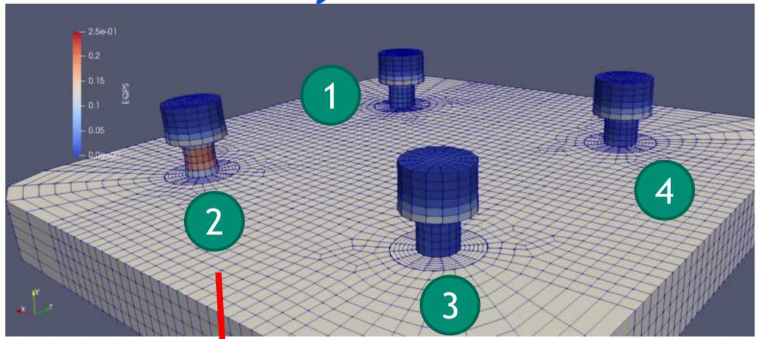
Plug model (low fidelity)
- 1,920 elements
- Minimum element edge: 0.022 – time step ~ 1e-07
- Tied contact b/w shank and nut



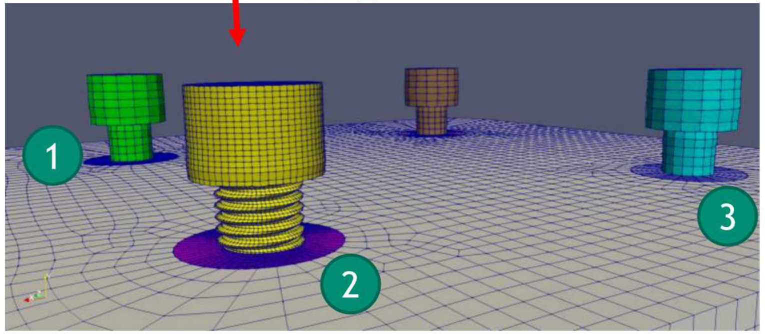
Threaded model (high fidelity & truth)
- 180,000 elements
- Minimum element edge: 0.0027” – time step ~ 1e-08
- Frictional contact b/w shank and nut threads

Miscellaneous (but important) details

Lofi model



Hifi$_2$ model

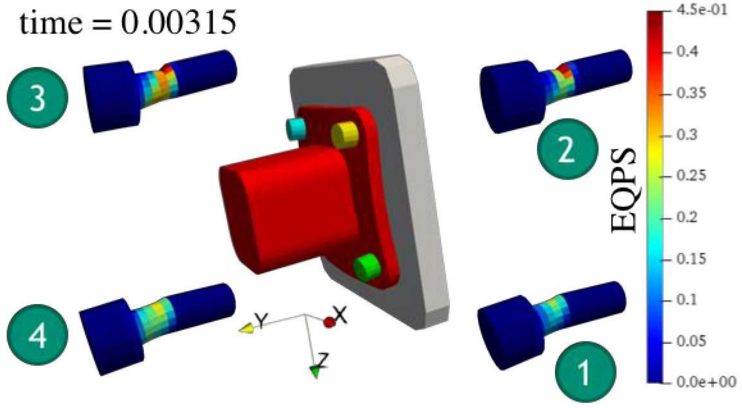


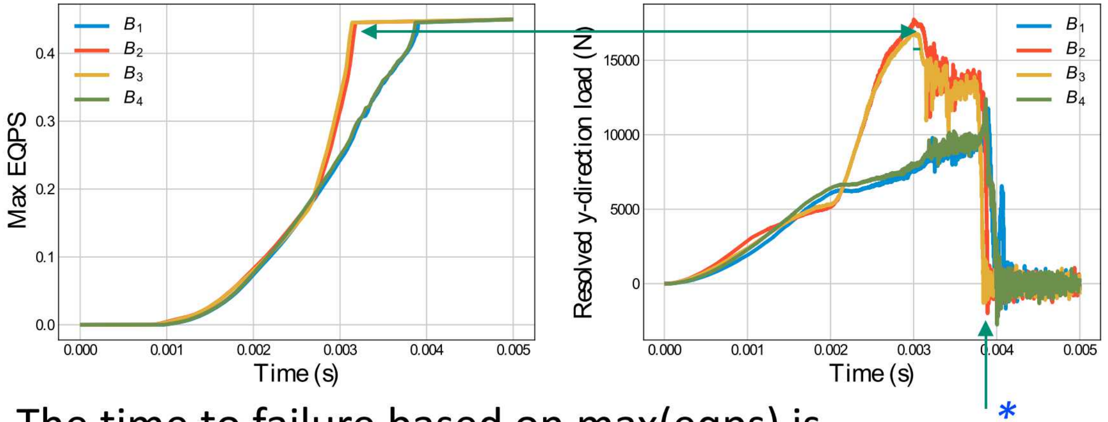
1. We use "plug" for low fidelity and (one or two) full threads for high fidelity.
2. We compare with "truth," which employs threaded models at all 4 locations.
3. Material properties are from tension data on fasteners, calibrated using the lofi model.
4. LoFi will be plugs at all 4 locations.
5. HiFi will be full thread at one, then two, location(s) selected based on lofi results.
6. There are convenient properties of multifidelity models (combinations of 3 & 4 above) that we are still exploring, but at least we expect it to be convergent because we recover "truth" when you include HiFi everywhere.
7. Hardening is hardening – recovery form w/ 3 parameters = initial_yield, hardening, recovery. (Allows us to parameterize the hardening and include them as random variates.)
8. System fails when first bolt "fails." This is hard to define. Presently, we use a mesh-dependent metric: max(eqps) = 0.45

Deterministic lofi & truth results

Lofi model

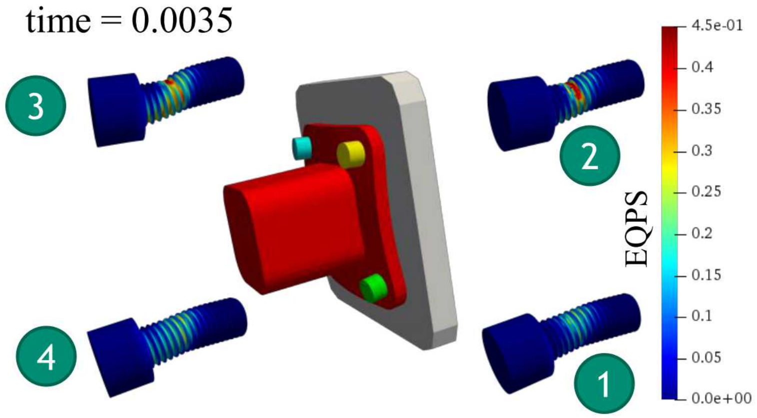
Deterministic calculations assume $\delta x = 0$.

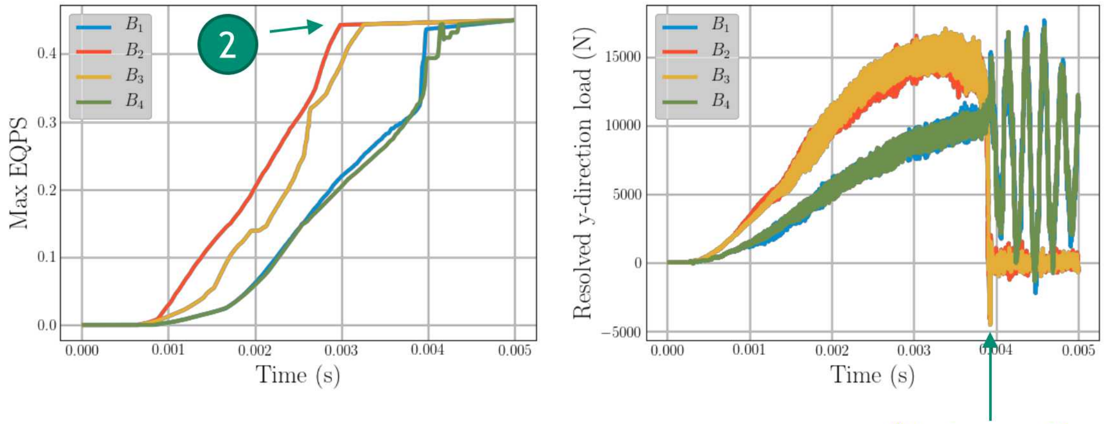




The time to failure based on max(eqps) is approximately coincident with load drop in the bolts.

Truth model

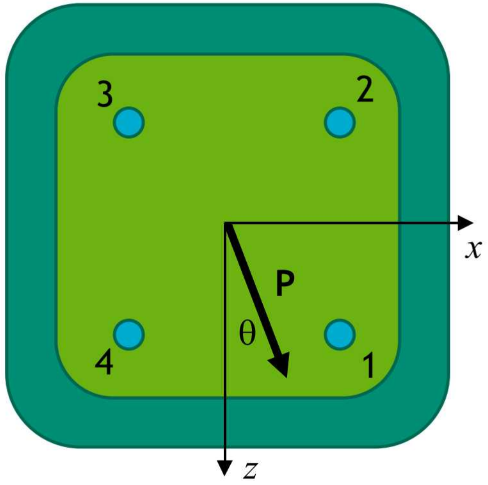




Interesting

Model for randomness

- Suppose, upon assembly, bolts 1 and 4 were the last two in the box, so that bolts 2 and 3 were the first two from a new box, *i.e.*, different batch. Bolt properties are correlated as shown in the matrix below. Hardening is weakly (and negatively) correlated with yield, and bolts 1, 4 and 2, 3 are weakly correlated. And there's some quantifiable uncertainty in loading.
- Bolts have random initial yield strength and hardening modulus, and the horizontal loading angle θ is random.
- Yield is Beta distribution calibrated to aluminum data but scaled to have mean = 111,660.8 and standard deviation = 1,353.3 (psi).
- Hardening is uniform calibrated to aluminum data, scaled to have mean = 898,637.0 (psi) and standard deviation = 135,497.0 (psi).
- θ is assumed uniform random between $-\pi/16$, $+\pi/16$ (mean 0).

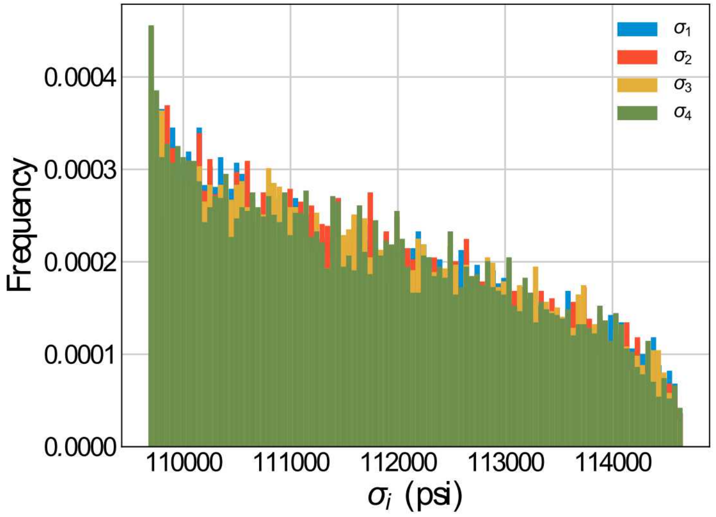


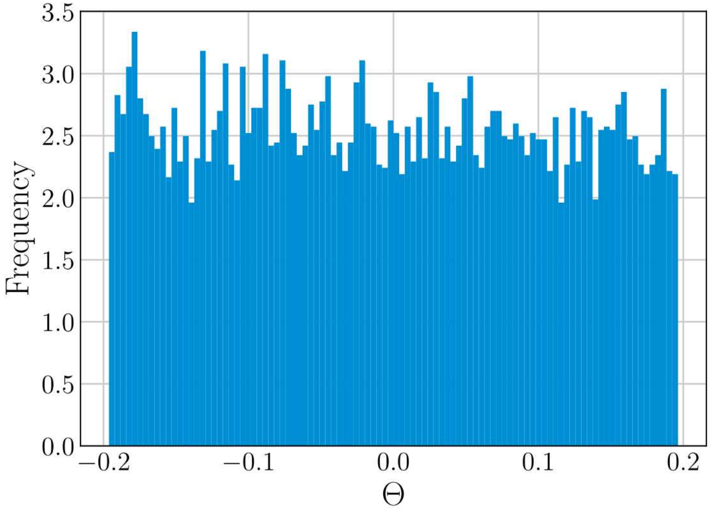
	Θ	σ_{y1}	h_1	σ_{y2}	h_2	σ_{y3}	h_3	σ_{y4}	h_4
Θ	1.	0.	0.	0.	0.	0.	0.	0.	0.
σ_{y1}	0.	1.	-0.2	0.	0.	0.	0.	0.5	0.
h_1	0.	-0.2	1.	-0.2	0.	0.	0.	0.	0.5
σ_{y2}	0.	0.	-0.2	1.	-0.2	0.5	0.	0.	0.
h_2	0.	0.	0.	-0.2	1.	-0.2	0.5	0.	0.
σ_{y3}	0.	0.	0.	0.5	-0.2	1.	-0.2	0.	0.
h_3	0.	0.	0.	0.	0.5	-0.2	1.	-0.2	0.
σ_{y4}	0.	0.5	0.	0.	0.	0.	-0.2	1.	-0.2
h_4	0.	0.	0.5	0.	0.	0.	0.	-0.2	1.

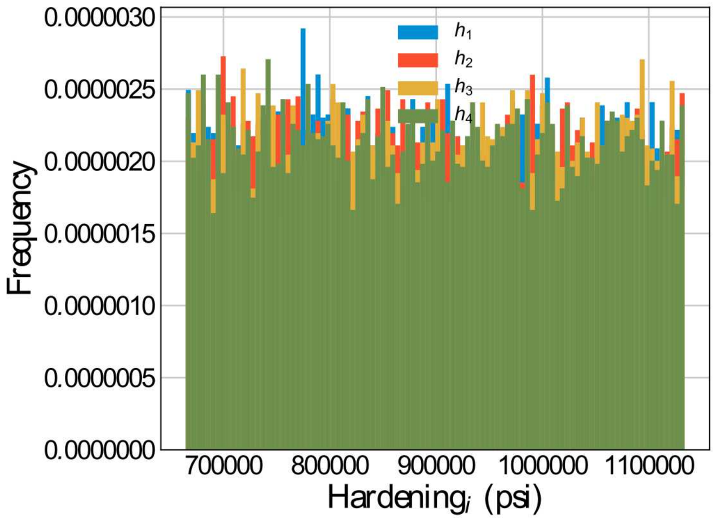
10,000 Samples -- Histograms and correlation

We use a translation model to obtain samples of this random vector. Here is the outcome from generating 10,000 samples.

$$
\begin{bmatrix}
1.00 & 0.00 & 0.00 & -0.01 & 0.01 & 0.00 & 0.01 & 0.01 & -0.02 \\
0.00 & 1.00 & -0.19 & -0.01 & -0.01 & -0.01 & 0.01 & 0.48 & 0.00 \\
0.00 & -0.19 & 1.00 & -0.01 & 0.01 & 0.00 & 0.01 & -0.01 & 0.48 \\
-0.01 & -0.01 & -0.01 & 1.00 & -0.20 & 0.48 & 0.00 & 0.01 & -0.01 \\
0.01 & -0.01 & 0.01 & -0.20 & 1.00 & 0.00 & 0.48 & 0.00 & -0.01 \\
0.00 & -0.01 & 0.00 & 0.48 & 0.00 & 1.00 & -0.19 & 0.01 & 0.00 \\
0.01 & 0.01 & 0.01 & 0.00 & 0.48 & -0.19 & 1.00 & 0.00 & 0.00 \\
0.01 & 0.48 & -0.01 & 0.01 & 0.00 & 0.01 & 0.00 & 1.00 & -0.19 \\
-0.02 & 0.00 & 0.48 & -0.01 & -0.01 & 0.00 & 0.00 & -0.19 & 1.00
\end{bmatrix}
$$

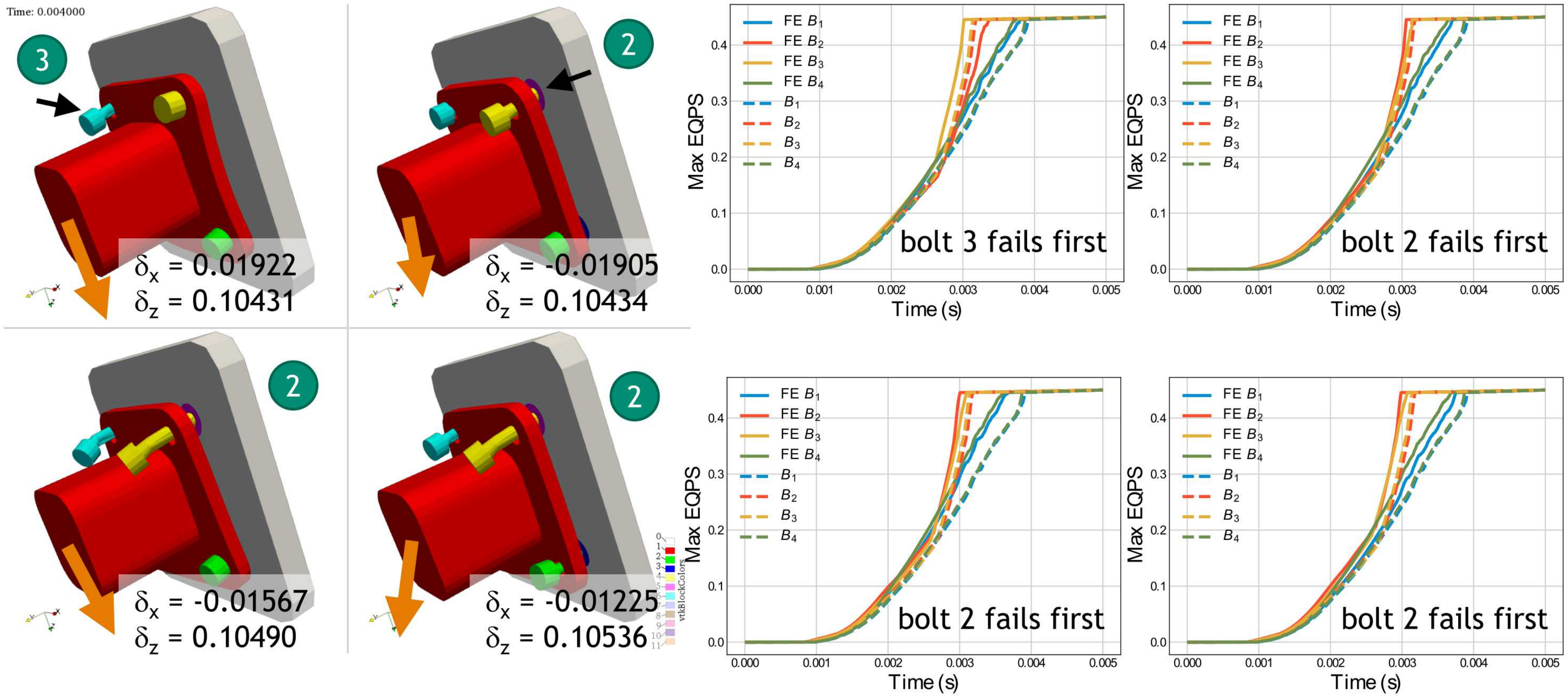






Lofi FE w/ 4 samples of random properties and loading angle

Low fidelity simulations of the first four samples. The dashed lines are from the deterministic calculation, for comparison.



Failure appears to be dictated by the sign of \Theta

Stochastic reduced-order model (SROM)

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 $\left(\tilde{\boldsymbol{\theta}}_k, \tilde{p}_k\right)$ $k = 1, \ldots, m$ that minimizes an objective function of the form:

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

Estimates of SROM statistics given SROM sample size m

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

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

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

Estimates of sample statistics given q samples of $\boldsymbol{\Theta}$

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

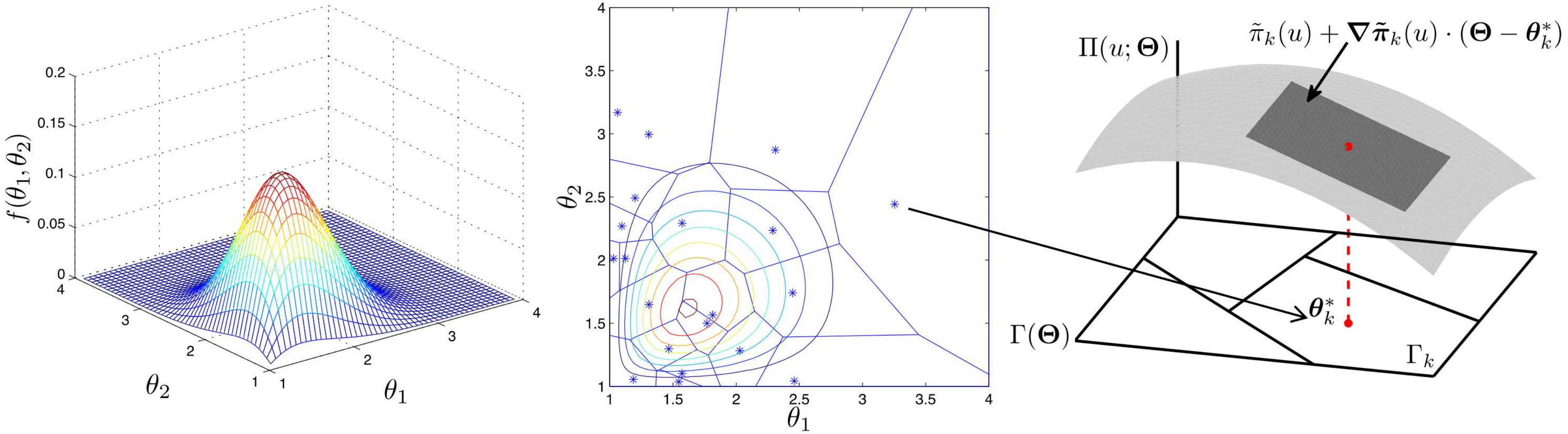
$$\hat{F}_s(x) = \sum_{i=1}^{q} (1/q) 1(\theta_{i,s} \le x)$$

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

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

Construction of SROM-based surrogate

Example 2D probability density | * SROM points | Response surface



- A response surface is constructed for the structural response of the component, $\Pi(u;\Theta)$
- The surface is a series of hyper-planes described with a first-order Taylor approximate of the structural response

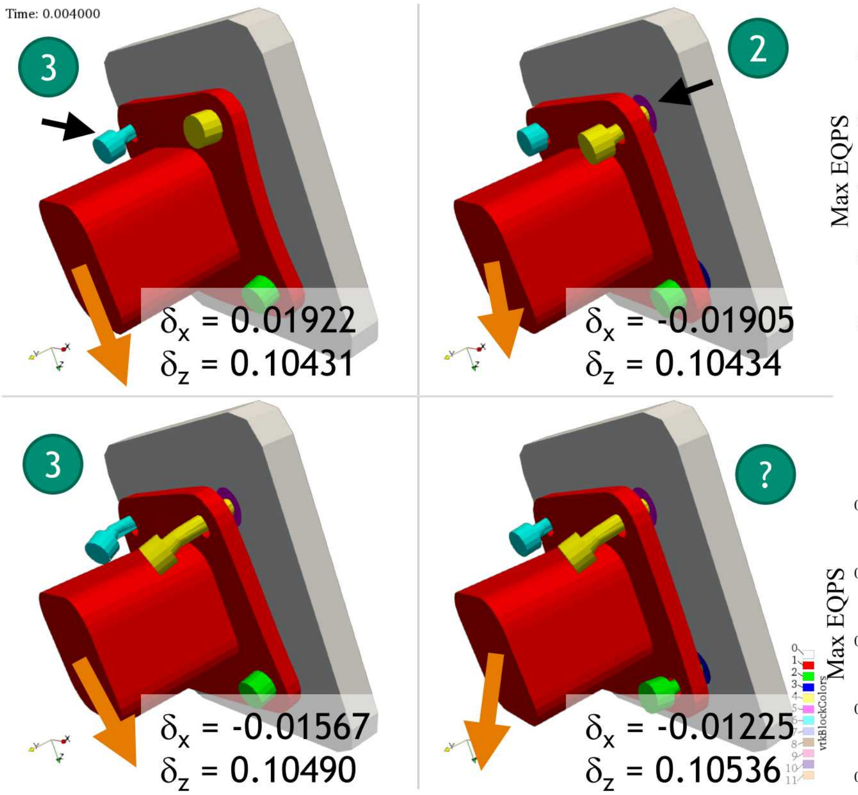
$$\tilde{\Pi}_L(u;\boldsymbol{\Theta}) = \sum_{k=1}^{m} 1(\boldsymbol{\Theta} \in \Gamma_k)[\tilde{\pi}_k(u) + \nabla\tilde{\pi}_k(u) \cdot (\boldsymbol{\Theta} - \theta_k^*)]$$

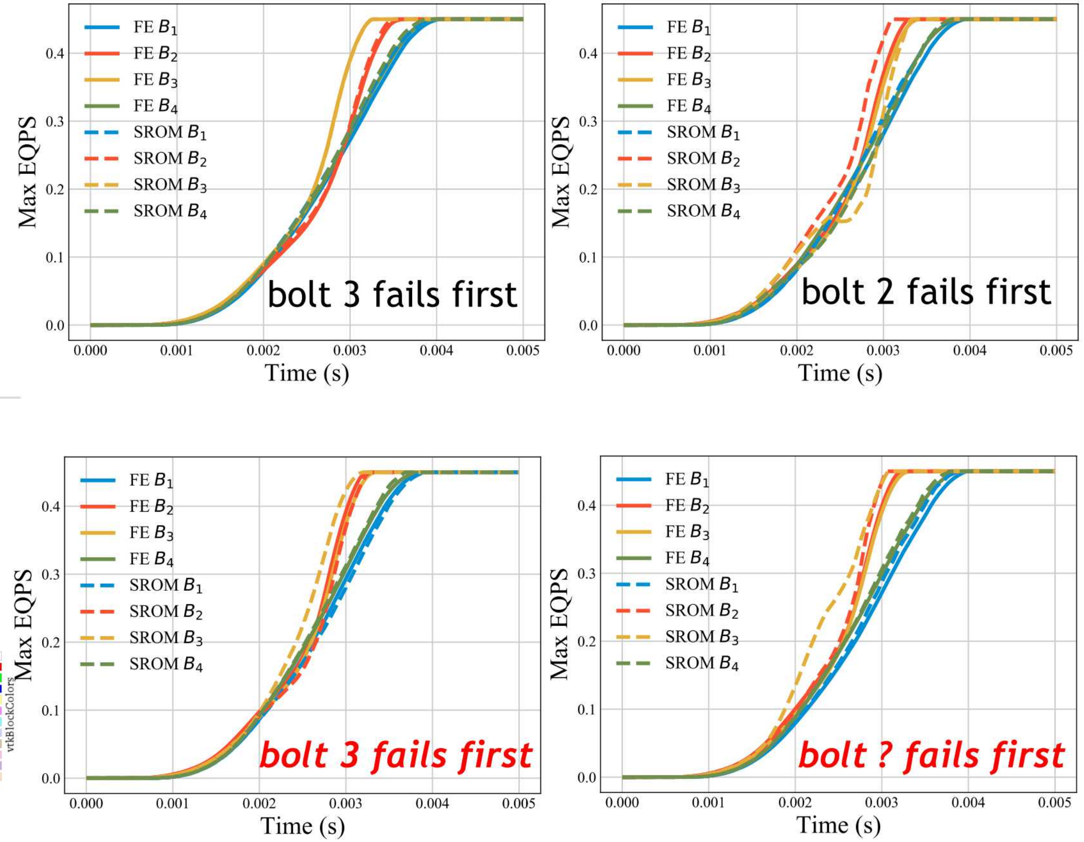
- The SROM samples are used as the expansion points θ_k^* and the domain Γ_k are determined by the Voronoi tessellation of the uncertain parameters
- Requires m*(d+1) FE calculations (we use m = 20 and d = 9, so 200 FE calculations)

Assumes the quantity of interest is differentiable.

Lofi SROM predictions (same 4 samples)

For the first four random samples, we plot eqps in bolts 1-4 per the low fidelity FE model and the SROM-based surrogate. There is error introduced with the SROM, but we've shown it can be quite accurate in the ensemble, even for highly nonlinear problems (Emery *et al.*, IJNME 2016).

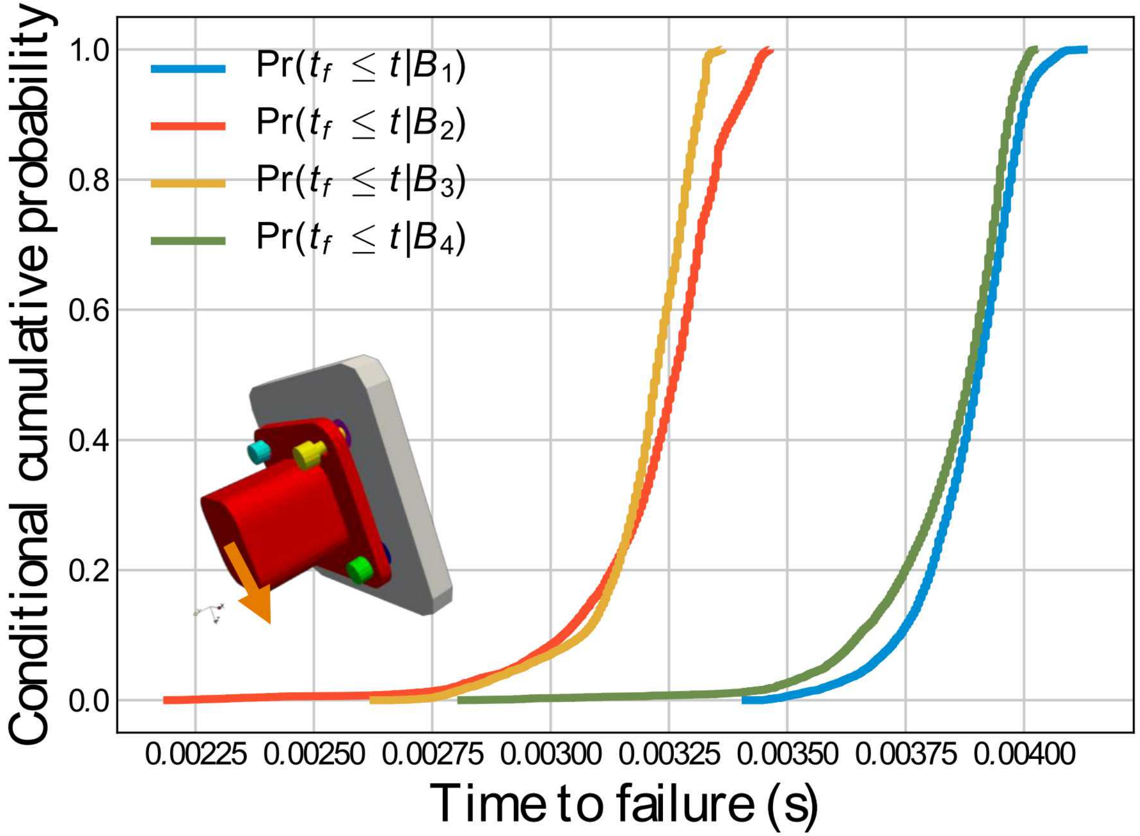




Failure appears to be dictated by the sign of \Theta

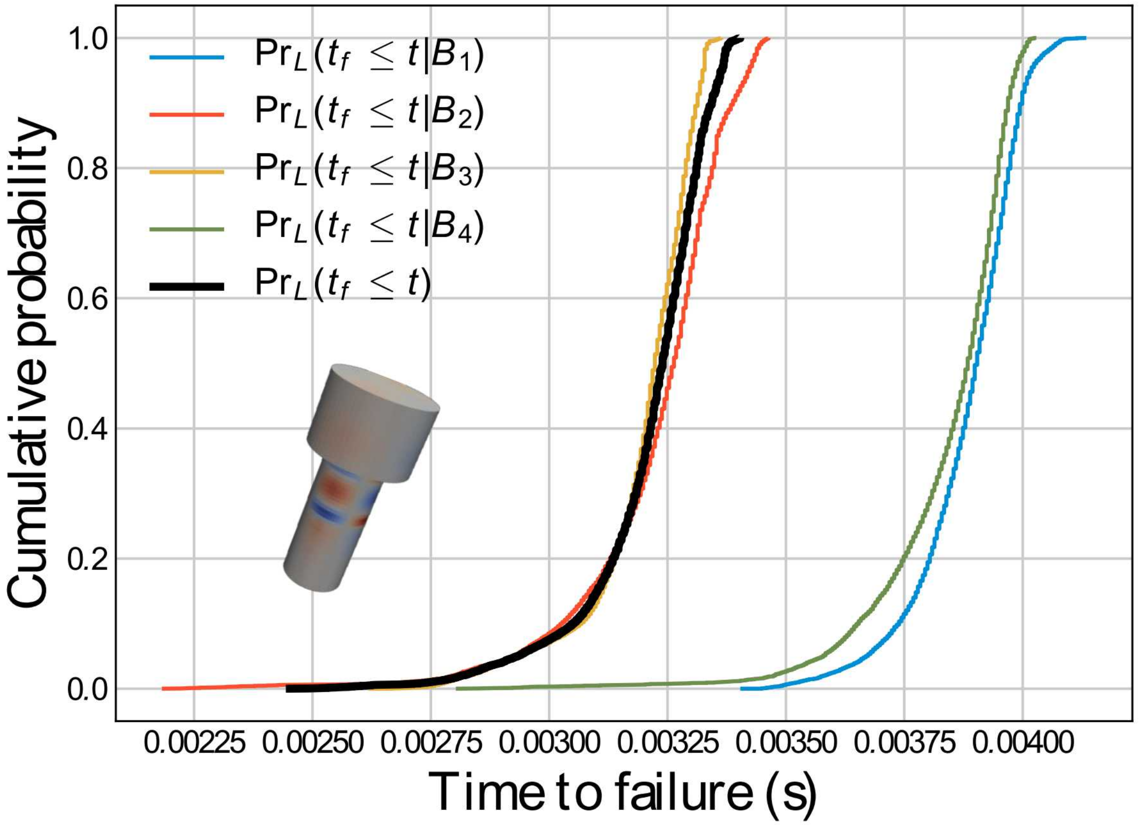
Low fidelity estimates of conditional probability

Thanks to the SROM-based surrogate, we can perform MCS w/ 10,000 samples for the cost of 200 lofi FE simulations.



Low fidelity estimate of total probability

The law of total probability allows us to compute the probability of failure (due to bolt fracture) for our component. $\Pr(B_i)$ is easy to compute as the fraction of occurrences when failure of bolt B_i governs.



$$\Pr(t_f \leq t) = \sum_{i=1}^{N} \Pr(t_f \leq t|B_i)\Pr(B_i)$$

Bolt	$\Pr(B_i)$
1	0.
2	0.3973
3	0.6027
4	0.

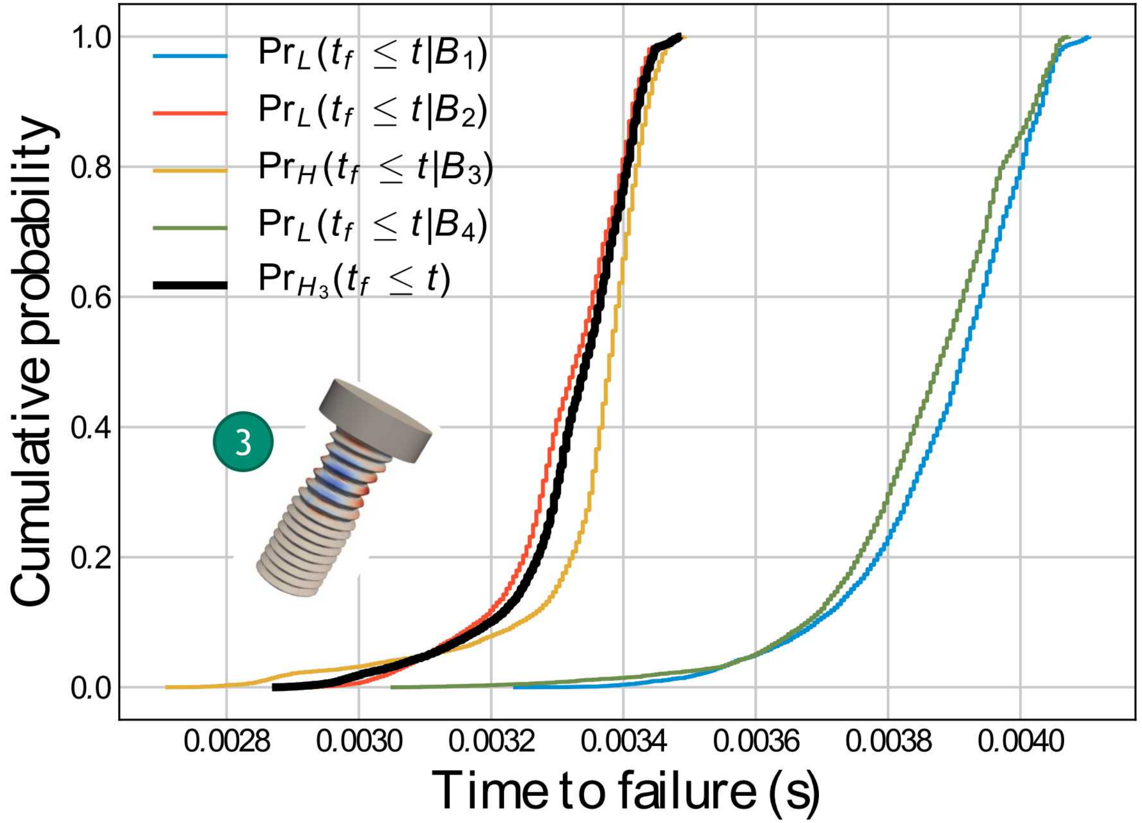
2nd (bolt 2), 1st (bolt 3)

Obvious choices for hifi simulation

Hifi$_3$ SROM estimate of total probability

We know our failure metric is mesh dependent (max[EQPS]) and sensitive to gradients, but the full thread model is at bolt 3 for this calculation whereas the emphasis (conditional probability) shifted to bolt 2.

What is this telling us? (Other than maybe the lofi model misled us in choosing bolt 3 for hifi.)



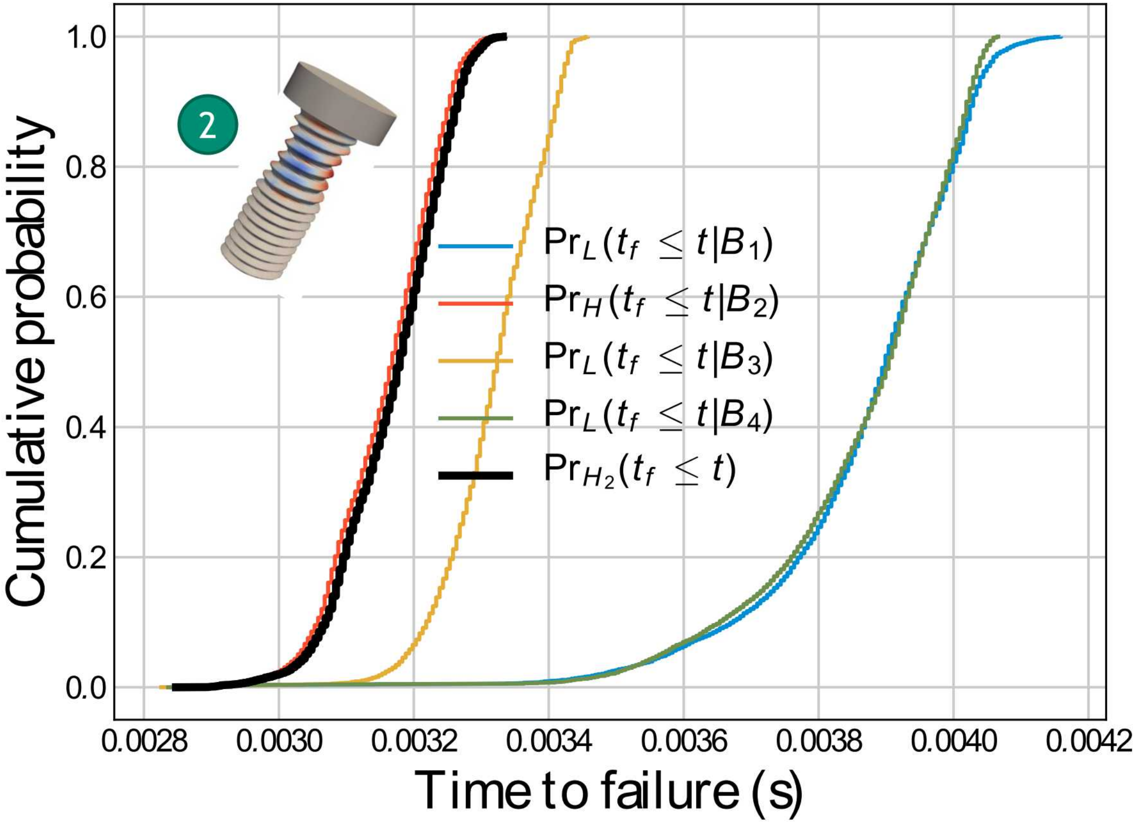
$$\Pr(t_f \leq t) = \sum_{i=1}^{N} \Pr(t_f \leq t|B_i)\,\Pr(B_i)$$

Bolt	$\Pr(B_i)$
1	0.0019
2	0.7263
3	0.2716
4	0.0002

IT SWITCHED!

Hifi$_2$ SROM estimate of total probability

Wow! Obviously, the lofi model dramatically underestimates the probability of failure at bolt 2. Hifi$_2$, no doubt, over estimates it since there are no threads and a coarse mesh in bolt 3. But what to believe and what to use for computing our multifidelity Pr?



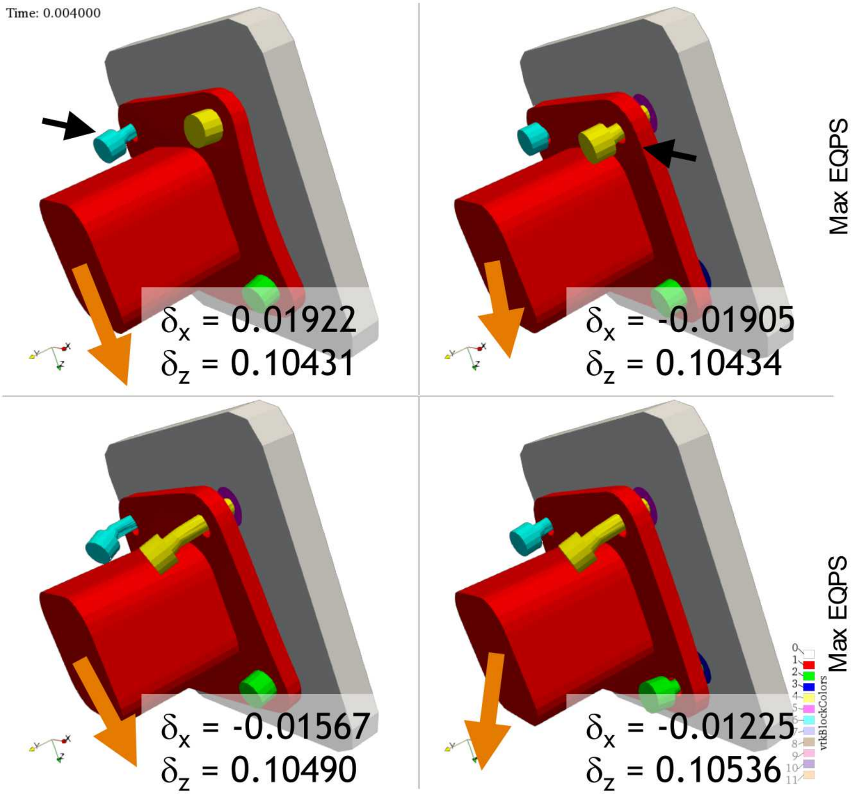
$$\Pr(t_f \leq t) = \sum_{i=1}^{N} \Pr(t_f \leq t|B_i)\,\Pr(B_i)$$

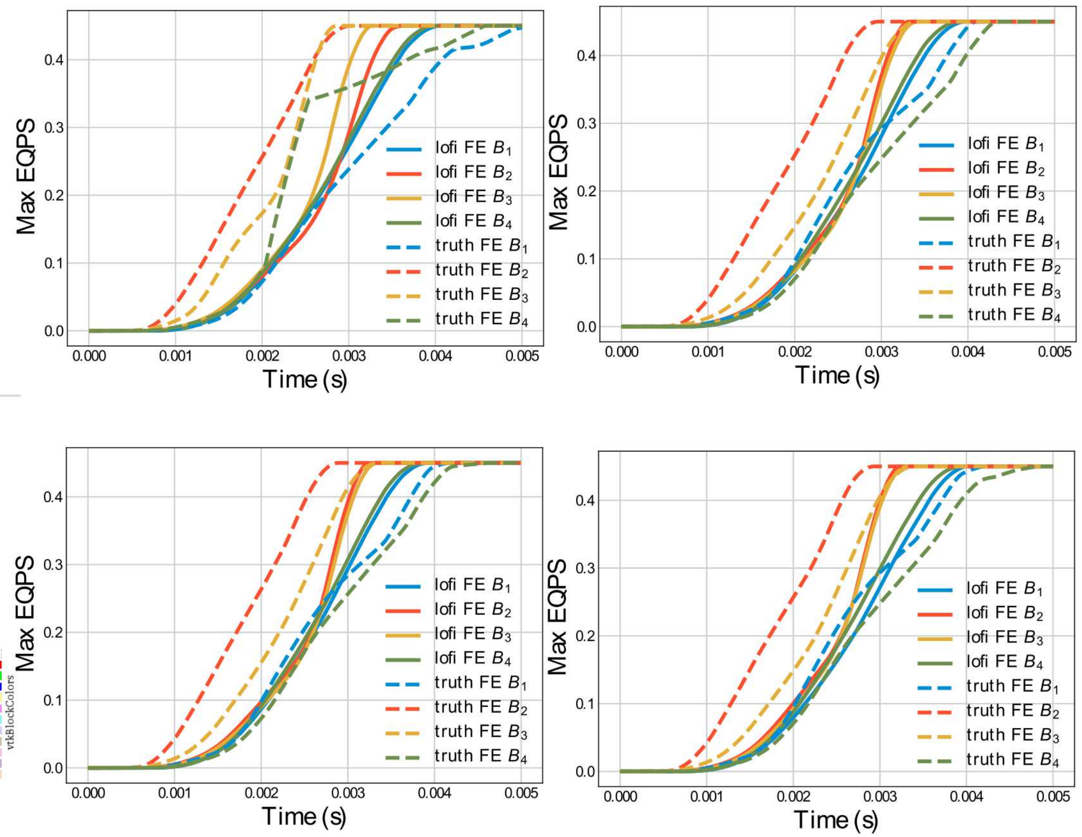
Bolt	$\Pr(B_i)$
1	0.
2	0.9375
3	0.0602
4	0.0023

← !!!

Comparing "truth" with lofi FE (same 4 samples)

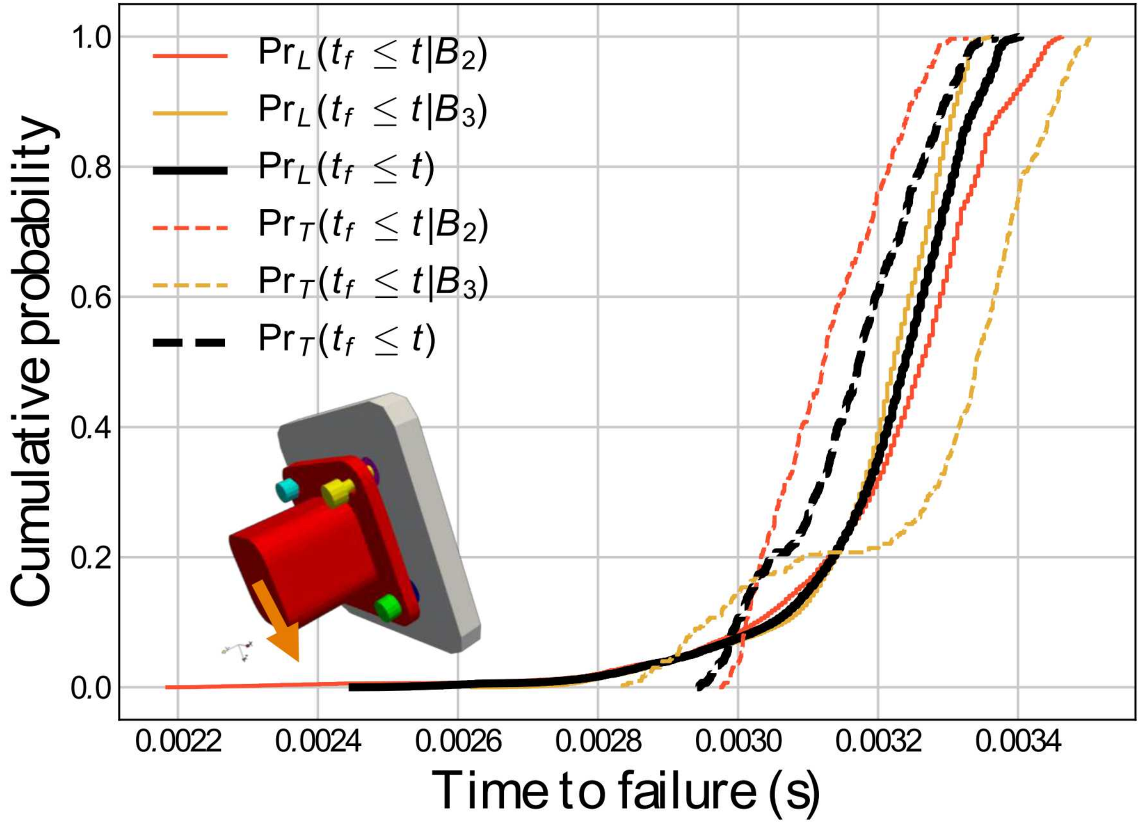
We expect to see differences based on choice of max(eqps).





Conditional and total probabilities: truth vs. lofi

Note the “truth” of the matter for the marginal probabilities.



$$\Pr(t_f \leq t) = \sum_{i=1}^{N} \Pr(t_f \leq t|B_i)\,\Pr(B_i)$$

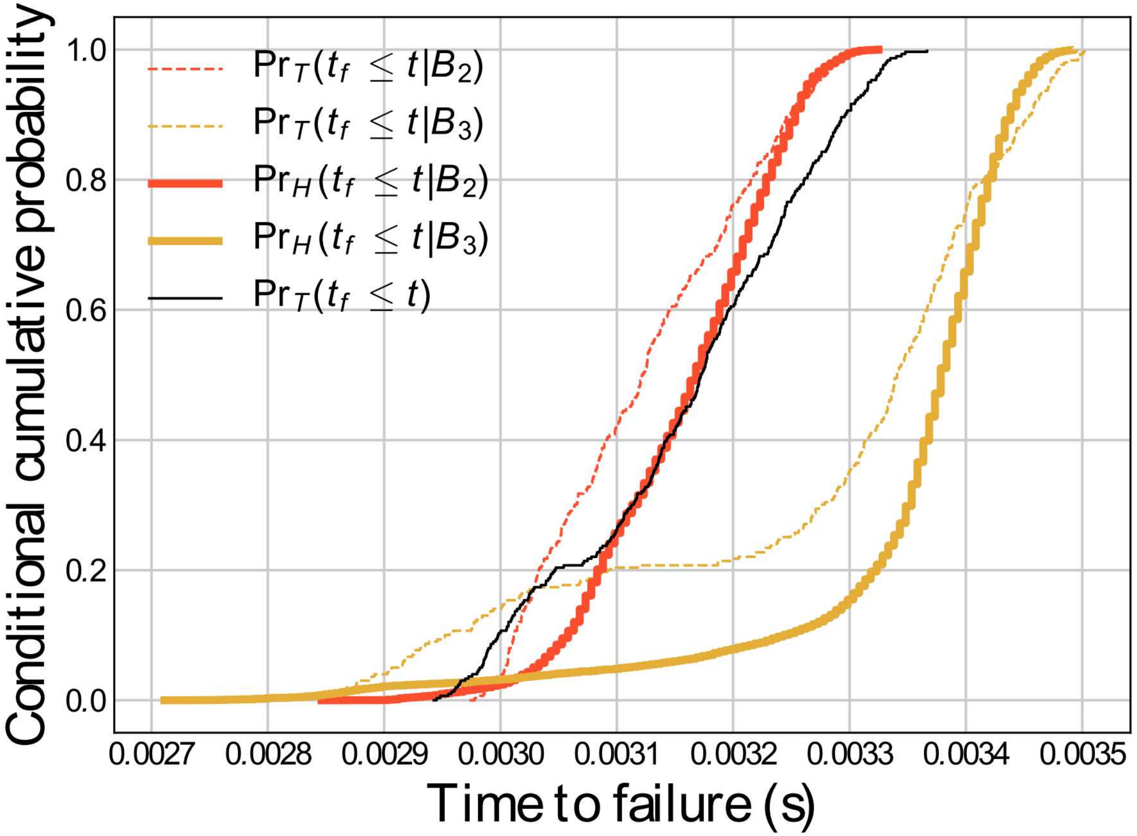
Bolt	$\Pr(B_i)$
1	0.
2	0.77
3	0.23
4	0.0

“truth”

Compare conditional probabilities for bolt 2, 3

As expected, when computed with the high fidelity model, the conditional probabilities for bolts 2 and 3 are reasonably close to the conditional "truth" predictions.

With proper weighting, these would closely approximate "truth's" total probability.



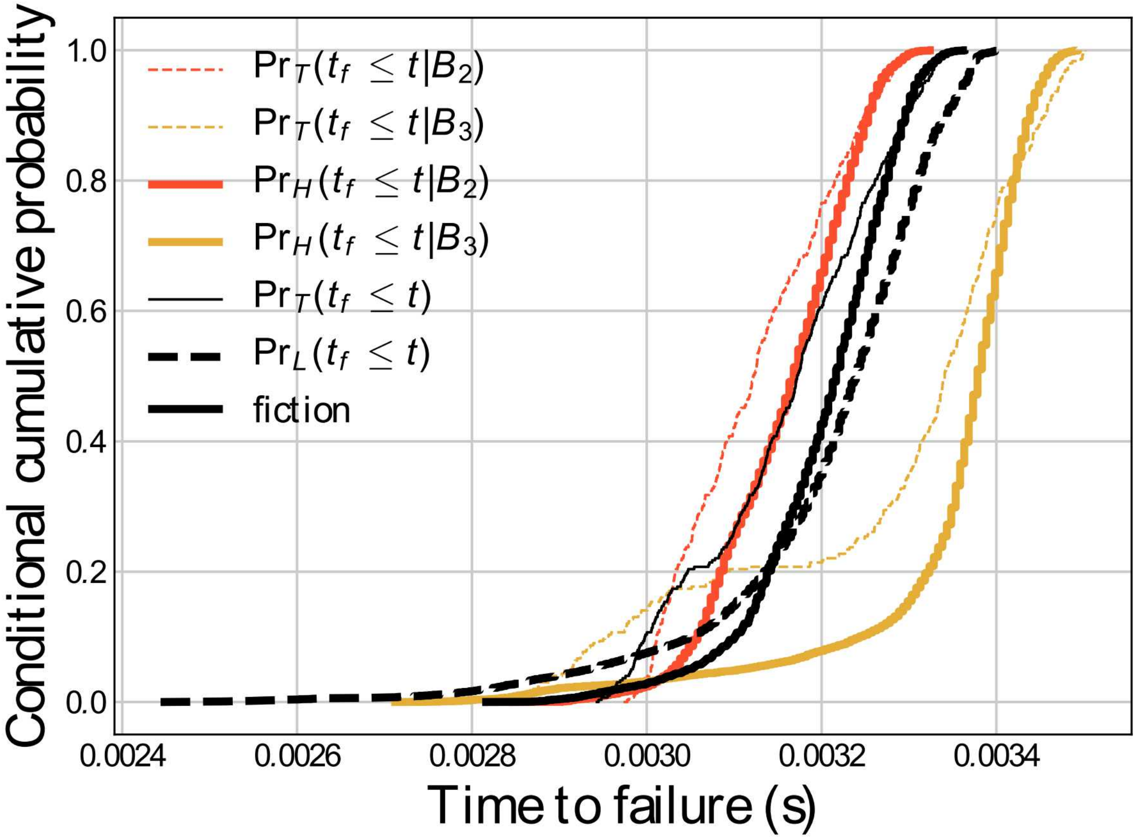
$$\Pr(t_f \leq t) = \sum_{i=1}^{N} \Pr(t_f \leq t|B_i) \Pr(B_i)$$

What to do with this?

If I cheat and pretend we somehow know the truth about the marginal probabilities $\Pr(B_i)$, *i.e.*, use weights from the truth calculation, then the total probability looks pretty reasonable. I am trying to understand how to improve the estimates for $\Pr(B_i)$ based on the information we have from the series of simulations. But…

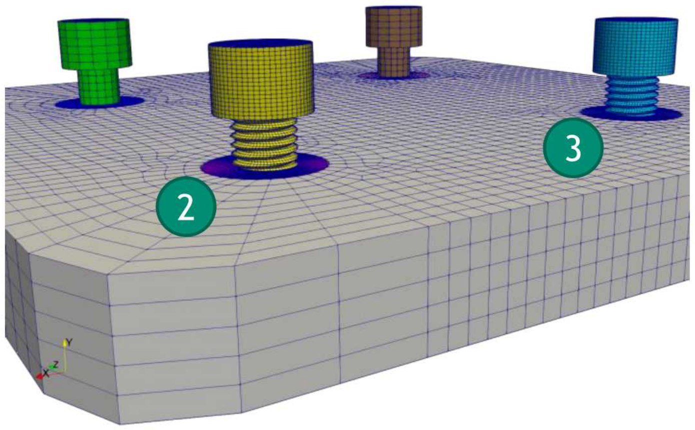
Summary of $\Pr(B_i)$

Bolt	lofi	hifi 2	hifi 3	truth
1	0.	0.	0.0019	0.
2	0.3973	0.9375	0.7263	0.77
3	0.6027	0.0602	0.2716	0.23
4	0.	0.0023	0.0002	0.0



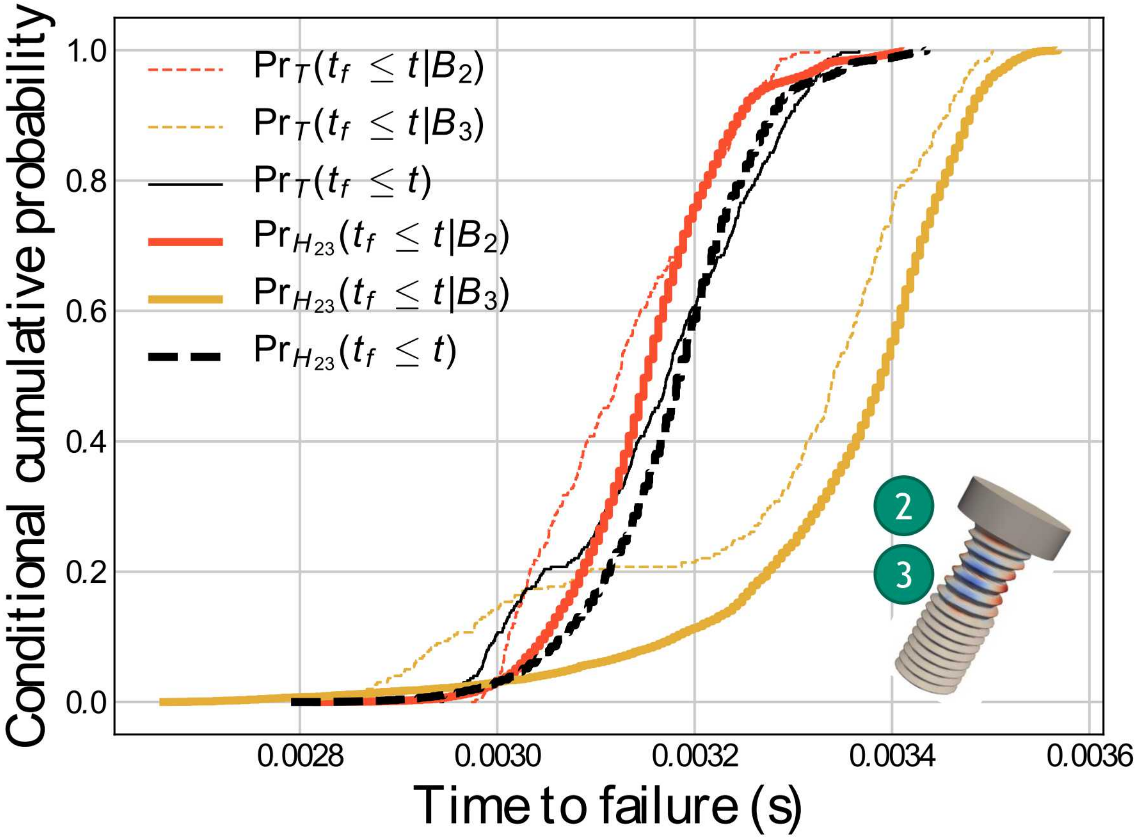
Hifi23

But based on the lofi estimates of $\Pr(B_i)$ and other obvious concerns about their interaction, and certainly after the emphasis switch in the prediction by hifi_3, it seems reasonable to assume that the hifi model should include threaded bolts at both locations 2 and 3 (simultaneously). And when you do…



Summary of $\Pr(B_i)$

Bolt	lofi	hifi 23	truth
1	0.	0.	0.
2	0.3973	0.86	0.77
3	0.6027	0.14	0.23
4	0.	0.0	0.0
cpu hours	196.7	82,300.	196,036.

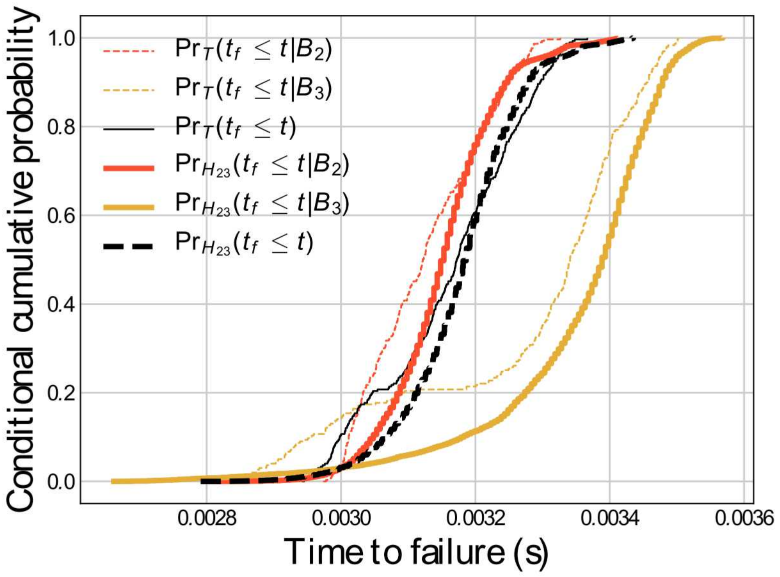


Summary

1. We propose a hierarchical model for efficient propagation of uncertainty that includes geometric parameters (θ).
2. We develop a reduced-order geometry model and a reduced-order probability model.
3. Our lofi model confuses the marginal probabilities, but highlights hot-spots.
4. When we listen carefully, we use hifi_{23} and do pretty well for less computational cost.

Summary of $\Pr(B_i)$

Bolt	lofi	hifi 23	truth
1	0.	0.	0.
2	0.3973	0.86	0.77
3	0.6027	0.14	0.23
4	0.	0.0	0.0
cpu hours	196.7	82,300.	196,036.



Research ideas

1. Use the lofi results to improve the SROM for the hifi calculations, *e.g.*, add SROM samples where the gradients are steep.
2. Use ideas from importance sampling to hierarchically improve the SROM, we care about the tails.
3. Improved failure models for the fasteners, both hifi and lofi.