SAND2015-3005C

Advanced UQ and V&V Procedures applied to Thermal-Mechanical Response and Weld Failure in Heated Pressurizing Canisters

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April 21-23, Detroit, MI

National Nuclear Security Administration

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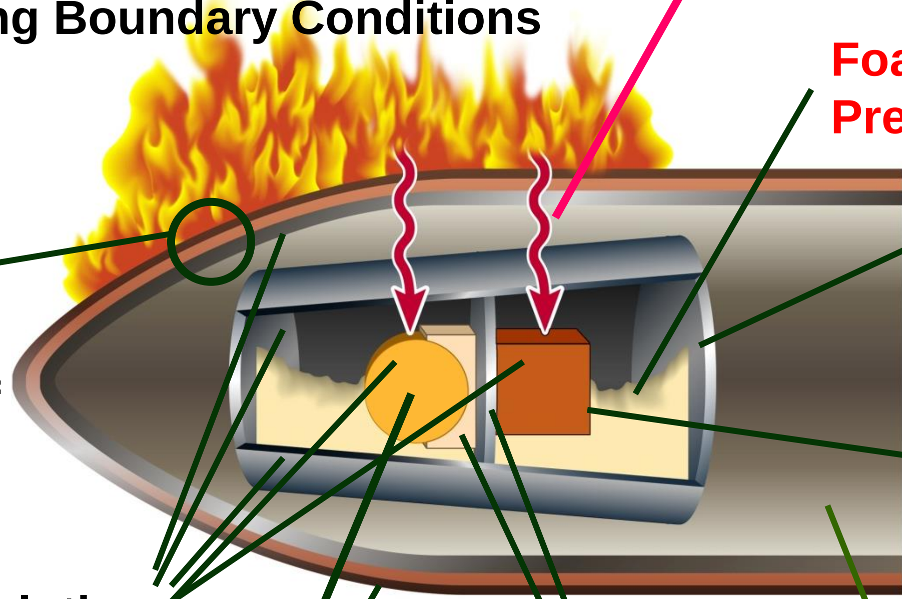
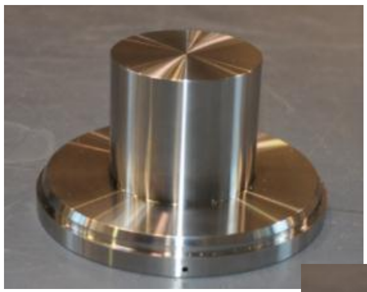
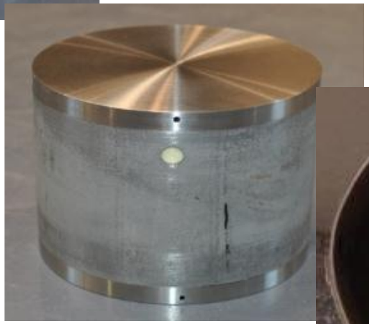
DOE drive toward Predictivity of Important Phenomena and Weapon Response in Fires



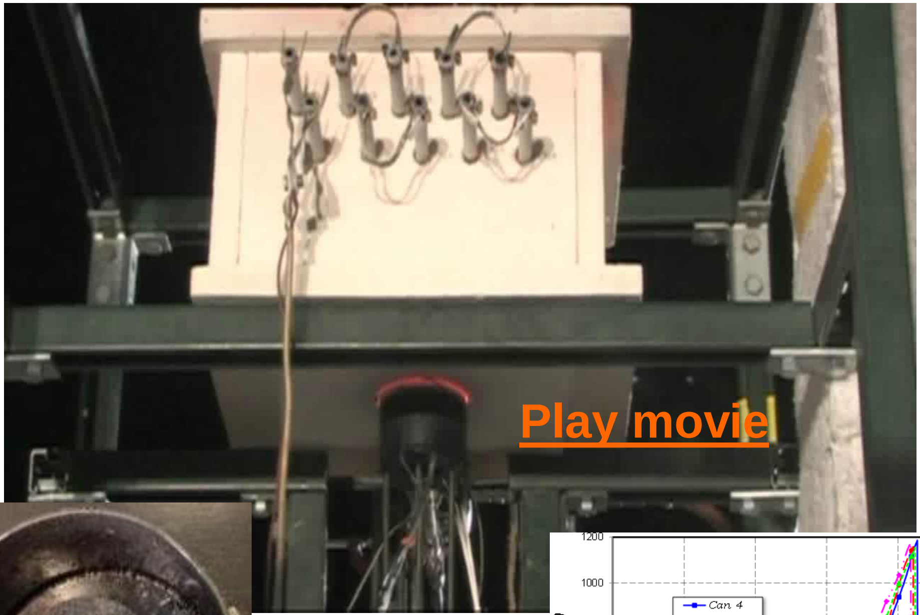
DOE Predictive Capability Assessment Project — Thermal-Mechanical Element

<u>Project Goal</u>: assess predictiveness of can pressurization from foam thermal decomposition and induced failure of weld around lid

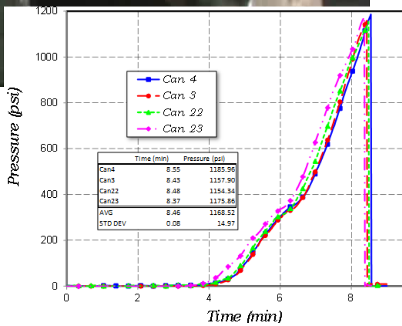





simplified geometry for phenomena V&V



internal pressure response



	Time (min)	Pressure (psi)
Can4	8.55	1185.96
Can3	8.43	1157.90
Can22	8.48	1154.34
Can23	8.37	1175.86
AVG	8.46	1168.52
STD DEV	0.08	14.97

5 Levels of Increasing Rigor in Treatment of Experimental and Simulation Uncertainties in Model Validation

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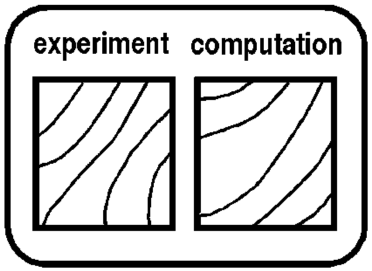
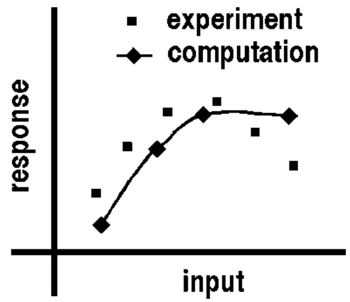
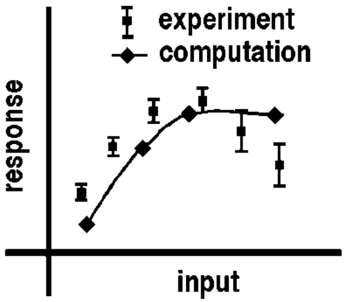


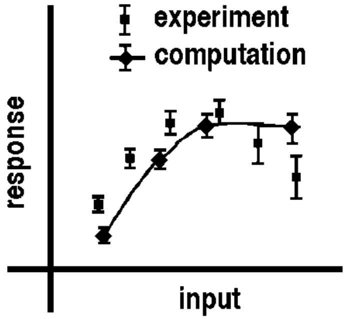
(a) Viewgraph Norm



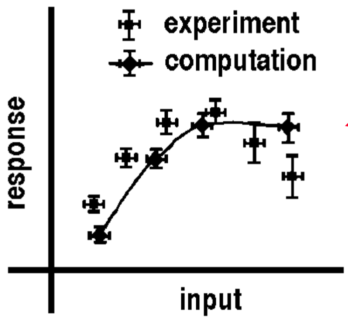
(b) Deterministic



(c) Experimental Uncertainty



(d) Numerical Error



(e) Nondeterministic Computation

"Real Space" validation approach appropriately and pragmatically treats all uncertainties on inputs & outputs of experiments and simulations

A “Real Space” Model Validation Approach is Used and Presented in the following

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- **advanced VVUQ approach**
- **general, versatile, practical**
- **Enables treatment of:**
  - Significant random/stochastic variability (aleatory uncertainty) in the models and physical systems, tests, and measurements.
  - Coupled with significant epistemic (systematic) uncertainty in the experiments and models
  - small #s of replicate tests (sparse data)
    - material characterization tests
    - integral tests at integral (can) level
  - Discrete random function data (matl. stress-strain curves)
  - Interval and Probabilistic characterizations of uncertainty

Aleatory – describes a set or population of multiple results (random or stochastic variability)
Epistemic – unknown single result within an uncertainty range (systematic uncertainty)

Real-Space Comparison of Experiment and Simulation Results

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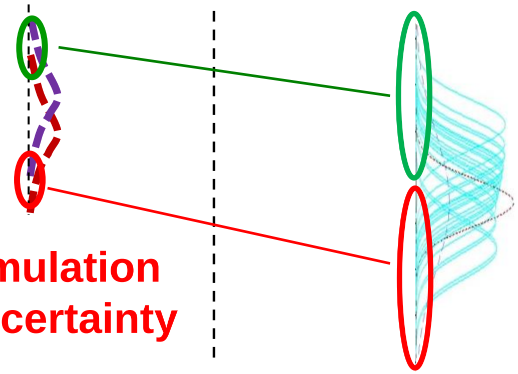
Approximate Probability Box (APbox) representation of aleatory & epistemic uncertainties



simulation uncertainty

experimental uncertainty

- **Aleatory/Random and Epistemic/Systematic uncertainties in experiments also accounted for.**
- **Intuitive visual indication of how accurate the model is, on several fronts:**
  - **<u>Variance</u>** of the predicted and experimental populations due to test-to-test random variability in geometry and stochastic phenomena
  - **<u>Means</u>** of the predicted and experimental populations
  - **<u>Percentiles</u>** of the predicted and experimental populations

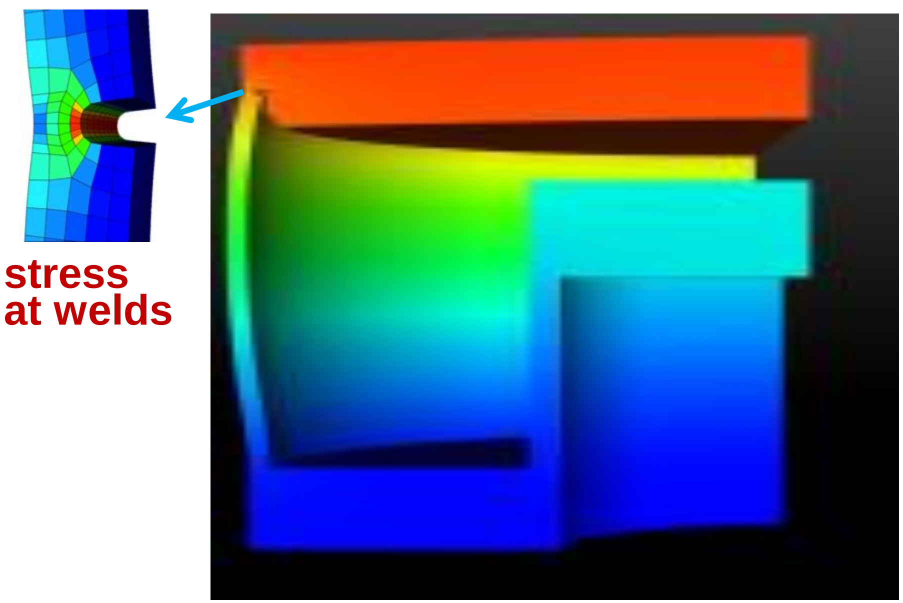
☛ **<u>granular</u> quantification of how the model is doing, as compared to validation metrics of integrated mismatch of distributions**

- **Percentile comparisons are particularly useful for validation assessment of models to be used in the analysis of performance and safety <u>margins</u>.**

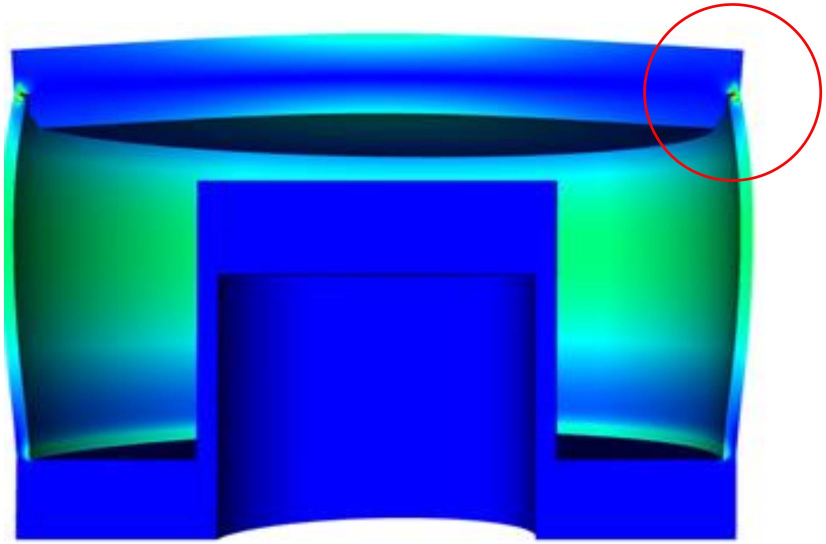
Treatment of Aleatory and Epistemic Uncertainties in Model Validation

- **Real Space approach can be viewed as an <u>extended hybrid</u> of other developed frameworks:**
  - **ASME V&V20 2009 *Standard for V&V in CFD and Heat Transfer***
    - geared for validation of non-stochastic (non-aleatory) systems
    - no aleatory-epistemic differentiation
    - equivalent to Real Space for probabilistic and epistemic-only uncer.
  - **ASME V&V10 2012 *Supplement for V&V in Computational Solid Mechanics***
    - built for validation of stochastic systems
    - segregates aleatory and epistemic uncertainties (Prob. boxes)
    - uses Ferson & Oberkampf "area" validation metric (CDF matching)
    - ignores some important types of experimental epistemic uncertainty that ASME VV20 and Real Space include

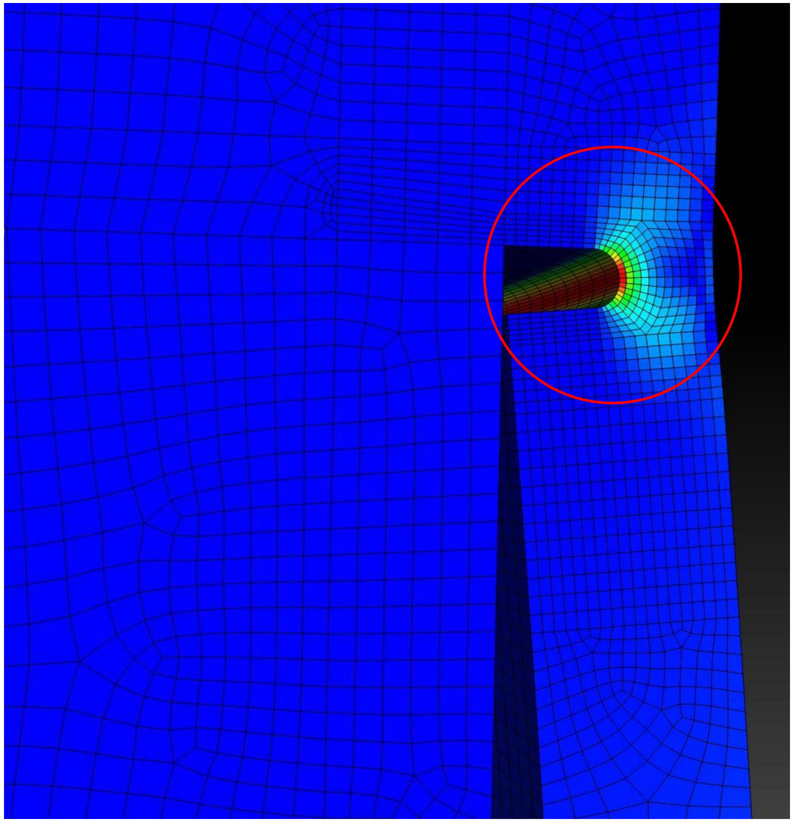
Weld Failure Predictions and their VVUQ Processing

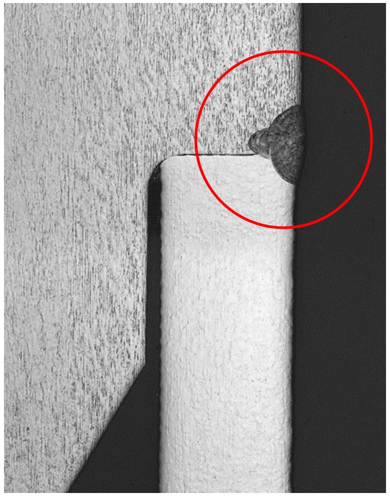


Some Aspects of Weld Modeling Approach



- idealization of weld as circular notch
- multilinear elastic-plastic constitutive model with temperature-dependent mtl. strength (more on later slides)





Material Characterization:

Aleatory and Epistemic uncertainties from Sparse samples of Discrete Random Functions

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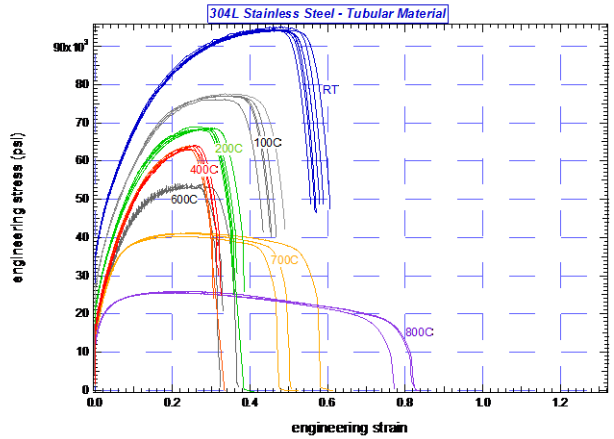
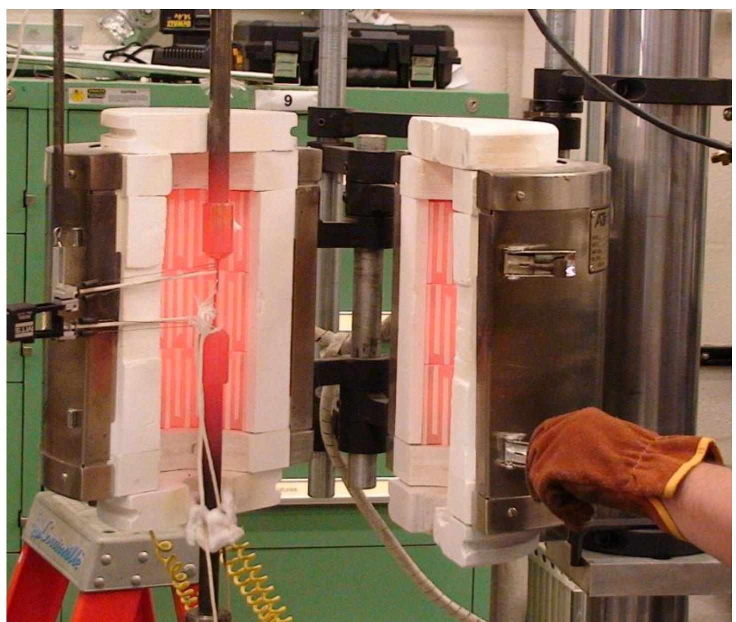
- **Variability of stress-strain curves of material response in cylinder tension tests at various temperatures**





Thermo-mechanical Failure Tensile Characterization of Can Materials

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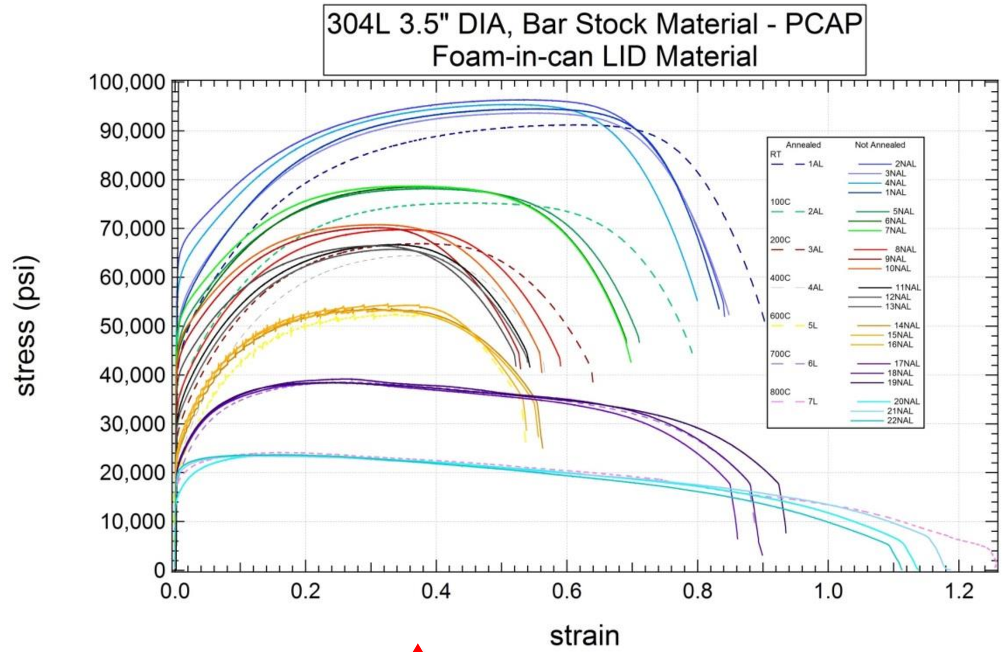
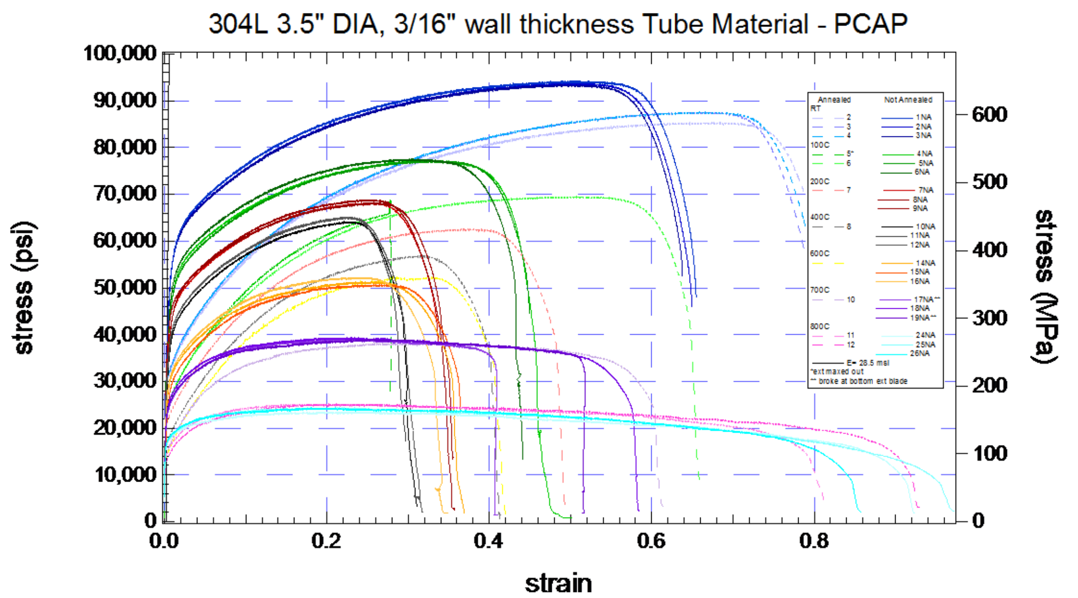


- Temperatures =
  20, 100, 200, 400, 600, 700, 800°C
- Material Characterization Tests
  - Lid Tensile Tests = 8 temps x 3 repeats = 24
  - Tube Tensile Tests = 8 temps x 3 repeats = 24

304L Lid Material

304L Wall Material



Inversion Procedure

to extract Cauchy-Stress/Logarithmic-Strain from Experimental Stress-Strain Curves

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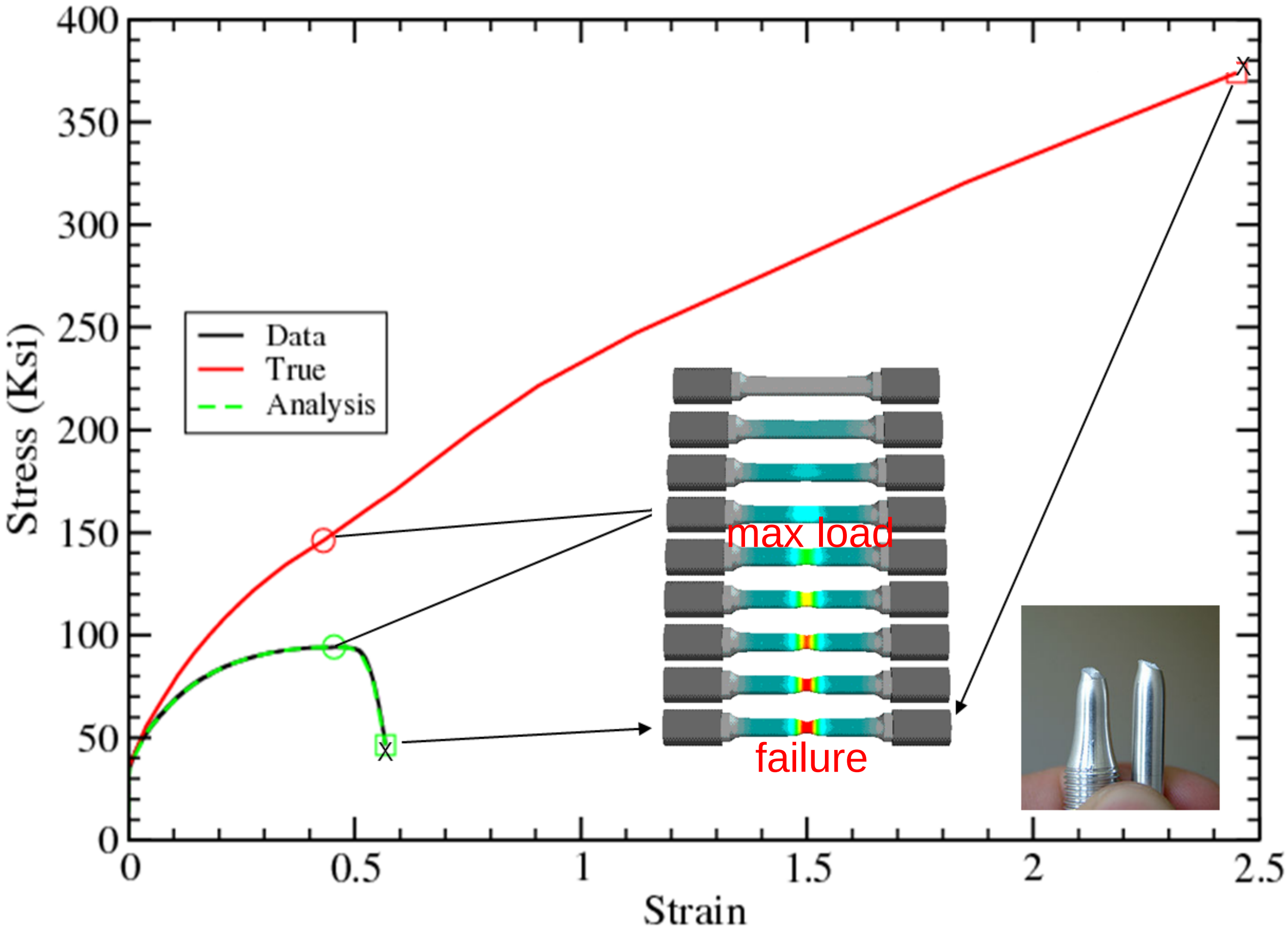
Quasi-Static Thermal-Elastic-Plastic Stainless Steel Constitutive Model



Solution Verification in Material Model Calibrations

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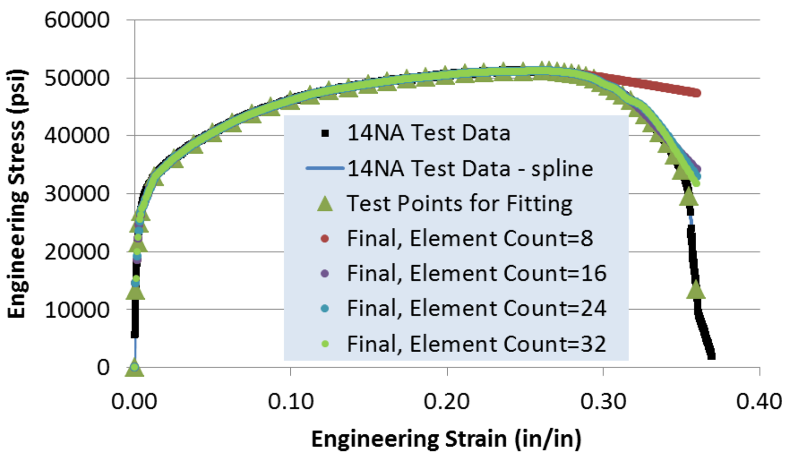
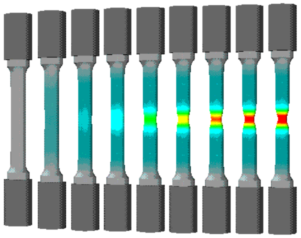
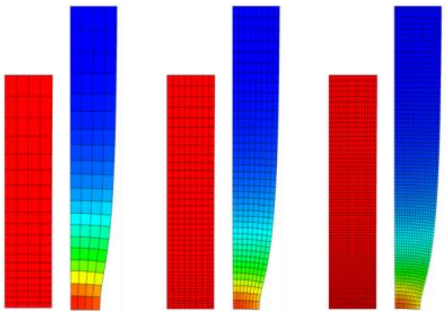
Negligible discretization sensitivity established for portion of material curves relevant in can-level calculations.

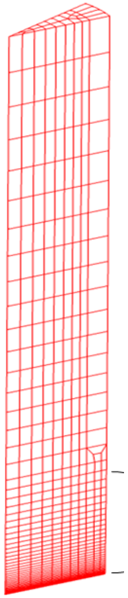
<u>Explored</u>:

- **Element type, size, & aspect ratios**
- **Solver parameters (including Hourglass treatment options)**





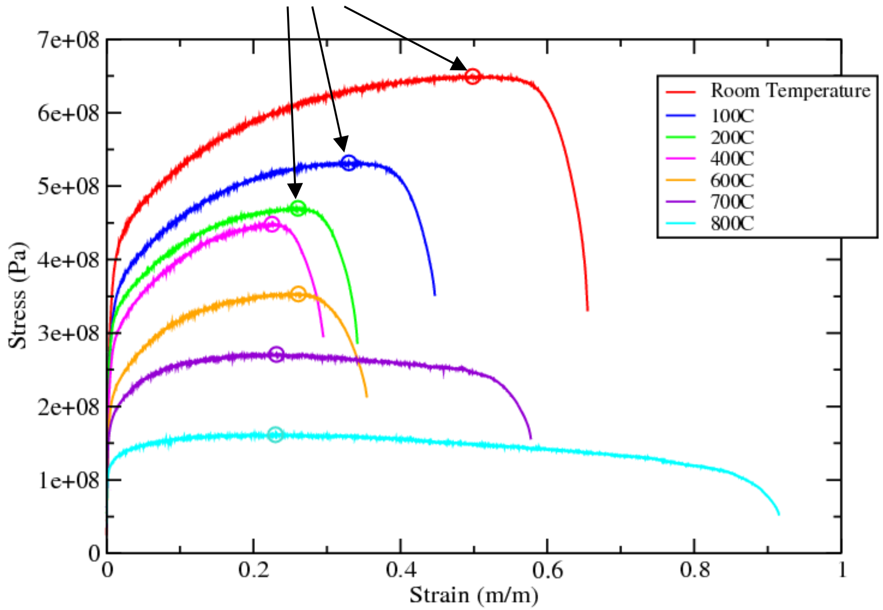




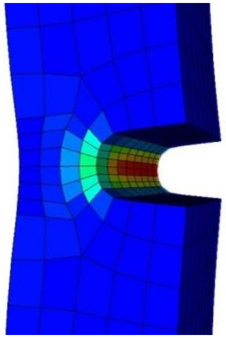
- Mesh independent up to max load (uniform stress/strain field)
- Very mesh sensitive past max load where necking occurs (strain-rates increase by orders of magnitude)
- Unable to get a converged solution for the last part of the data curve
- Tensile shape and material model form are incorrect past max load

Material Damage Metrics and Critical "Failure" Values for Welds

- Material damage Metrics:
  - Tearing Parameter (TP), tri-axial measure
  - Equivalent Plastic Strain (EQPS), uni-axial measure
- Critical failure levels are taken to be calculated values of TP, EQPS at <u>maximum load</u> points in round bar tension tests



- Failure said to occur when the first element in weld notch reaches critical TP and EQPS failure levels



UQ with Discrete Random Functions

Item 1: rank stress-strain (σ-ε) curve strengths for Wall, Lid, Weld materials

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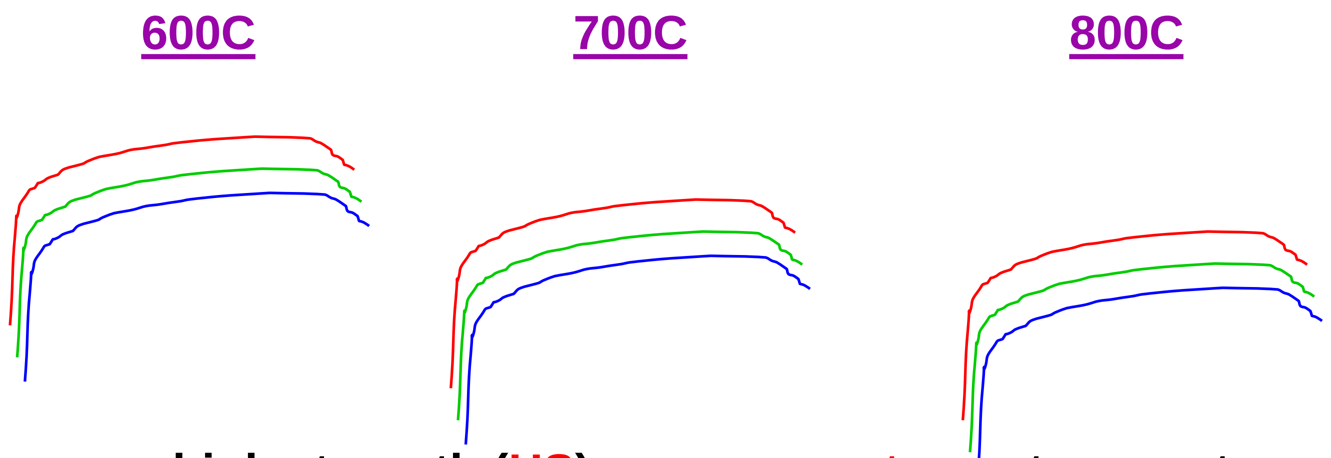
– ***For a given material type (wall, lid, weld):***

- *Rank the strengths of the multiple replicate σ-ε curves from the material tests at a given temperature by running isothermal can model with each σ-ε curve at that temperature.*
- *Down-select to 3 curves per temperature: highest strength, median strength, lowest strength, e.g.*



Red curves = high strength (HS) σ-ε curve set over temperatures

Green curves = medium strength (MS) set over temperatures

Blue curves = low strength (LS) set over temperatures

UQ with Discrete Random Functions

Item 2: strength-correlated interpolation across temperatures

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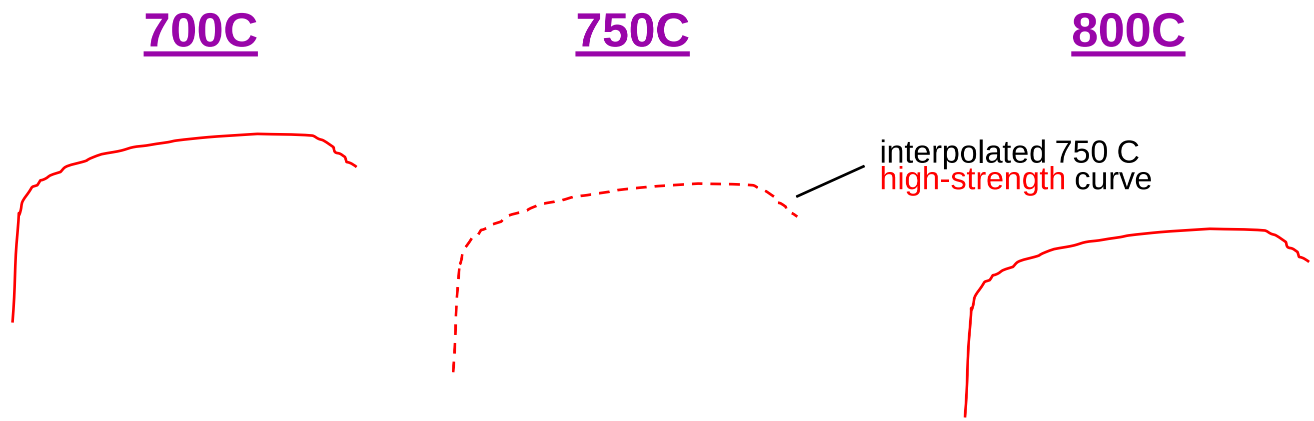
Make a physically reasonable assumption that is key for computational UQ feasibility:

Assume σ-ε curve strengths are strongly correlated over temperature, then linearly interpolate like-strength σ-ε curves and their TP, EQPS failure values across temperatures.

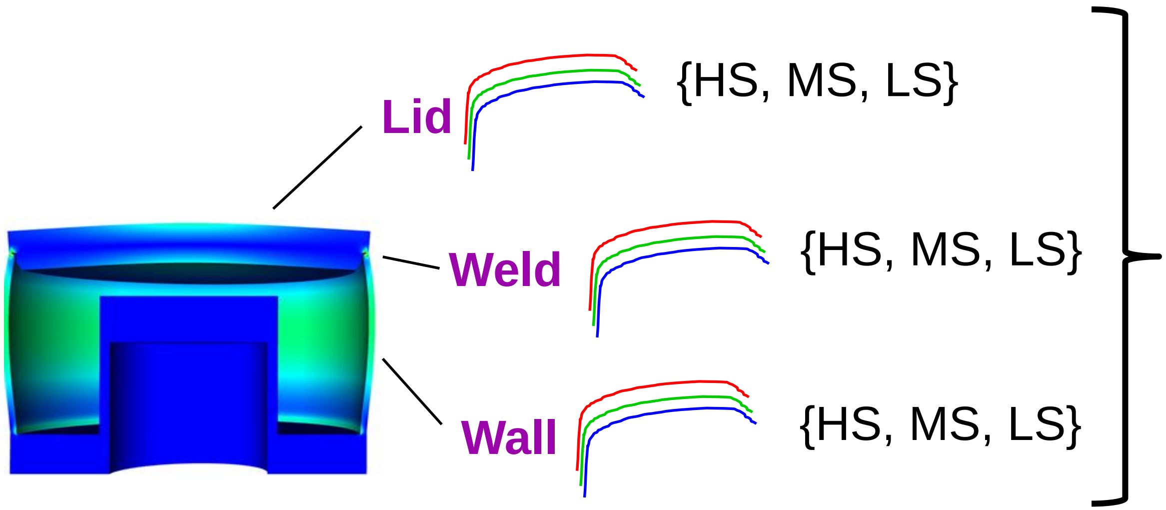
E.g., for high-strength curves at 700C, 800C:



Effectively gives high-strength, median-strength, and low-strength temperature-dependent material functions for each material.

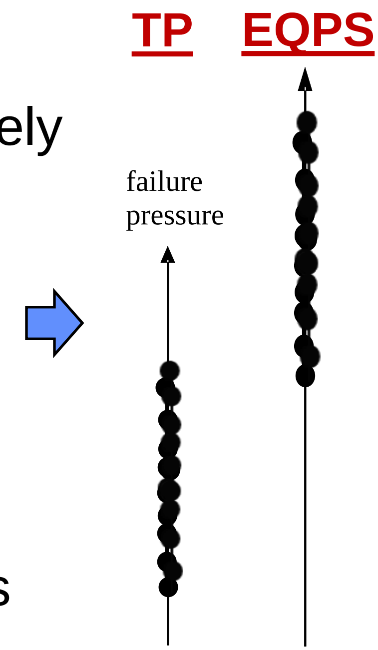
UQ with Discrete Random Functions

<u>Item 3</u>: propagation of material strength variability in Can simulations



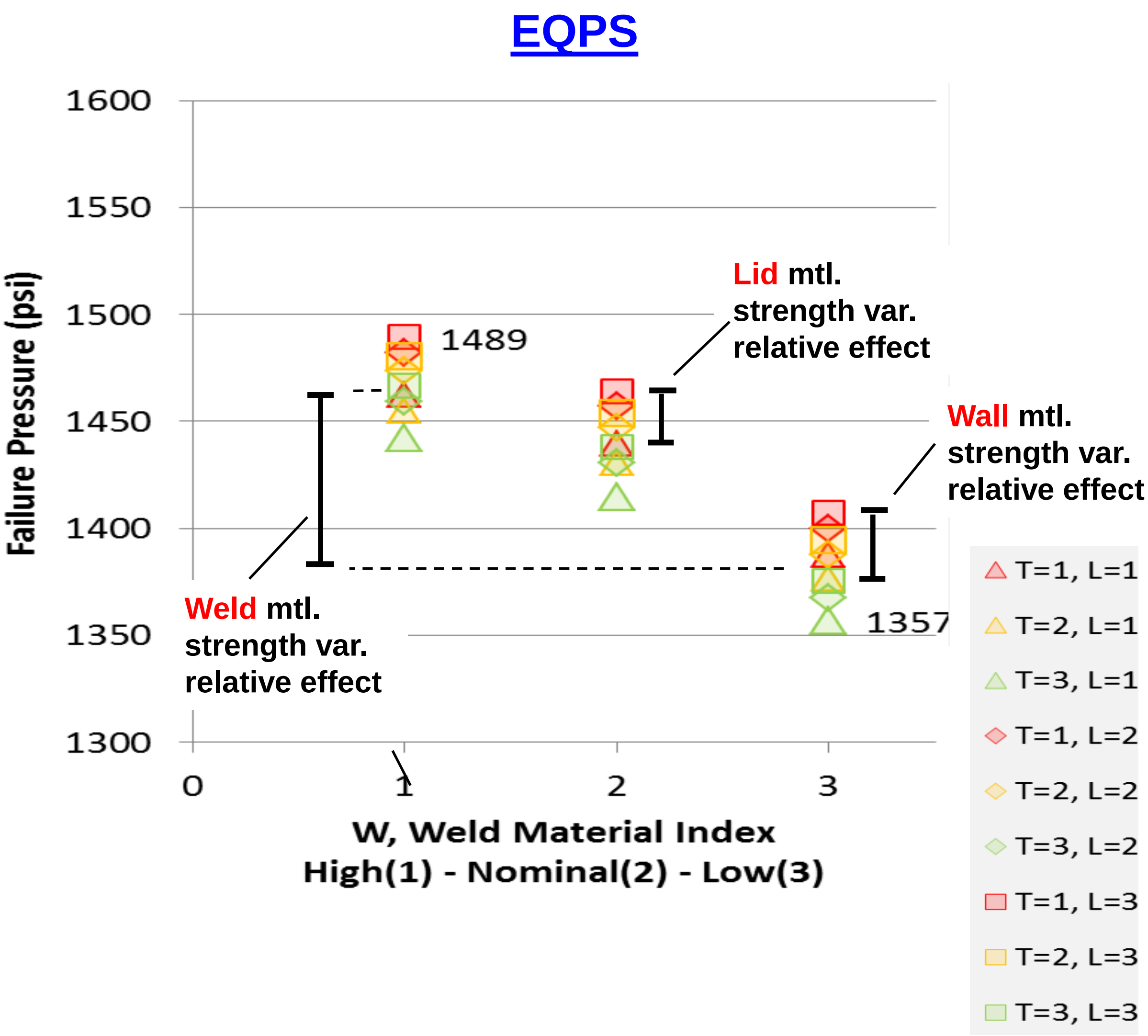
27 ~equally likely curve-strength combinations,

27 simulations with other uncertainties held at their nominal values



- ❑ Heating conditions of reference nominal Test #6 applied

Sensitivity of Predicted Failure Pressure to Material Strength Variations



Weld mtl. strength variations have largest effect as expected, but Lid and Wall strength variations also have significant effect – a global structural stress/deformation/ relaxation problem

- Similar sensitivities for failure pressures by Tear. Param.

Propagation of Other Traveling Aleatory Uncertainties and Aggregation with Material Strength Variability Effects

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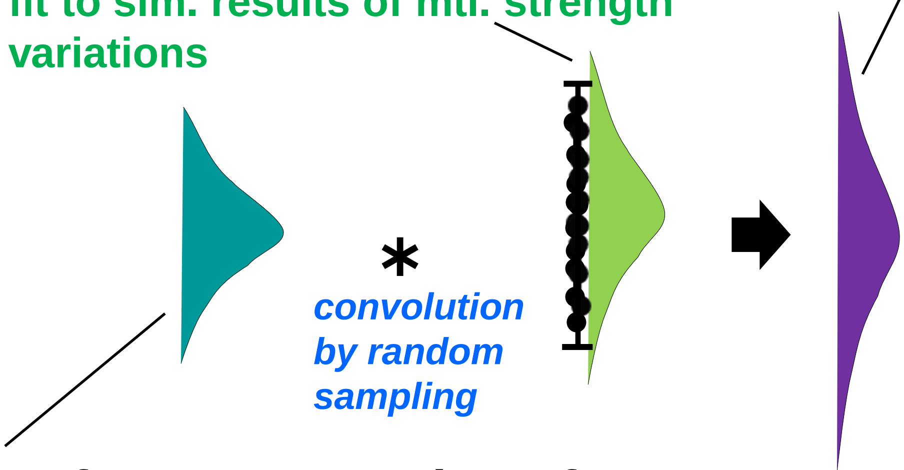
Equivalent Normal PDF from 0.95/0.90 Tolerance Interval fit to sim. results of mtl. strength variations

Net PDF of traveling Aleatory Uncertainty



variance decomposition (TP)

70% - material strength

23% - weld depth

6% - thermal contact

1% - wall thickness

variance decomposition (EQPS)

52% - material strength

41% - weld depth

6% - thermal contact

1% - wall thickness

PDF from propagation of 3 sources of random variability through 3D Linear-Quadratic Polynomial Surrogate Model

- Linear in wall thickness variations
- Linear in lid thermal contact variations
- Quadratic in weld depth variations

❑ All other uncertainties held at their nominal reference values and heating conditions for Test #6

“*Traveling*” and “*Non-Traveling*” Quantities in the Validation Assessment

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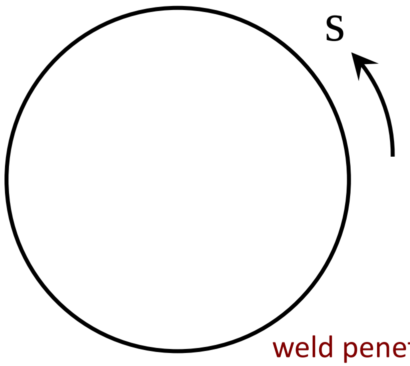
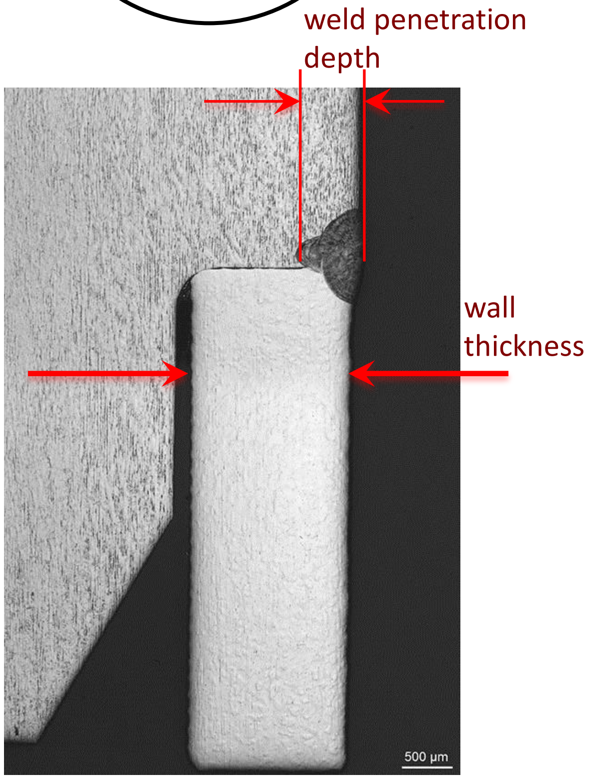
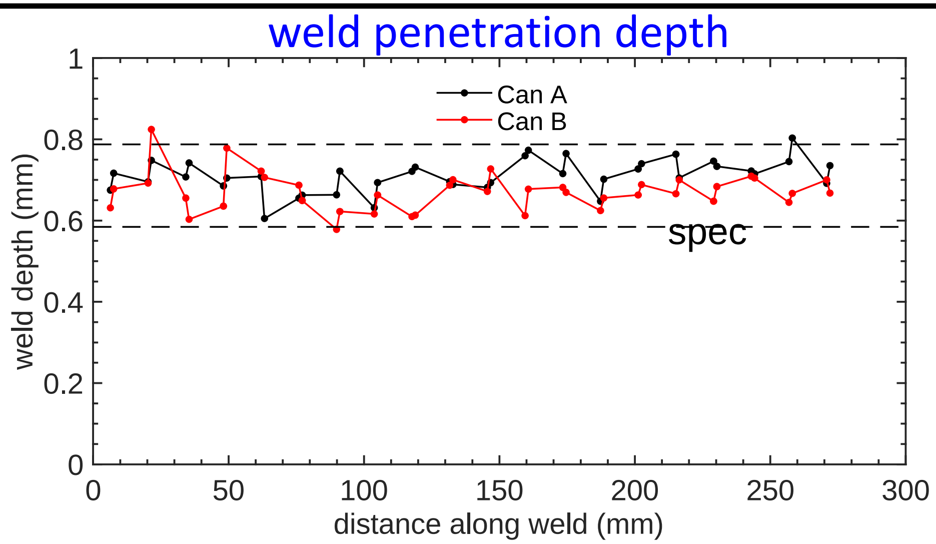
Traveling model quantities and their uncertainties are those proposed in the validation analysis to “travel” consistently to specified applications of interest beyond the validation study.

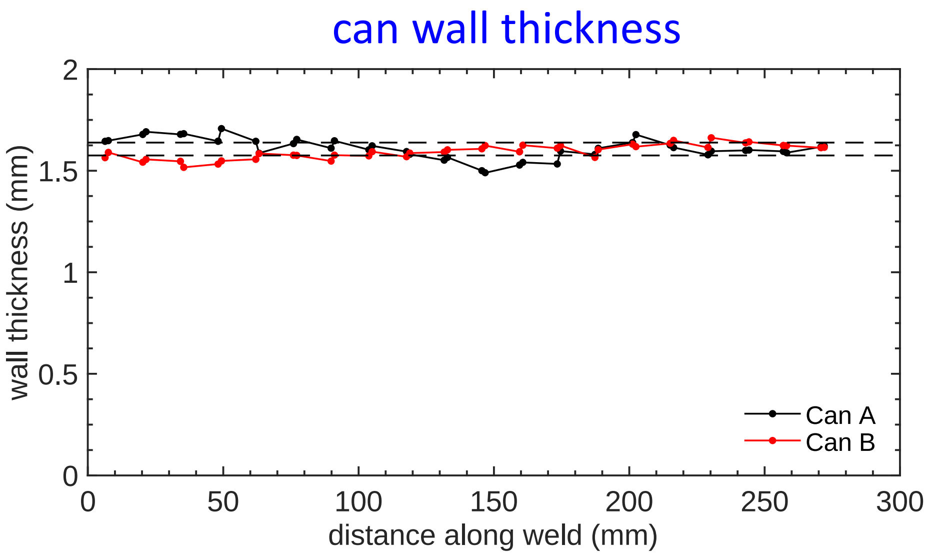
Non-Traveling quantities and uncertainties are deemed to be exclusive to the validation study and experiments—including some model quantities/uncertainties such as discretization error that do to not reasonably extrapolate consistently to the new application space.

Measured Variations of Weld Depth and Wall Thickness







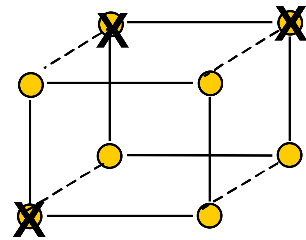


Propagation of Traveling Model's Epistemic Uncertainties

Model's Epistemic Uncertainties – all Interval

- ss304 conductivity: *f(temp.)* … [±20%]
- ss304 specific heat: *f(temp.)* …[±20%]
- foam conductivity: *f(temp.)* … [±20%]
- foam specific heat: *f(temp.)* … [±20%]
- foam activation energy: value…[±4%]
- foam pressure multiplier … [0.5, 2.64]

6D Staged Mixed-Order Polynomial Surrogate Model



Linear terms in all 6 factors

Linear sens. analysis →

go higher-order in dominant 3 factors— Quadratic main-effects terms

quadratic main effects identify best corners to sample for interactn. effects →

quadratic interaction terms in dominant 3 factors

f(x1,..,x6) = c0 + c1*x1 + c2*x2 + c3*x3 + c4*x4 + c5*x5 + c6*x6 + c1,1*x1*x1 + c3,3*x3*x3 + c6,6*x6*x6 + c1,3*x1*x3 + c1,6*x1*x6 + c3,6*x3*x6

row	Const	x1	x2	x3	x4	x5	x6	x1^2	x3^2	x6^2	x1*x3	x1*x6	x3*x6		coeffs. {c}		True Y
1	1	0	0	0	0	0	0	0	0	0	0	0	0		962.4044		974.94
2	1	0.2	0	0	0	0	0	0.04	0	0	0	0	0		-77.2912		959.64
3	1	0	0.2	0	0	0	0	0	0	0	0	0	0		64.5844		975.32
4	1	0	0	0.2	0	0	0	0	0.04	0	0	0	0		-67.7611		964.34
5	1	0	0	0	0.2	0	0	0	0	0	0	0	0		70.2356		976.45
6	1	0	0	0	0	0.04	0	0	0	0	0	0	0		271.5542		973.27
7	1	0	0	0	0	0	1.64	0	0	2.6896	0	0	0		27.7711		1069.43
8	1	-0.2	0	0	0	0	0	0.04	0	0	0	0	0		446.7097		994.64
9	1	0	0	-0.2	0	0	0	0	0.04	0	0	0	0		414.3498		987.36
10	1	0	0	0	0	0	-0.5	0	0	0.25	0	0	0		24.0210		951.39
11	1	-0.2	0	0.2	0	0	1.64	0.04	0.04	2.6896	-0.04	-0.328	0.328		2454.5500		933.00
12	1	0.2	0	-0.2	0	0	-0.5	0.04	0.04	0.25	0.04	-0.1	0.1		115.9472		1064.35
13	1	0.2	0	-0.2	0	0	1.64	0.04	0.04	2.6896	-0.04	0.328	-0.328		-124.3182		1087.76

Net Aleatory and Epistemic Uncertainties in Predicted Failure Pressure (Mesh 4)

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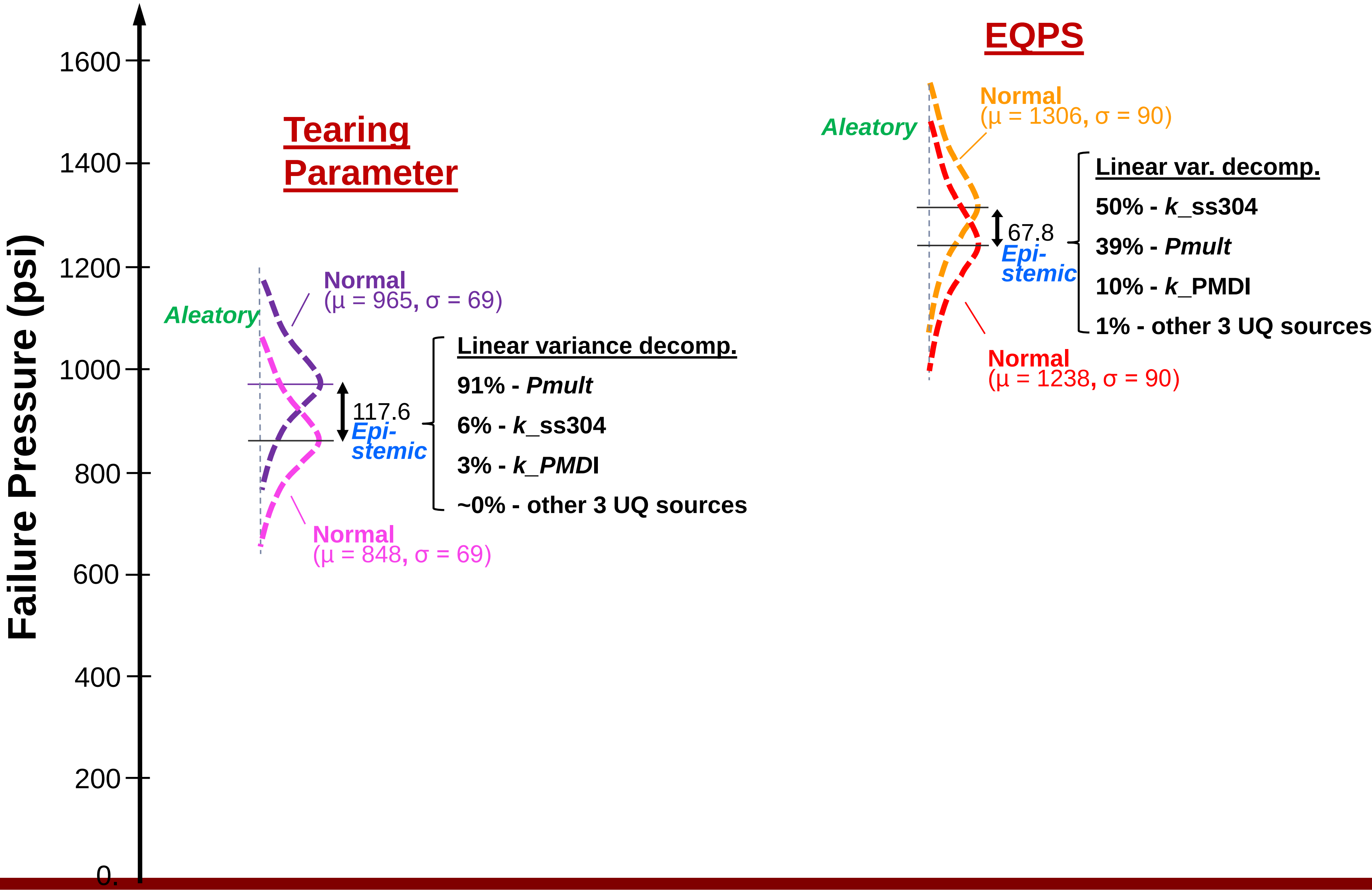

Traveling and Non-Traveling Uncertainties in Thermo-Mechanical validation problem

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Non-Traveling Uncertainties

Experimental Aleatory

- lid TC measurement/redundancy test-test variations: I[±2%]
- ss304 emissivity can-can variations: I[±0.03]
- ambient temperature test-test variations I[±10C]
- pressure measurement/redundancy test-test variations: I[±2%]

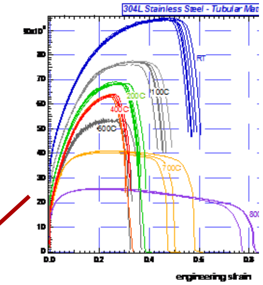
Experimental Epistemic

- ss304 emissivity effective value over time, space: 0.69 + I[±20%]
- effective temperature for radiative, convective losses: 29C + I[±15C]
- convection coeff. effective value over time, space: 10W/m^2-K + I[±40%]

Model Epistemic

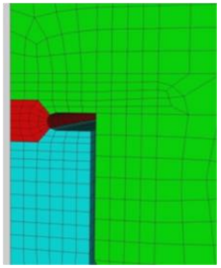
- mesh size error
- solver error

Traveling Uncertainties



Model Aleatory

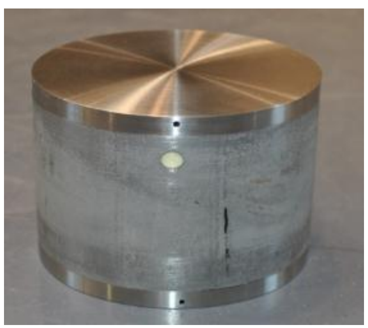
- material stress-strain curves for lid, weld, & wall
- lid thermal contact: I[20%, 90%] of distance between modeled extremes of no heat transfer and perfect-contact heat transfer
- wall thickness: I[0.062,0.0645]in.
- weld depth: I[0.023, 0.031]in. (next slide shows measured values)

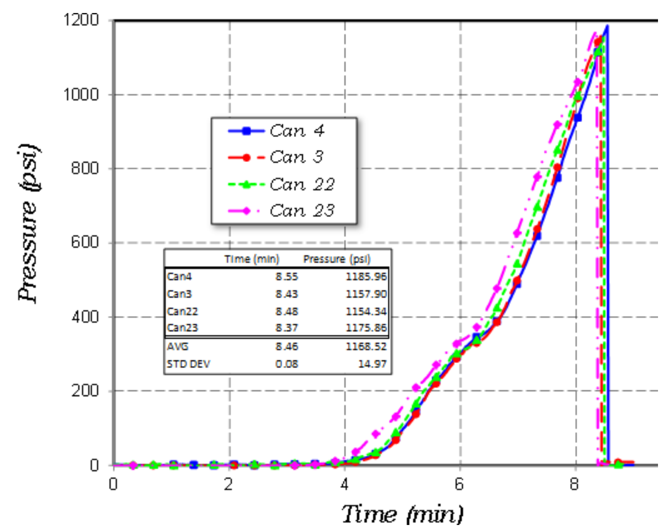


Model Epistemic

- foam conductivity: *f(temp.)* + I[±20%]
- foam specific heat: *f(temp.)* + I[±20%]
- foam activation energy: value + I[±4%]
- foam pressure multiplier: I[0.5, 2.64]
- ss304 conductivity: *f(temp.)* + I[±20%]
- ss304 specific heat: *f(temp.)* + I[±20%]

Processing of Experimental Failure Pressures





	Time (min)	Pressure (psi)
Can4	8.55	1185.96
Can3	8.43	1157.90
Can22	8.48	1154.34
Can23	8.37	1175.86
AVG	8.46	1168.52
STD DEV	0.08	14.97

Spreadsheet Processing of Experimental Results & Uncertainties

- *Normalize experimental results to the same reference input conditions for "Apples-to-Apples" comparisons*

- **Account for sparse data (small # of replicate tests)**

- **Normalize for:**
  - **known (measured) variations in experimental inputs among tests**
  - **random and systematic measurement/ estimation uncertainties of experimental inputs & outputs (account for uncertain correlated and uncorrelated errors across replicate tests)**

Systematic uncertainties; correlated across the 5 replicate experiments

Random; uncorrelated across experiments

	A	B	C	D	E	F	G	H	I	J
1										
2		RAND# =	6734							
3										
4			realization	v1sys = ΔemisMult = Unif[-0.2, 0.2]	v2sys = ΔconvCoeffMult = Unif[-0.4, 0.4]	v3sys = ΔTambMult = Unif[-0.03, 0.03	v4sys = ΔTlidTCmult = Unif[-0.003, 0.]	v3ind = ΔTambMult = Unif[-0.02, 0.02	v4ind = ΔTlidTCmult = Unif[-0.01, 0.01]	v5ind = ΔmeasPres = Unif[-10, 10]psi
5	RNGseeds	->		5301	4105	6999	9724	7490	52	4485
6			1	0.011786	-0.07179	0.011921	-8.9E-05	0.009904	-0.00987	-1.03732
7			2	-0.18207	0.190814	-0.02911	-0.00043	-0.01718	-0.00415	-2.313
8			3	0.040376	0.060903	-0.0119	-0.00032	0.019232	0.009941	4.824061
9			4	0.1541	0.078237	0.019105	-0.0002	-0.00455	-0.00478	3.046663
10002			9997	0.118528	0.117203	0.012582	-0.00156	0.004796	-0.00029	-2.00415
10003			9998	0.132505	-0.21164	0.009023	-0.00195	-0.00206	0.006737	-6.05335
10004			9999	0.107163	0.179485	0.028414	-0.00137	-0.01185	0.008592	-0.78829
10005			10000	0.177795	-0.02533	-0.01103	-3.6E-05	0.004812	-0.00551	0.653401
10006										
10007										
10008	stats		mean =	0.0011	0.0005	0.0001	-0.0015	-0.0001	0.0000	-0.0317
10009	from		max =	0.2000	0.3999	0.0300	0.0000	0.0200	0.0100	9.9969
10010	10000		min =	-0.2000	-0.4000	-0.0300	-0.0030	-0.0200	-0.0100	-9.9988
10011	samples		stdev =	0.1156	0.2323	0.0173	0.0009	0.0115	0.0058	5.7716
10012										

Linear-Quadratic Mixed-Order Polynomial surrogate for these MC samples of pressure meas. and experimental boundary conditn. uncertainties

UQ Rollup for Experiments

Uncertainty of 0.025 & 0.975 percentiles of Failure Pressure

- these %iles combine uncertainties in both mean & variance of response

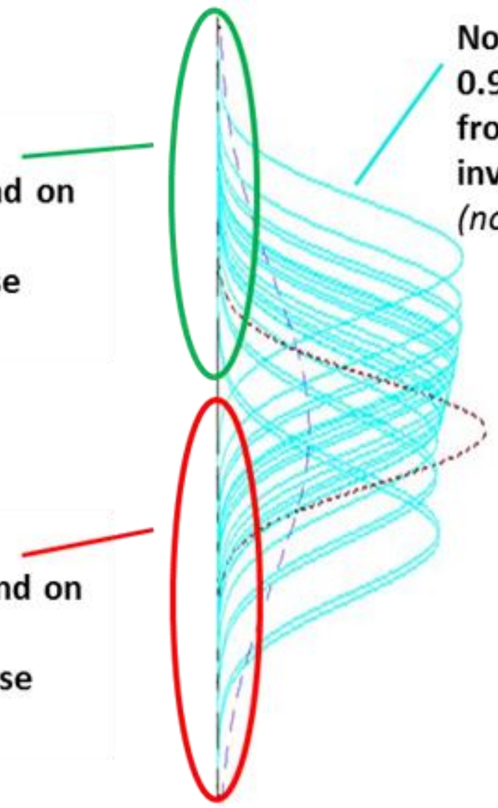
assoc. w/ experimental factors in the tests:
- *differing test conditions*
- *uncertainties in measurement and estimation of test conditions, responses, and normalization quantities*

assoc. w/ # of tests

assoc. w/ response variability attributed to stochastic elements/behaviors in the systems tested

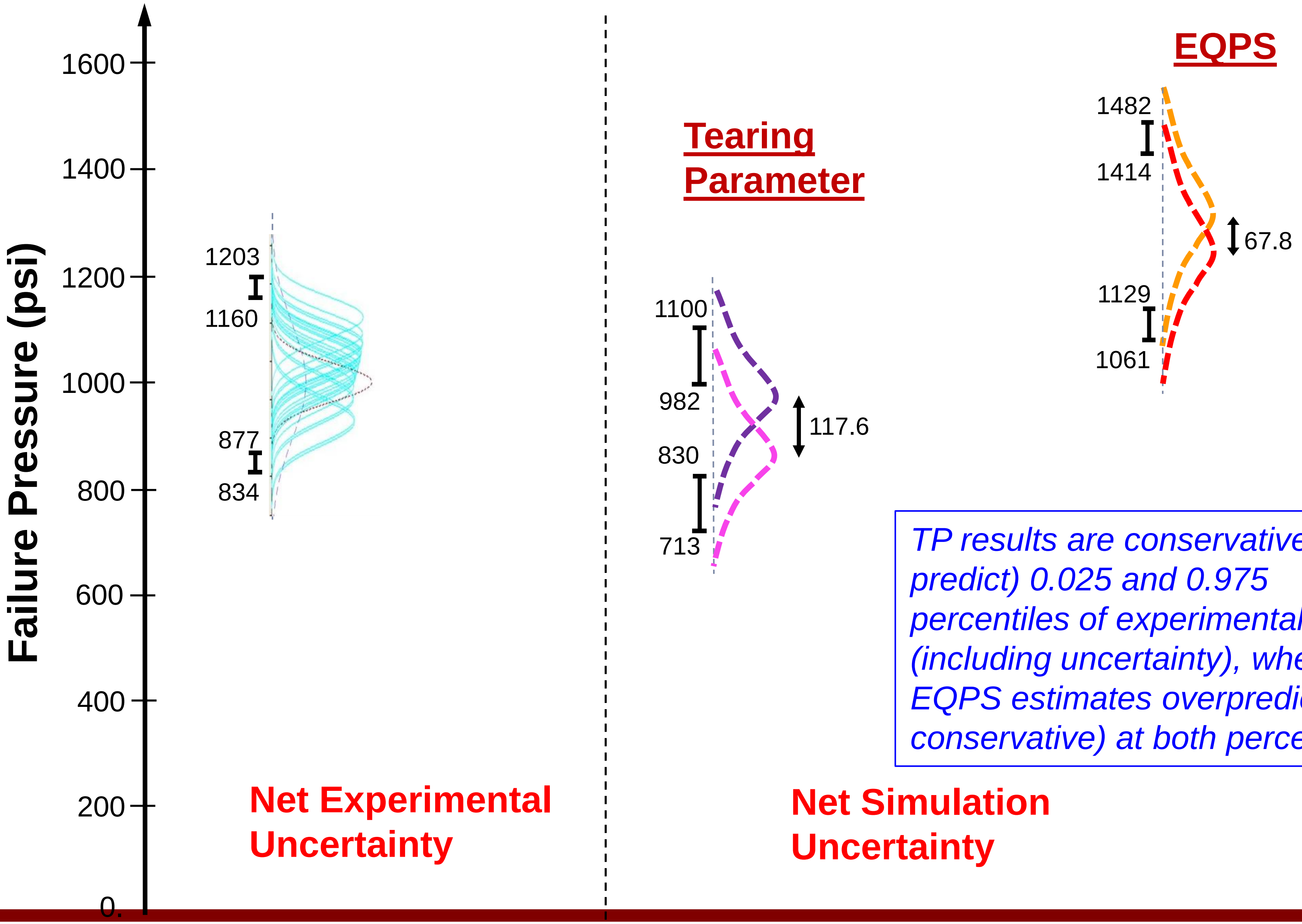
Uncertainty of 90% conf. upper bound on 0.975 percentile of experimental response *(failure pressure)*

Uncertainty of 90% conf. lower bound on 0.025 percentile of experimental response *(failure pressure)*



Normal PDFs fit to 0.95/0.90 Tolerance Intervals from Small # of Tests involving uncertainty *(notional PDFs for illustration)*

Validation Comparisons of 0.025 and 0.975 Percentiles of Failure Pressure (Mesh 4)

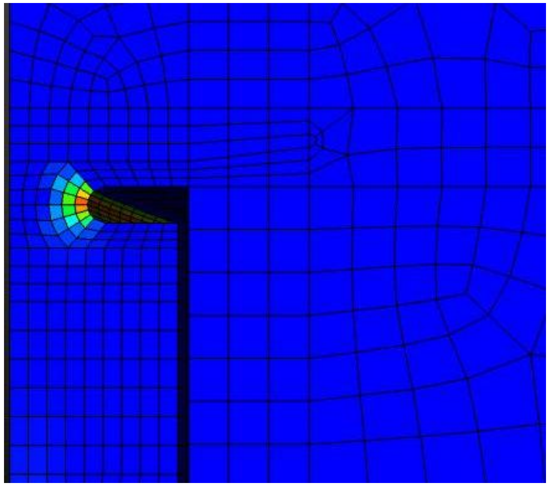


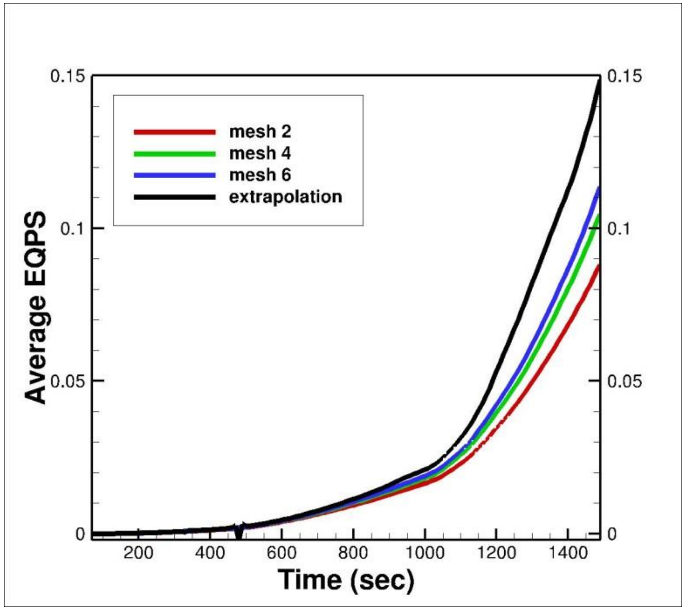
TP results are conservative (under-predict) 0.025 and 0.975 percentiles of experimental data (including uncertainty), whereas EQPS estimates overpredict (non-conservative) at both percentiles

Solution Verification assessment of Discretization Effects

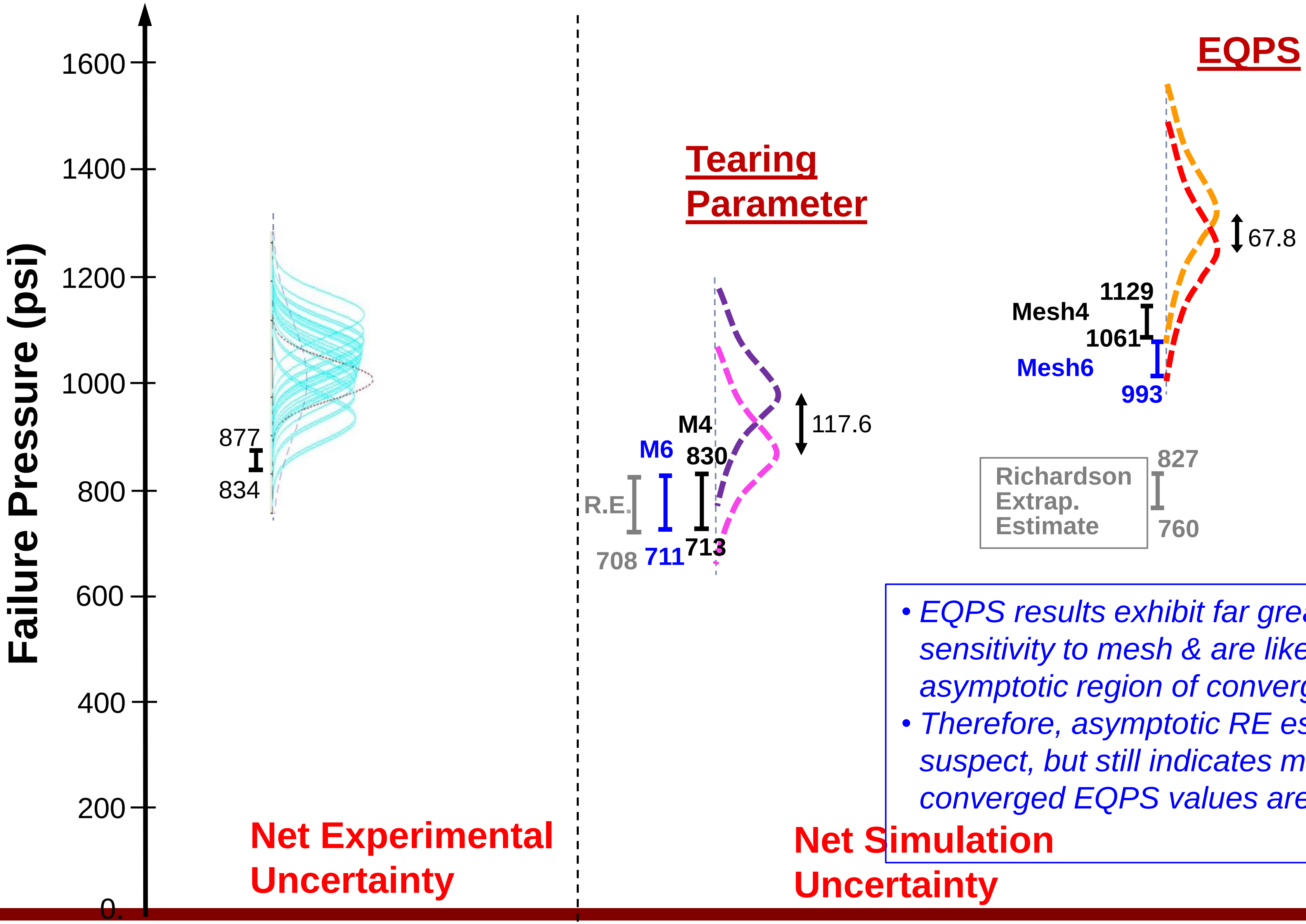
Mechanical Deformation and Breach

- Load Step (10.0, 1.0, 0.1)
  - Solver tolerances were set to small values, 1.0e-06
- Element Size: 6 meshes – ¼ symmetry geometry
  - Mesh 1 = 370,440; Weld block = 6,048 (6x6)
  - Mesh 2 = 694,936; Weld block = 10,752 (8x8)
  - Mesh 3 = 1,190,721; Weld block = 16,800 (10x10)
  - Mesh 4 = 1,850,944; Weld block = 24,192 (12x12)
  - Mesh 5 = 2,639,996; Weld block = 32,928 (14x14)
  - Mesh 6 = 3,684,285; Weld block = 43,008 (16x16)
- Element Type
  - Mean-Quadrature (MQ) Element - Uniform Gradient with Total Hourglass Formulation
  - Selective Deviatoric (SD) Element - Fully Integrated Gradient, Hourglass control isn't required





Mesh Effects on Validation Comparisons of 0.025 Percentile of Failure Pressure



- *EQPS results exhibit far greater sensitivity to mesh & are likely outside asymptotic region of convergence*
- *Therefore, asymptotic RE estimate is suspect, but still indicates mesh-converged EQPS values are closer to TP values.*

Closing Remarks

- **Many types and sources of uncertainty exist in model V&V and UQ, several illustrated in this talk**
- **"Real Space" Validation metrics were presented that:**
  - separate aleatory and epistemic uncertainties
  - are relatively straightforward to interpret
  - are especially relevant for assessing models/quantities to be used in the analysis of performance and safety margins (QMU)
- **The Real Space validation methodology presented is versatile and practical, geared for:**
  - Very expensive computational models (minimal # of simulations)
  - Sparse experimental data
  - Multiple replicate experiments
  - Stochastic phenomena and models
  - Rollup of various types, sources, and representations of uncertainty