SAND2017-0908C

Chapter 11: Application of UQ and V&V to Experiments and Simulations of Heated Pipes Pressurized to Failure

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MSS Special Session on Release of JANNAF Volume:
Simulation Credibility—Advances in V&V and UQ

JANNAF Meeting, Dec. 7, 2016, Phoenix, AZ

National Nuclear Security Administration

VERIFICATION VALIDATION™

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Elements of this VVUQ Case Study

- Material-strength experimental characterization and associated constitutive-model calibration
- Model-assisted design and analysis of validation experiments to characterize and reduce uncertainty
- Mesh and solver discretization studies (simulation verification) to control and characterize solution error and uncertainty
- Model validation comparison of experimental and simulation results with uncertainties and interpretation of the results

Challenging/Advanced VVUQ Aspects of this Application Problem

- **Material variability is characterized by discrete random functions (**temperature dependent stress-strain curves**)**
- **Very limited (sparse) experimental data**
  - at material testing/characterization level
  - at pipe-test validation level
- **Boundary condition reconstruction uncertainties from spatially sparse sensor data**
- **Normalization of pipe experimental responses for:**
  - measured input-condition differences among multiple replicate tests
  - random and systematic uncertainties in measurements and processing of experimental inputs & outputs
- **Very high computational cost → very limited # of model runs for UQ, and significant discretization errors/ uncertainties to manage, quantify, and account for**

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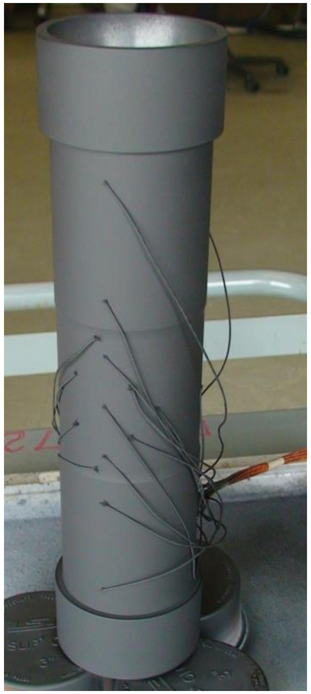
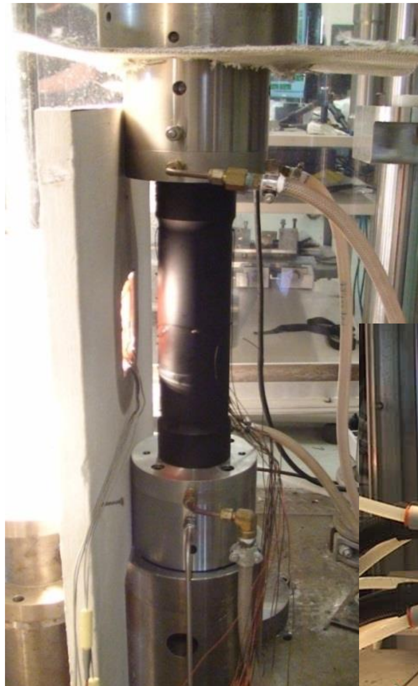
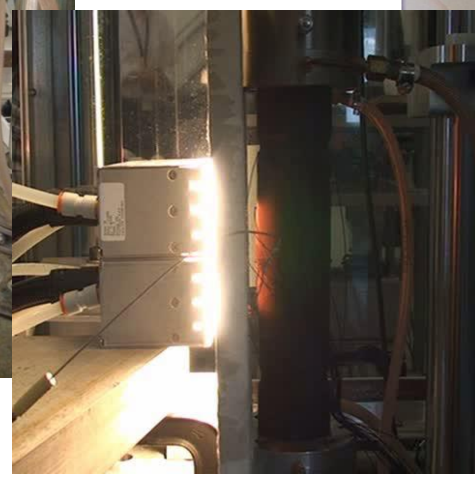
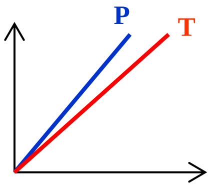
“Pipe Bomb” Validation Experiments

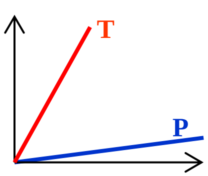


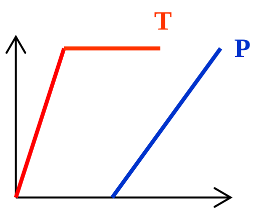




Ramp temperature and pressure independently to failure





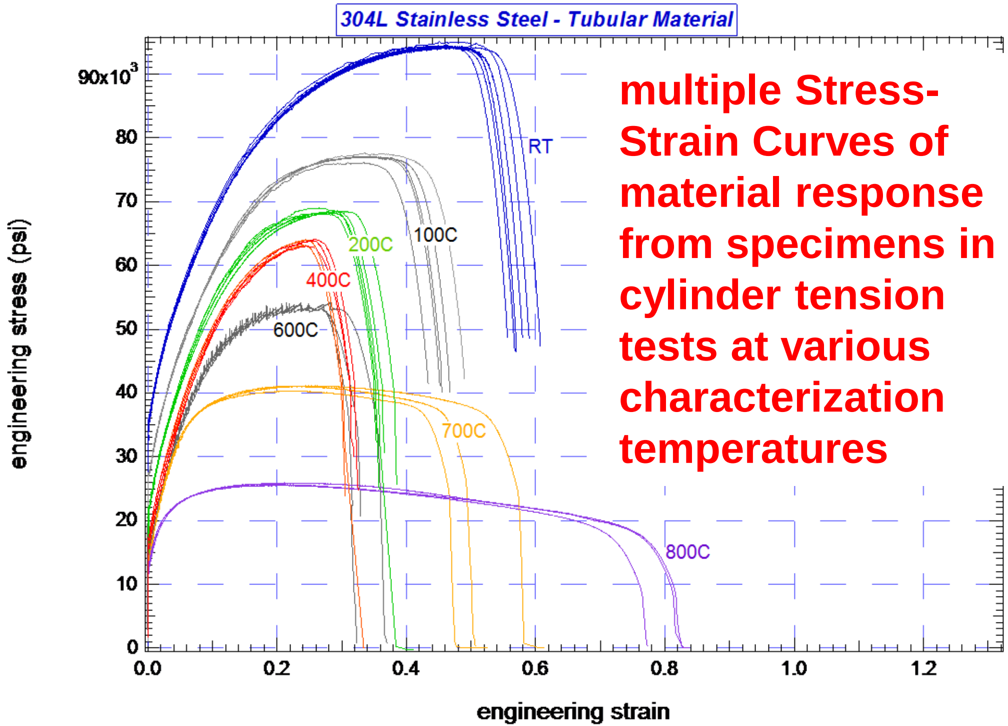


Material Characterization:

Aleatory and Epistemic uncertainties from Sparse samples of Discrete Random Functions

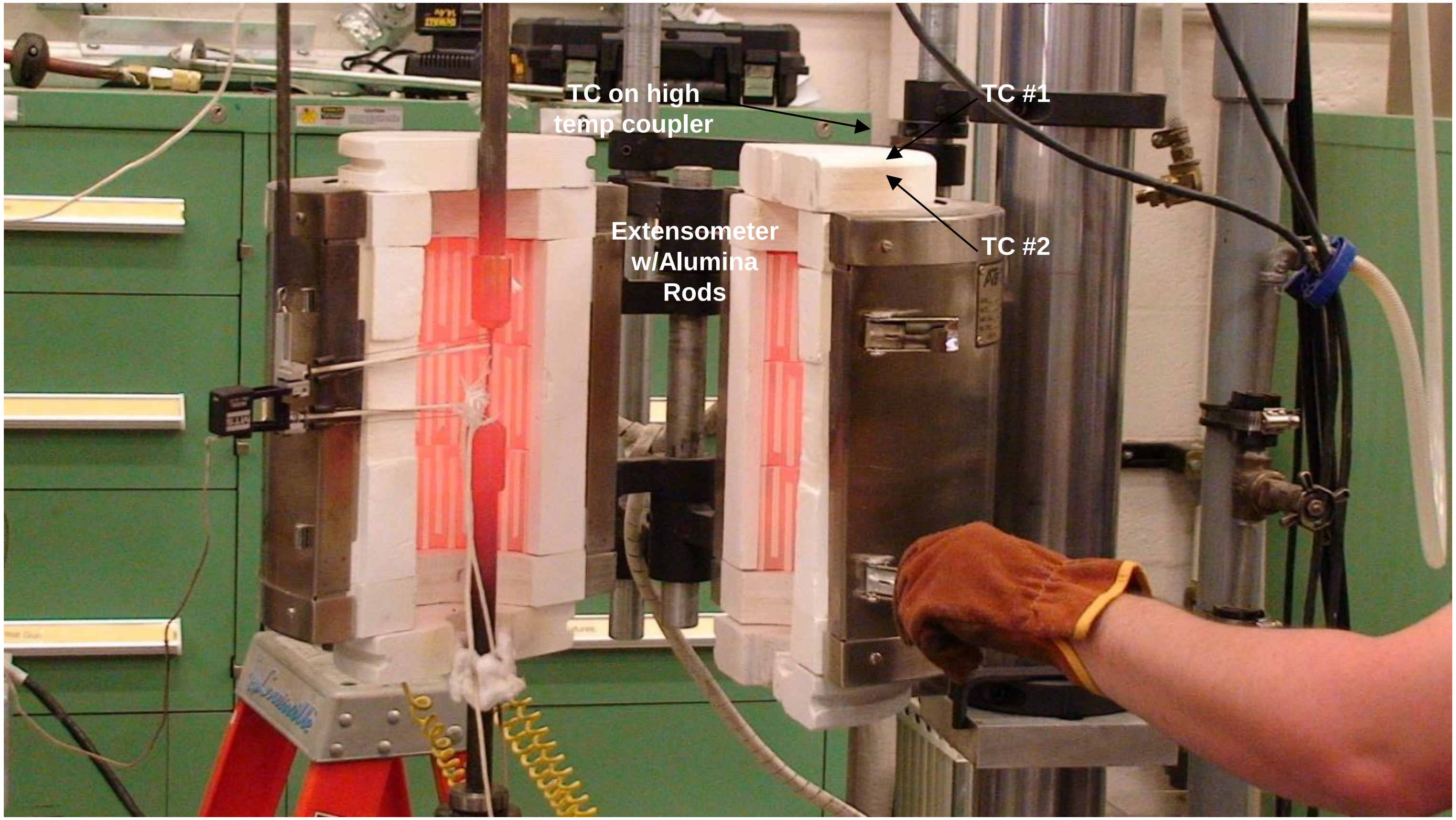
- **Example: multiple Stress-Strain Curves of material variability in calibration of constitutive model**
- **Similar issues in e.g. electonics modeling – calibration to experimental response curves of electronics yields discrete parameter sets considered non-interpolable in-between.**

cylinder Tension-test specimens



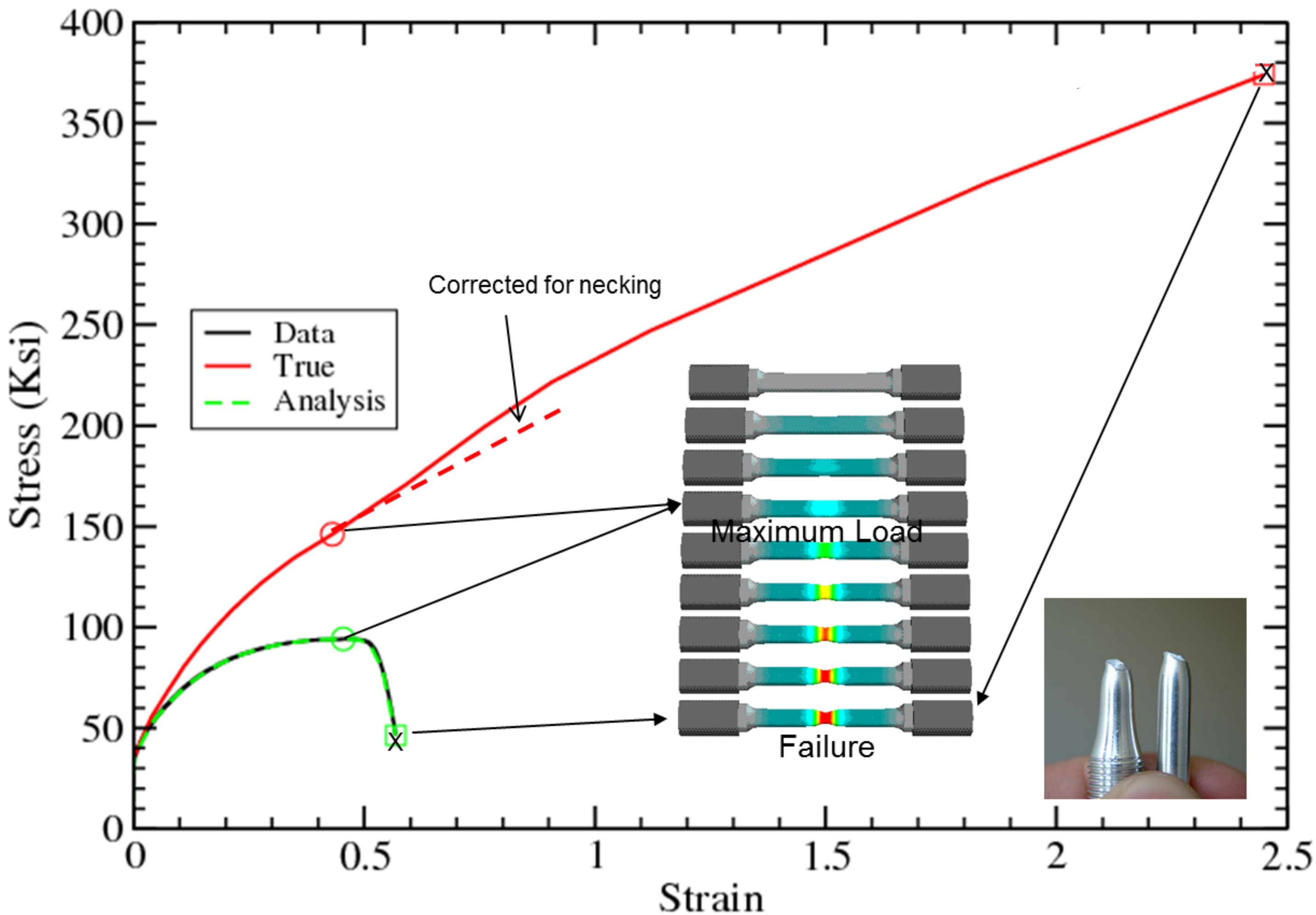
multiple Stress-Strain Curves of material response from specimens in cylinder tension tests at various characterization temperatures

Cylinder Material Specimen Tension Test at 800C

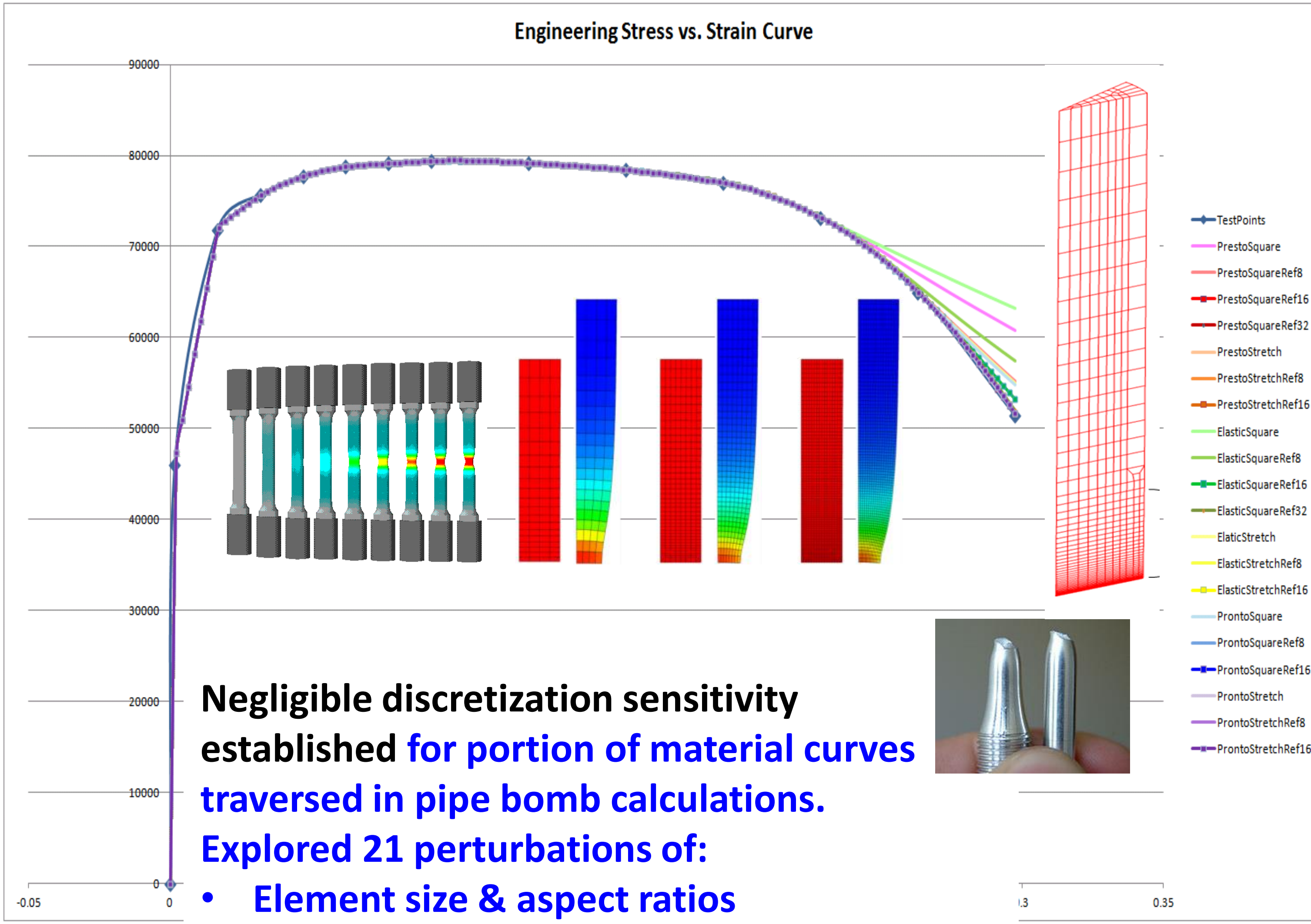


Inversion Procedure to extract Cauchy-Stress/Logarithmic-Strain from Experimental Stress-Strain Curves

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



Mesh and Solver Effects
in modeled necking/failure in material characterization tests



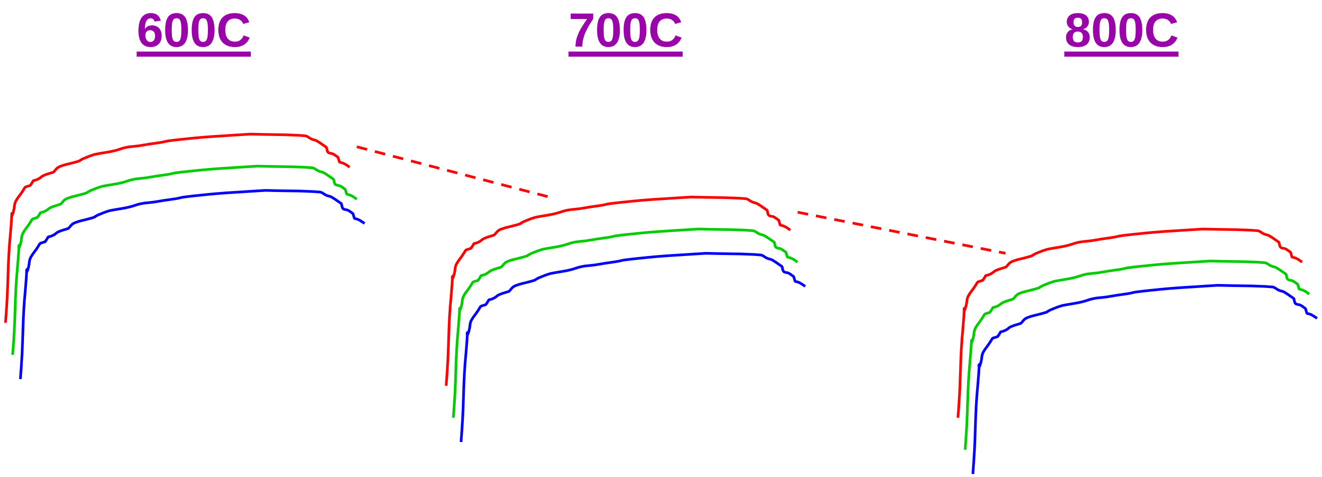
Negligible discretization sensitivity established for portion of material curves traversed in pipe bomb calculations.

Explored 21 perturbations of:

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

Correlation of Like-Ranked S-S Curves across Characterization Temperatures

- Assume material strength (as indicated by model-predicted failure pressure) is strongly correlated across temperatures
- Enables interpolation to other temperatures for spatial and/or temporal variations of material temperatures



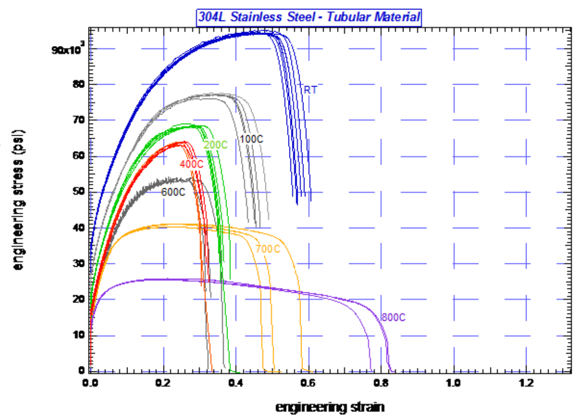
Red curves = high strength (HS) σ-ε curve set over temperatures

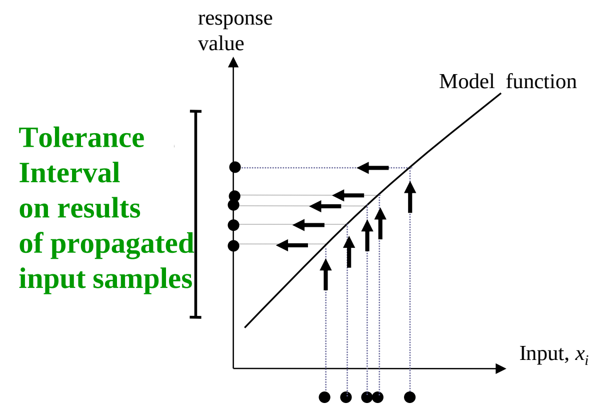
Green curves = medium strength (MS) set over temperatures

Blue curves = low strength (LS) set over temperatures

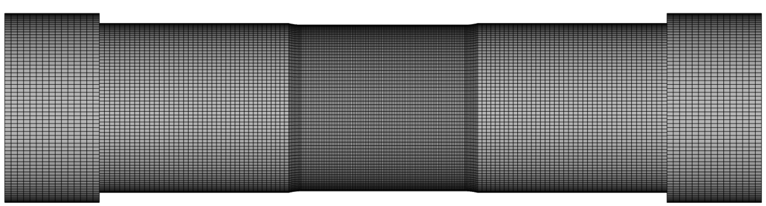
Predicted Variability of Failure Pressures due to Variability of Material Stress-Strain Curves

- Model is run for the individual Stress-Strain Curves at a test temperature
- 0.9/0.95 Tolerance Intervals are formed on the set of calculated failure pressures at that temperature

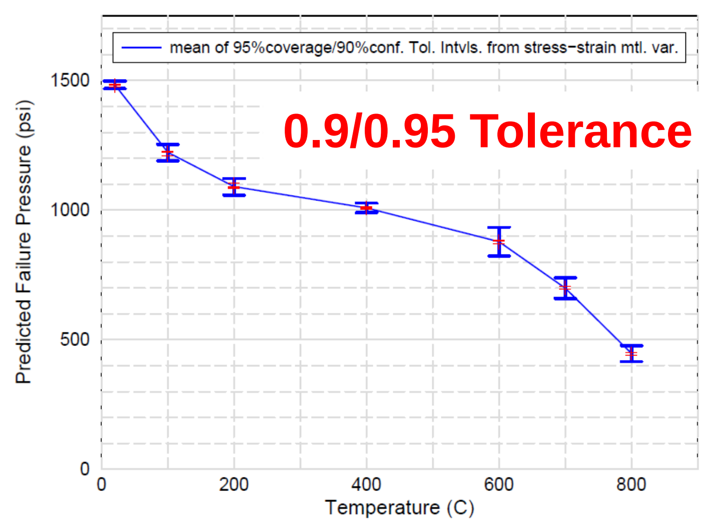




Propagate realizations of input variability, then form Tol Intvl. on realizations of response



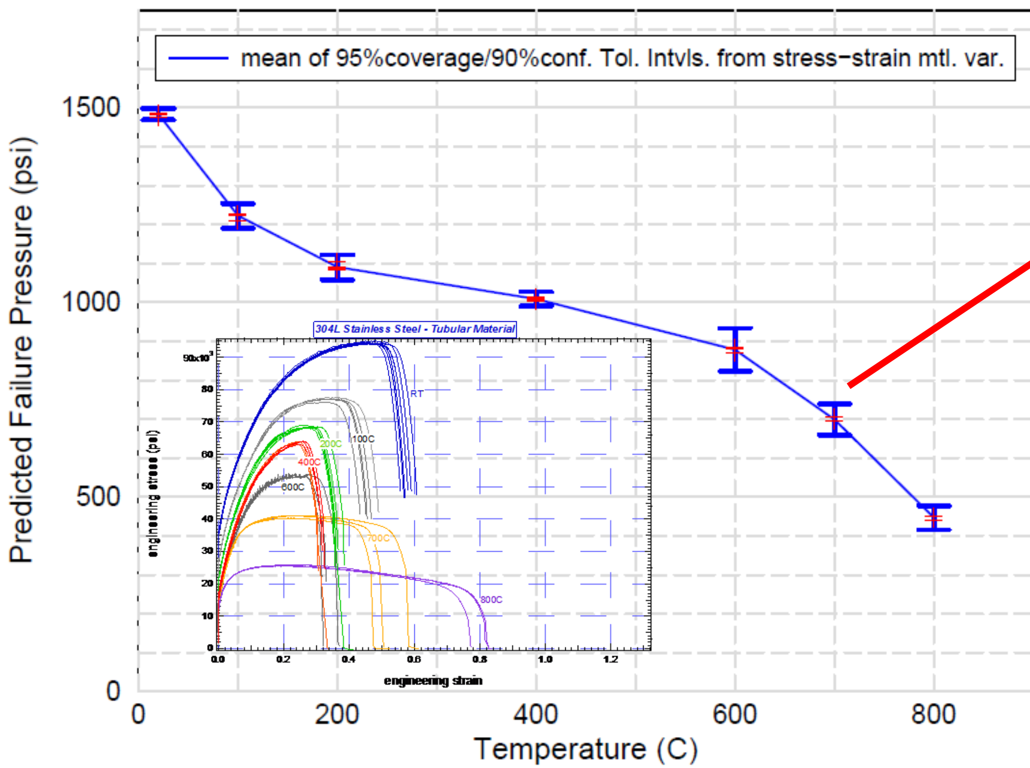
Pressure ramped uniform-temperature HEX finite element model of quasi-static solid mechanics

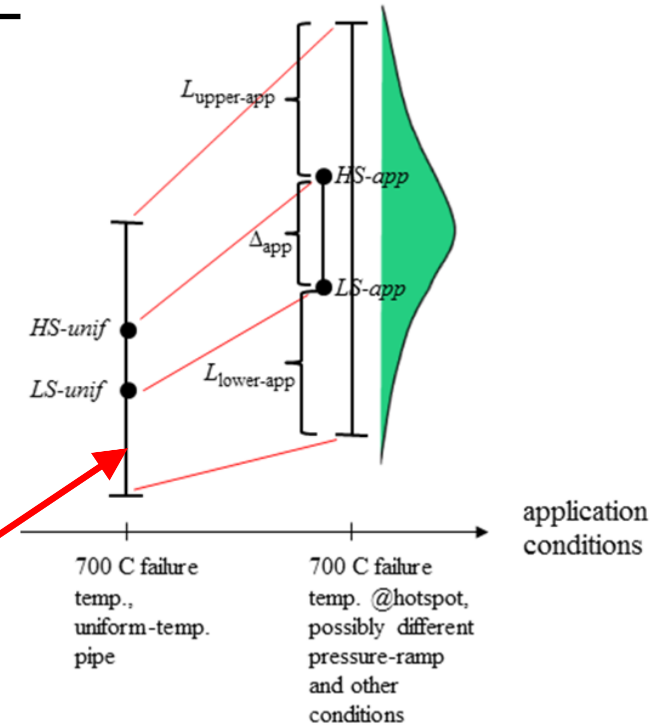


0.9/0.95 Tolerance Intervals

Economical Parameterization of TIs by High & Low Strength Material Curves

- **Tolerance Intervals are constructed from multiple stress-strain curves**
- **But TIs can be parameterized by 2 s-s curves for only 2 Val./UQ sims. w/ full-geom. model**





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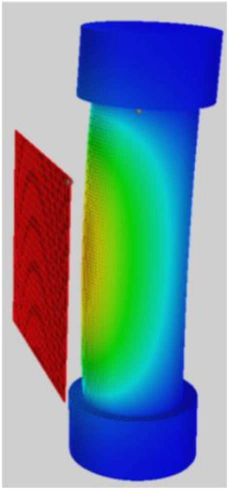
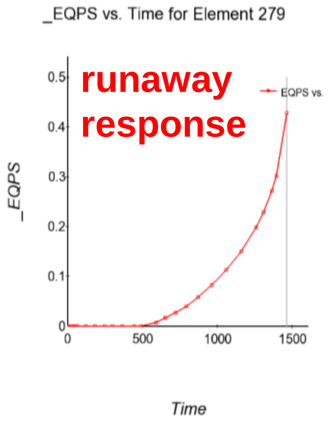
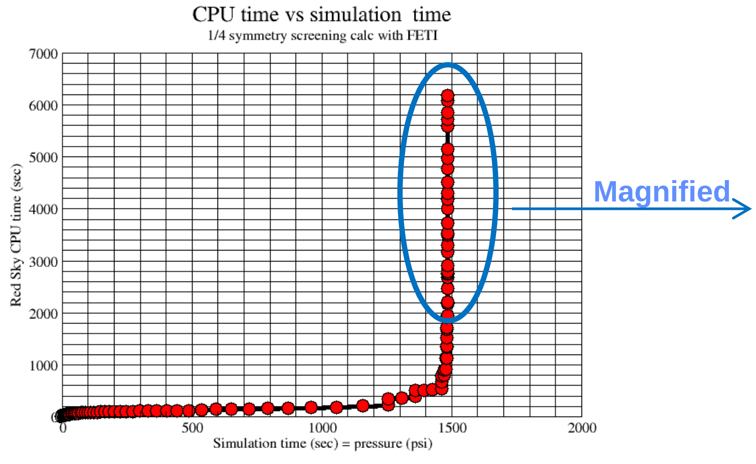
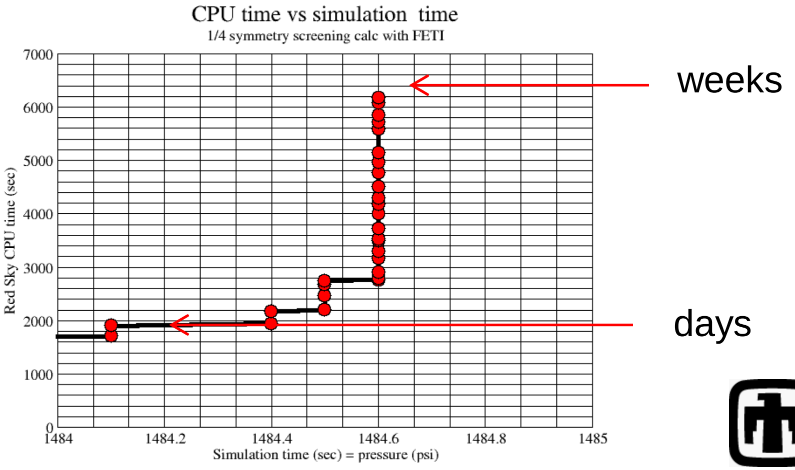
Simulation Difficulty:
creep up to a physical instability point

- **Pipe wall failure is indicated when the quasi-static calculations reach a physical instability point**
  - when the internal pressure exceeds the material's resisting force no static equilibrium is attainable and no inertia terms to stabilize the calculation through breakup
- **large sensitivity to mesh and solver settings**
- **excessive run times**
- **highly distorting elements**









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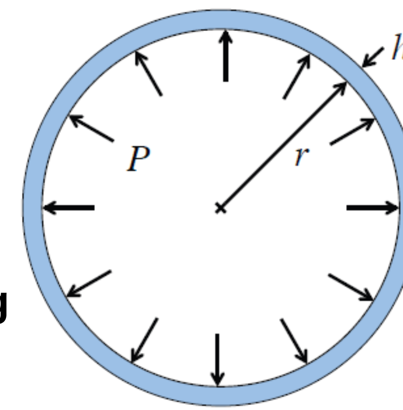
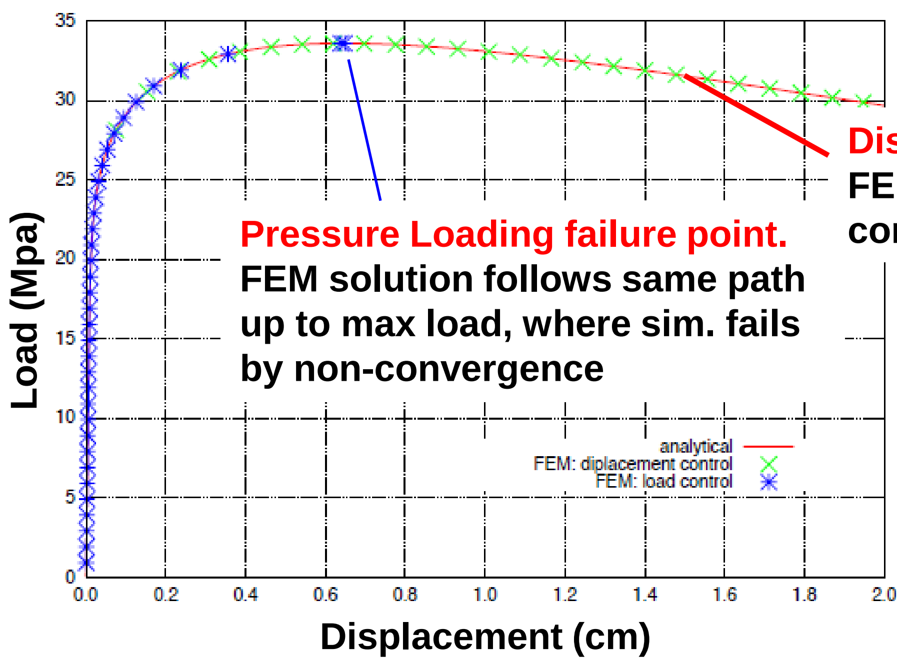
Calculation Instability signifying Structural Failure is Confirmed by 2D Test Problem with Analytic Solution

- **Test Problem w/same Code & Constit. Model**
  - **Ring internally loaded to failure (plain strain)**
  - **Two types of loading:**
    - ***displacement controlled* — radial displacement loading**
    - ***load controlled* — internal pressurization**





Displacement Controlled
FEM and Analytical solutions continue past max load

Work performed by Bill Scherzinger, Sandia Labs

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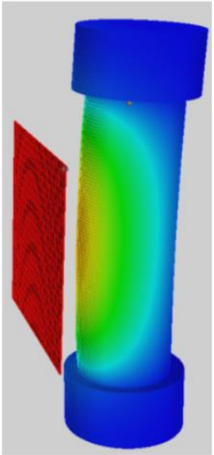
Solver Accuracy and Speed Assessment for Accurate Curve "Strength" Rankings

Test & temperature cases	CG 10^{-6} Failure psi (CPU time*)	FETI-CG 10^{-4} Failure psi (CPU time*)	FETI-CG 10^{-5} Failure psi (CPU time*)	FETI-CG 10^{-6} Failure psi (CPU time*)
try26-700C	704.0 (40.30)	702.0 (20.3)	703.8 (5.87)	703.7 (5.24)
try27-700C	704.9 (40.29)	704.1 (19.1)	704.2 (5.28)	704.2 (6.21)
try3-20C	1485.9 (21.1)	1490.70 (12.1)	1484.5 (7.8)	1484.5 (9.78)
try6-20C	1486.3 (15.2)	1487.20 (4.6)	1485.0 (2.9)	1485.0 (4.39)
try5-20C	1486.4 (16.0)	1492.60 (41.3)	1485.2 (20.7)	1485.2 (8.26)

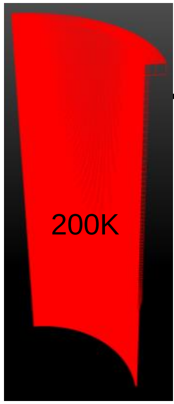
* CPU times reported in Adagio output file via global output variable *cpu_time*. CG and FETI sims. were run on 192 processors of Red Sky

- **Results effectively unchanged when solver tolerance is changed from 10^{-5} to 10^{-6} (for 4tt mesh).**
- **CPU time not >> for 10^{-6}**
- **Use 10^{-6} for production calcs.**

- **Various hourglass treatments also investigated**
- **verified to not have significant effect on predicted failure pressures**



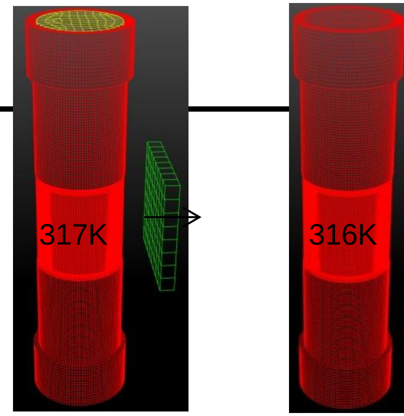
Models used for UQ



4tt

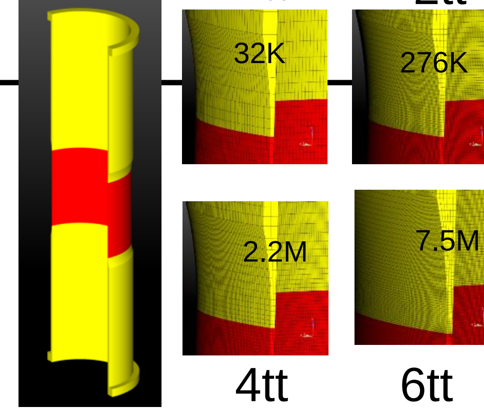
High-Low materials study
Isothermal - 1/8 symmetry

4tt

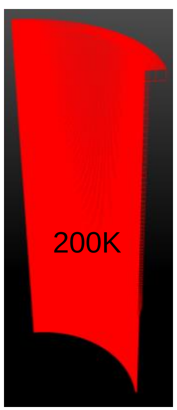


4tt

Coupled Self Check mapping
PB# 1 Nearby problem
Used ¼ symmetry



Mesh convergence
¼ symmetry



4tt

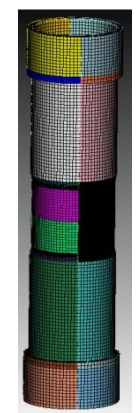
Solver parameters study
Isothermal - 1/8 symmetry

1tt-170K
2tt-1.5M
4tt-11.6M

No contact

1tt-83K
2tt-570K
4tt-4M

contact



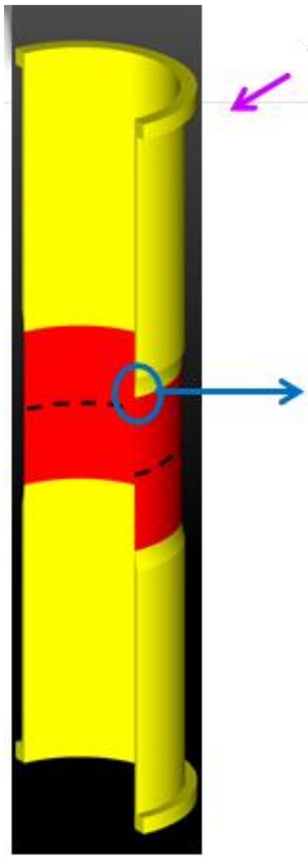
1tt-42K
2tt-285K
4tt-2M

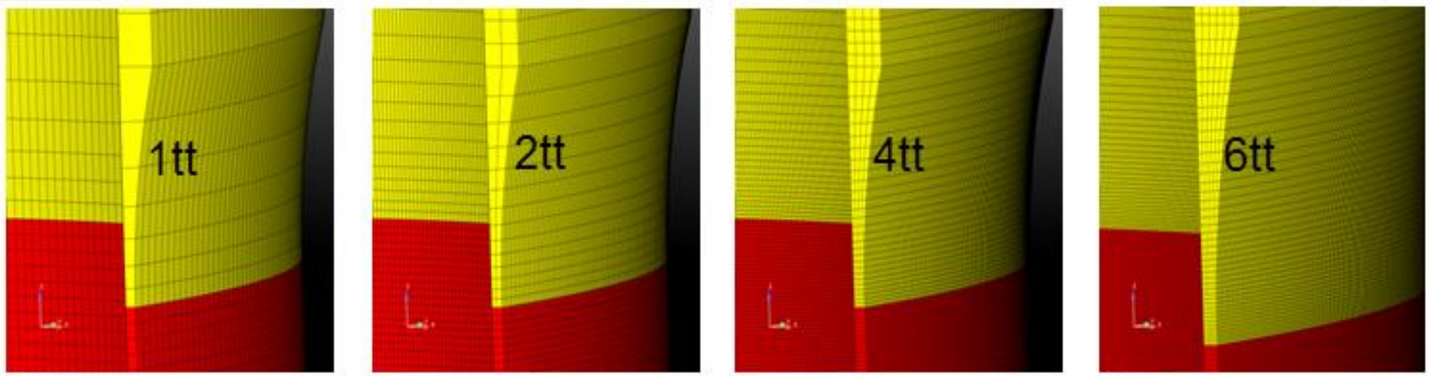
More contact

Validation to Experiments – Full symmetry

Pipe Bomb Calculation Verification
Mesh Refinement Studies

1/4 Pipe model = top ½ of half-pipe shown



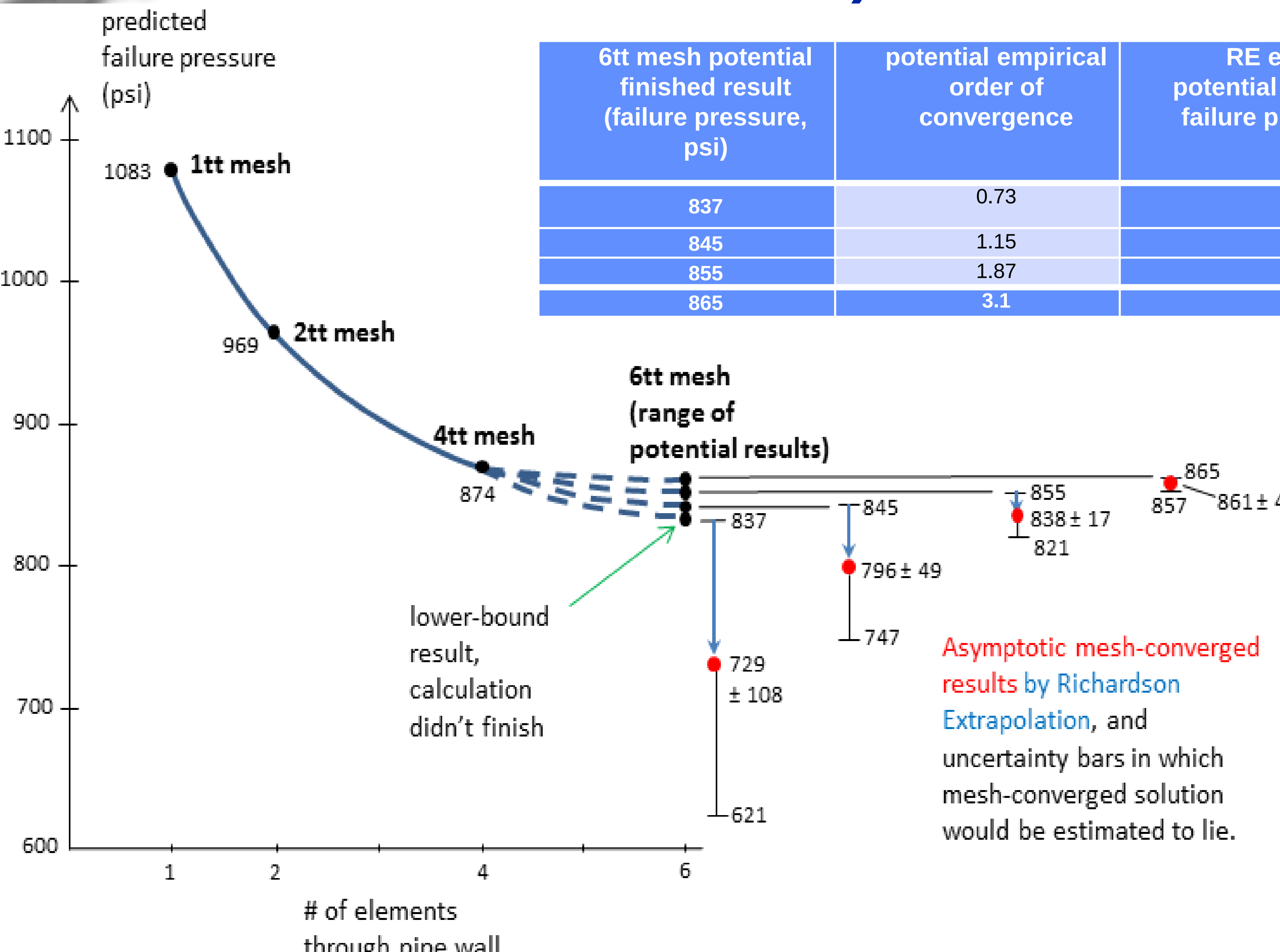


Geometrically similar **meshes**

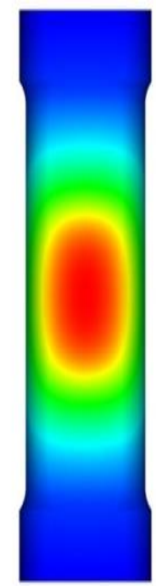
Number of Elements thru thickness of wall	1	2	4	6
# Elements (1/4 model)	32,368	276,080	2,173,600	7,458,912
Pressure at Fail (psi)	1069	955	850	819.1* (*didn't finish, 36 days on 400cpu's)

Calculation Verification
Mesh Study Results

6tt mesh potential finished result (failure pressure, psi)	potential empirical order of convergence	RE estimates of potential grid-converged failure pressure results (psi)
837	0.73	729
845	1.15	796
855	1.87	838
865	3.1	861



Asymptotic mesh-converged results by Richardson Extrapolation, and uncertainty bars in which mesh-converged solution would be estimated to lie.



Coupled Thermo-Mechanical modeling to Design Experiments & Thermocouple Locations to Reconstruct Temperature Field

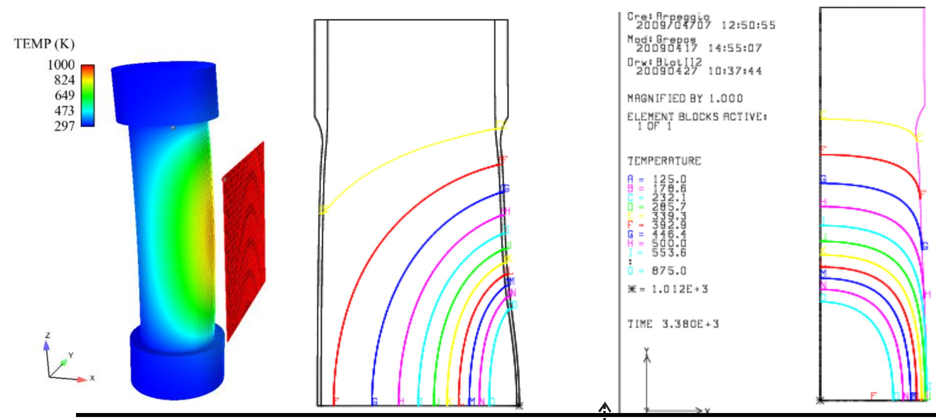
Model

- Pipe radiatively heated by plate
- Convection neglected
- Viewfactors change as pipe bulges toward plate at hot spot

Temperature Contours

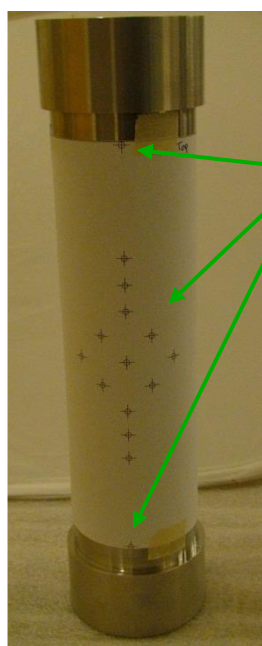
Side view, top half of pipe

Front view, ¼ symmetry



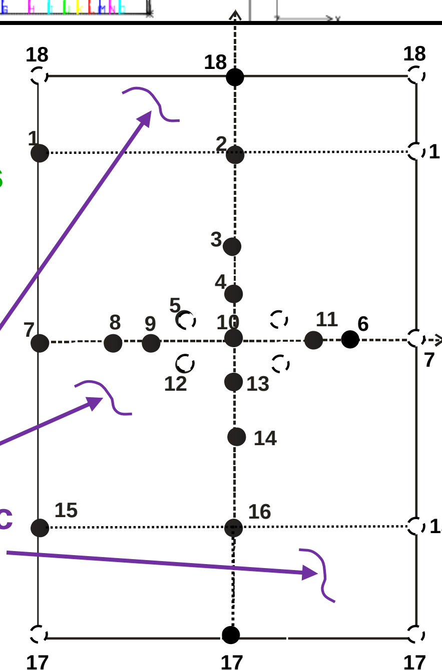
Experiment Design Quantities

- Size & location of plate relative to pipe
- # of thermocouples and locations to adequately reproduce temperature field on pipe surface
- in conjunction with design of interpolation method



Thermocouples (23 total, front & back)

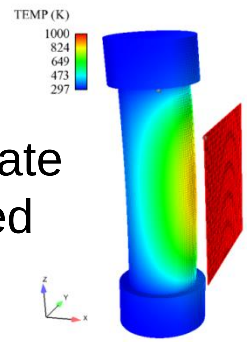
8 Linear to Cubic interpolation patches (C^0 continuous)



“Nearby Problem” to Quantify Error in Temperature Field obtained from TC Interpolation

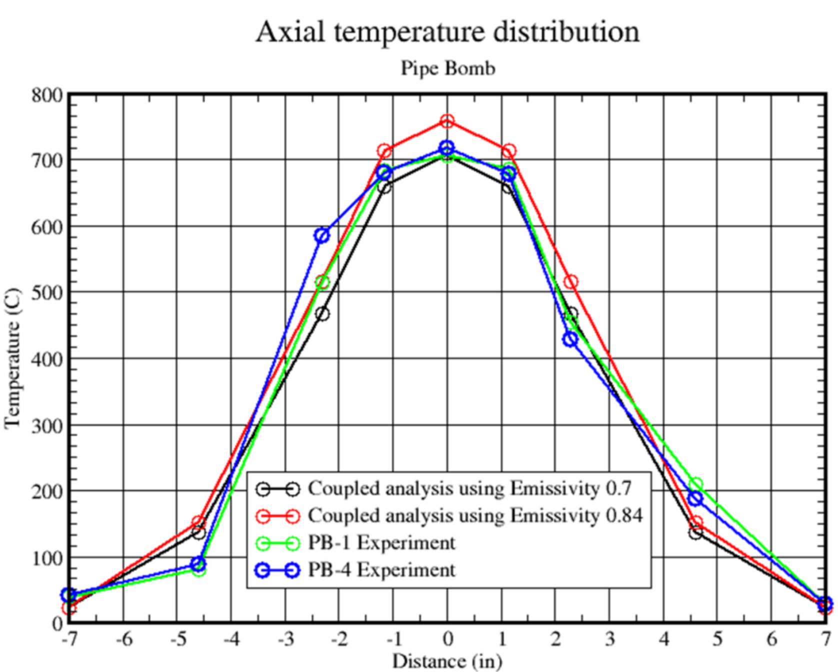
Nearby Problem:

- Pipe irradiated by plate
- Convection neglected



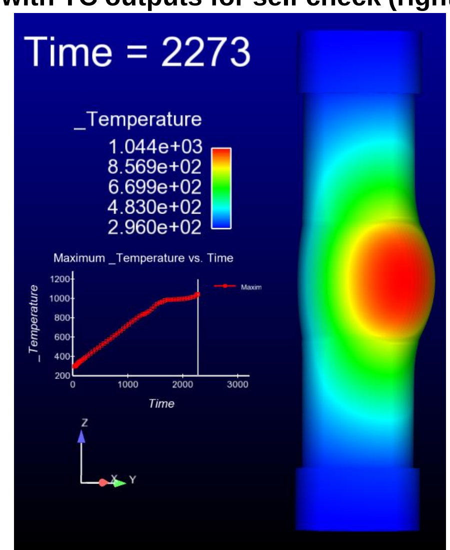
Run Matrix

Simulation case	Time @failure (sec.)	Temperature @failure (C)	Pressure @failure (psi)	Tear Param. @failure
Coupled-high-0.84	2277.1	759.0	809.9	6.23
Interp-high-0.84	2332.8	758.9	857.9	7.27
Coupled-low-0.84	2255.9	759.0	791.6	5.40
Interp-low-0.84	2299.3	759.0	829.0	7.46
Coupled-high-0.7	2386.0	706.9	903.7	3.9
Interp-high-0.7	2400.9	706.9	916.2	4.43
Coupled-low-0.7	2350.4	706.8	873.0	3.50
Interp-low-0.7	2353.6	706.8	875.8	3.86



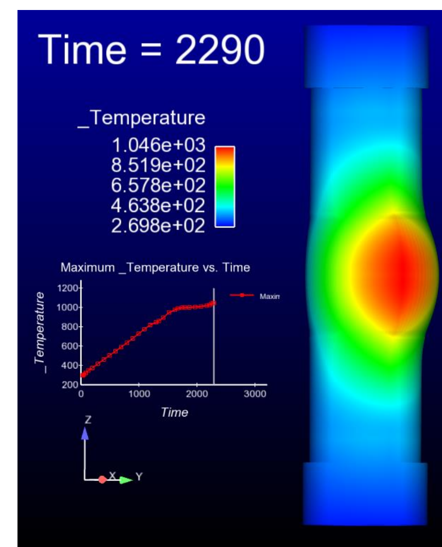
Coupled Thermo-Mechanical sim.

Coupled experiment calculation
High strength, Nominal Emissivity
with TC outputs for self check (right)



“Self-Check” sim. w/TC interp. temperatures

TC interpolation check calculation
Using coupled TC outputs (left)



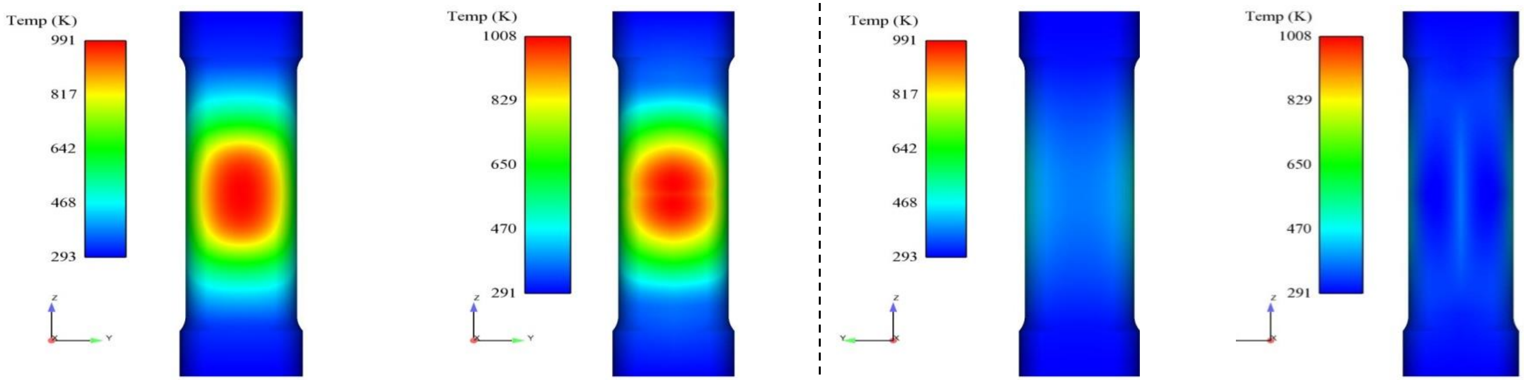
Temperature Field Reconstruction Error due to ***Spatially Sparse*** *TC data*

Exact Temperature Field *Front view, 3390sec.*

Interp. Temperature Field *Front view, 3386 sec.*

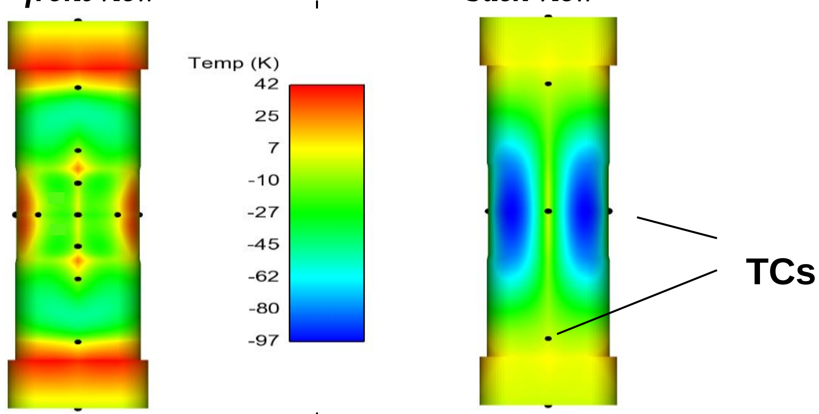
Exact Temperature Field, *Back view, 3390sec.*

Interp. Temp. Field *Back view,3386sec.*



Difference (error) Plots

front view *back view*



- **temperature interpolation error is characterized and corrected for validation predictions**
- **a ~4% (35 PSI) error in predicted failure pressure if not corrected for interp. error**

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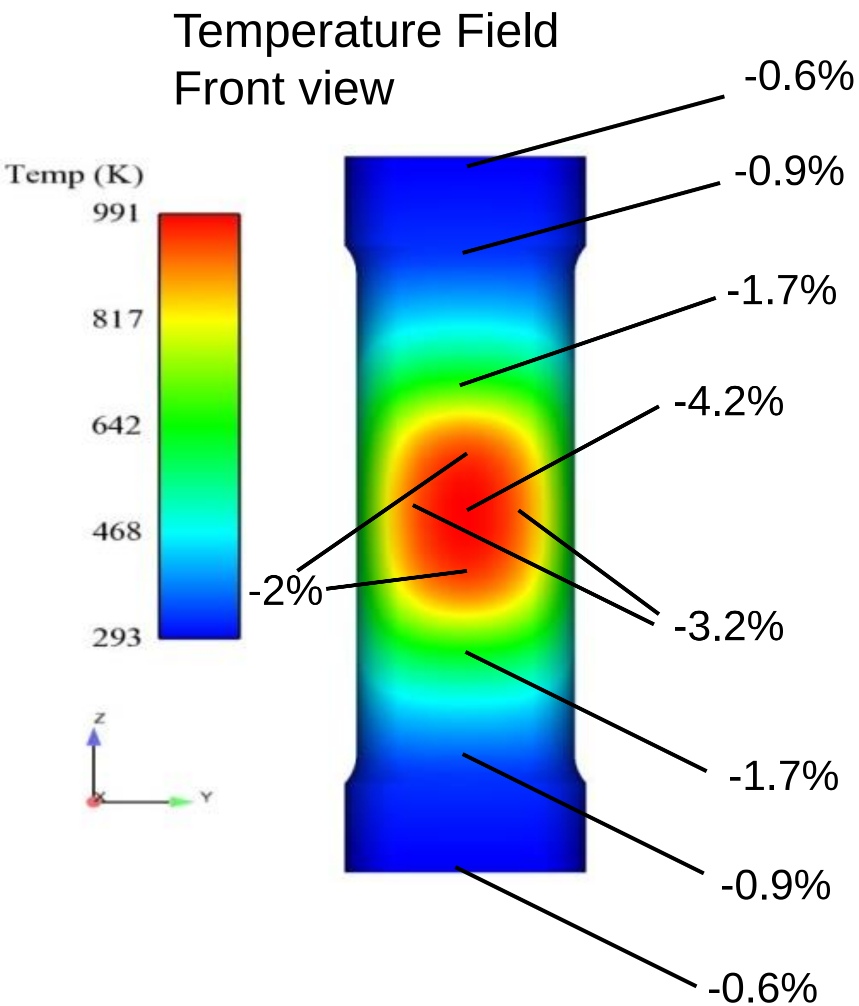
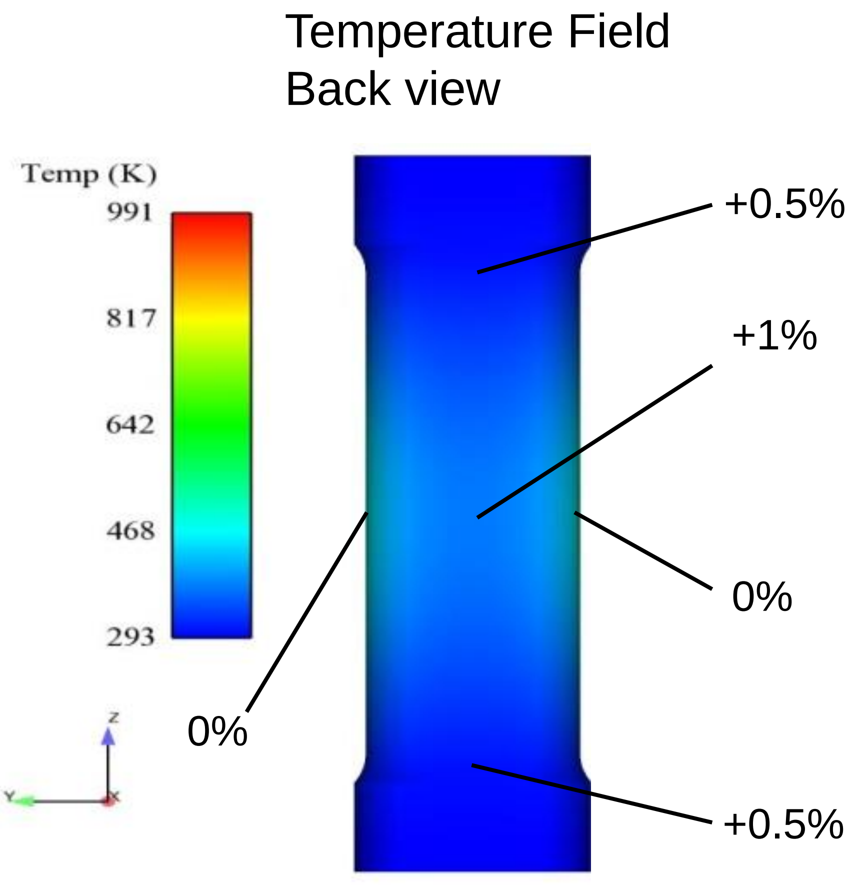
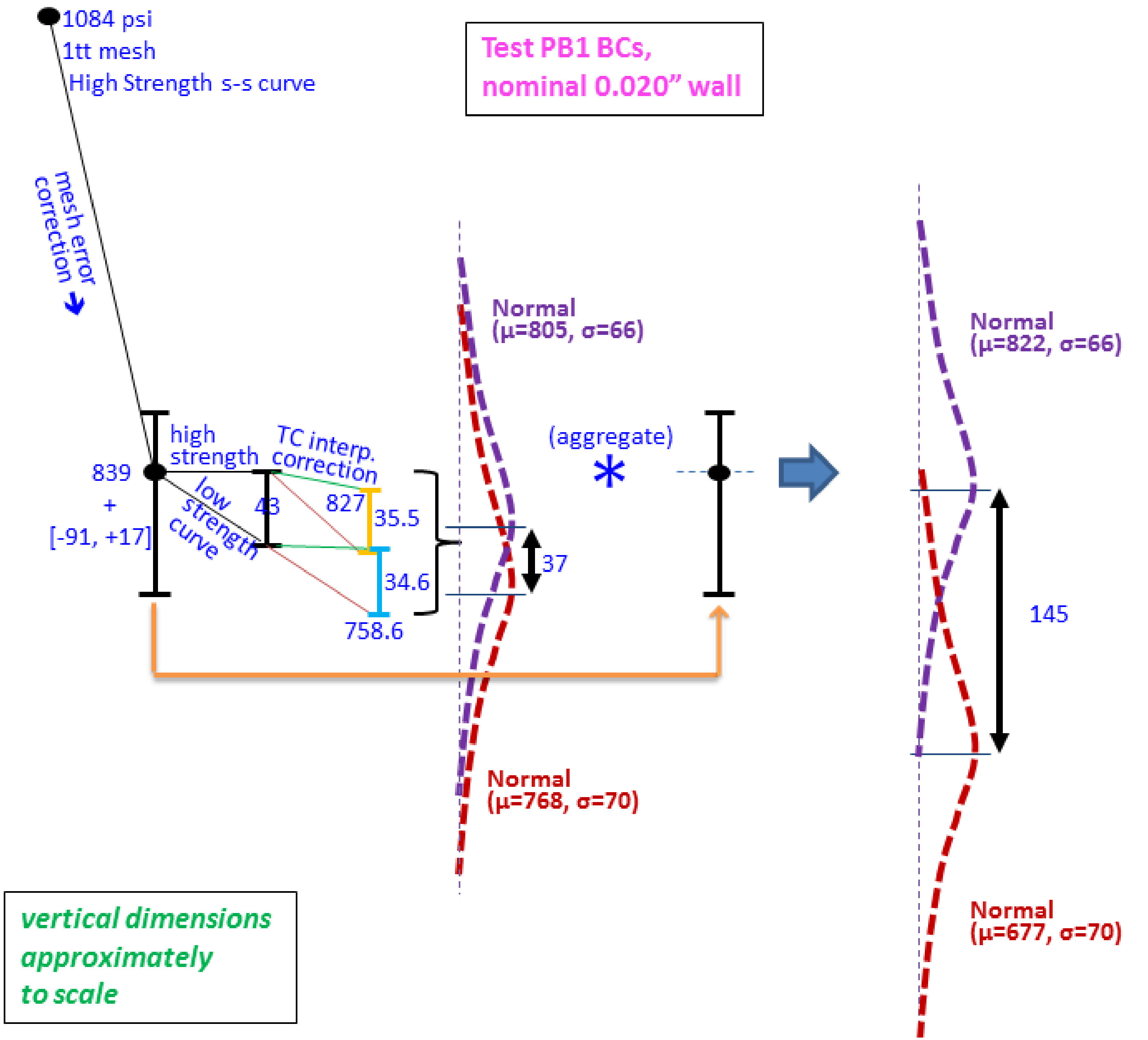
Bias Correction of TC Temperatures for Contact Resistance and Fin Effects



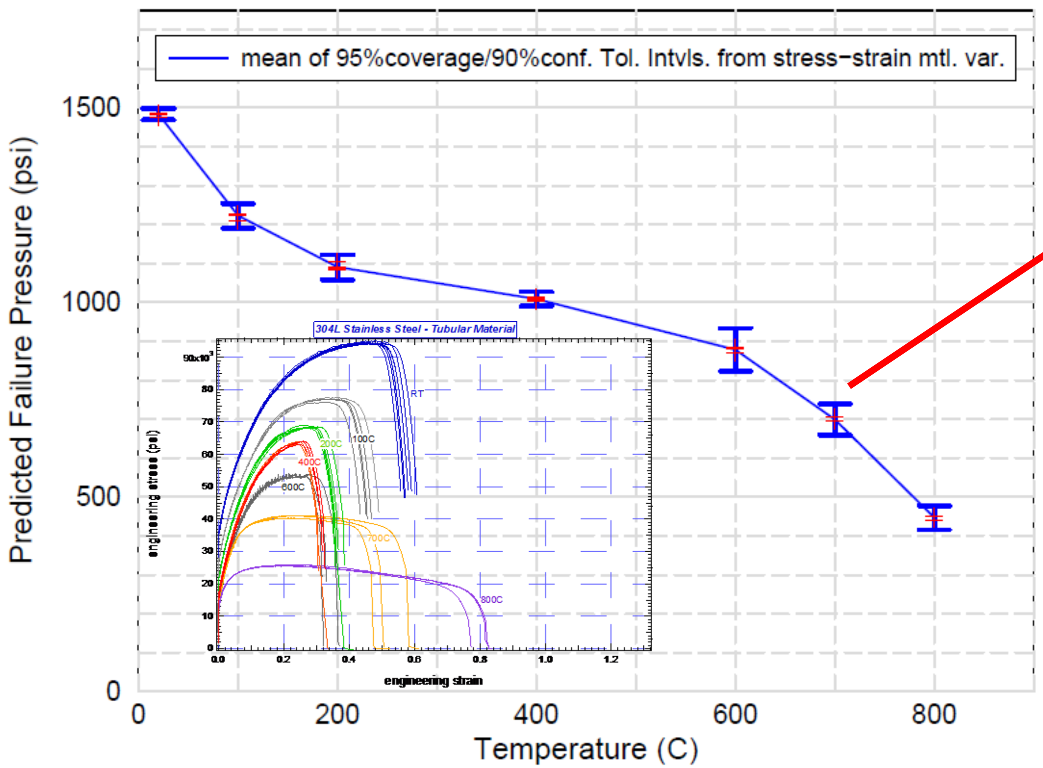


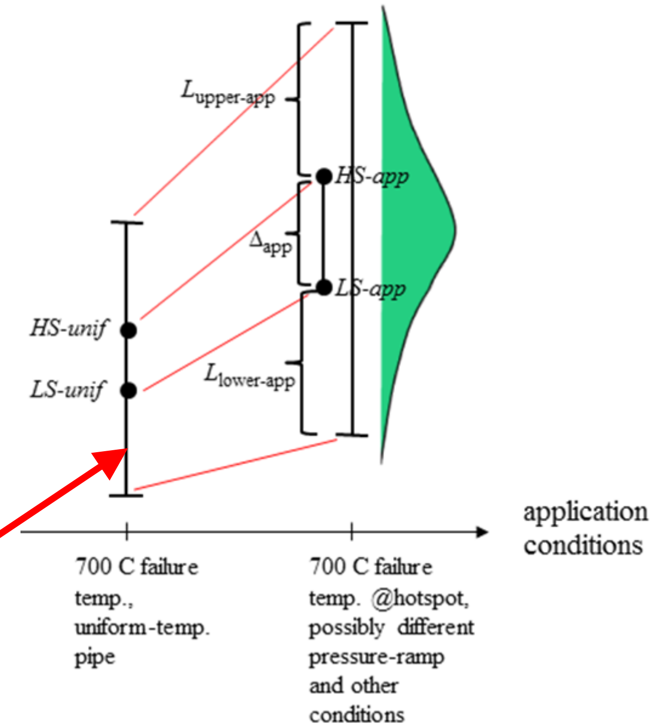
Simulation UQ Roll Up



Economical Parameterization of TIs by High & Low Strength Material Curves

- **Tolerance Intervals are constructed from multiple stress-strain curves**
- **But TIs can be parameterized by 2 s-s curves for only 2 Val./UQ sims. w/ full-geom. model**





Processing of Experimental Failure Pressures


Normalize Experimental Results to the same Reference Conditions Input to Model for “Apples to Apples” results comparisons

Taylor Series approach:

Example **Nominal wall thickness = 0.02”**

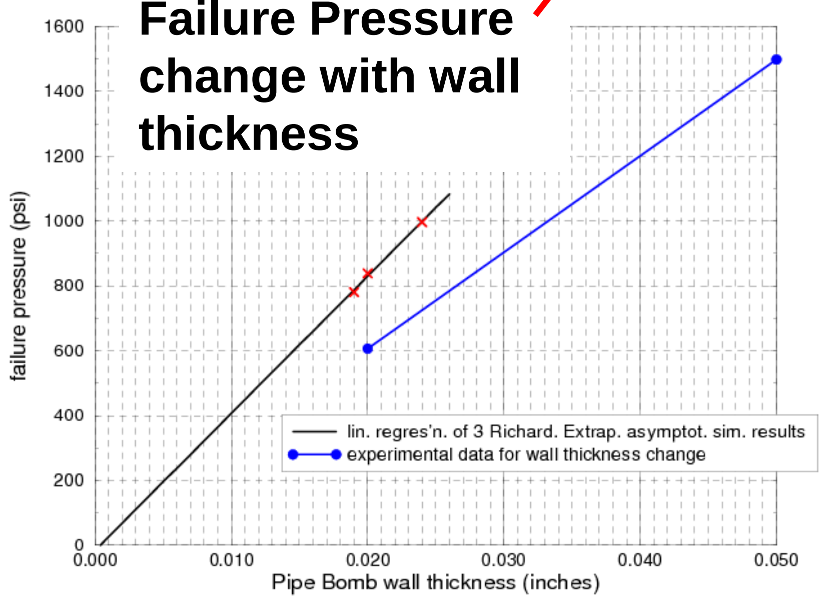
$$Pfail_{PB4}(\vec{x}_{PB1ref}) \approx Pfail_{PB4}(\vec{x}_{PB4}) + \sum \frac{\partial(PfailPB\ 4)}{\partial(x_i)} \bullet (x_{i\_PB1ref} - x_{i\_PB4})$$

Normalized Failure Pressure in Test PB4

Measured Failure Pressure in Test PB4

Failure Pressure change with wall thickness

wall thickness uncertainty



Part No.	Wall Thickness
1	.019/.022"
2	.020/.022"
4	.020/.024"
5	.020/.022"
7	.019/.022"
8	.020/.021"
9	.019/.0225"
10	.019/.021"

Spreadsheet Processing of Experimental Results & Uncertainties

***"Linear+"** propagation method samples uncertain sensitivities $\partial(Pfail)/\partial X_i$ as well as the uncertain input variables X_i*

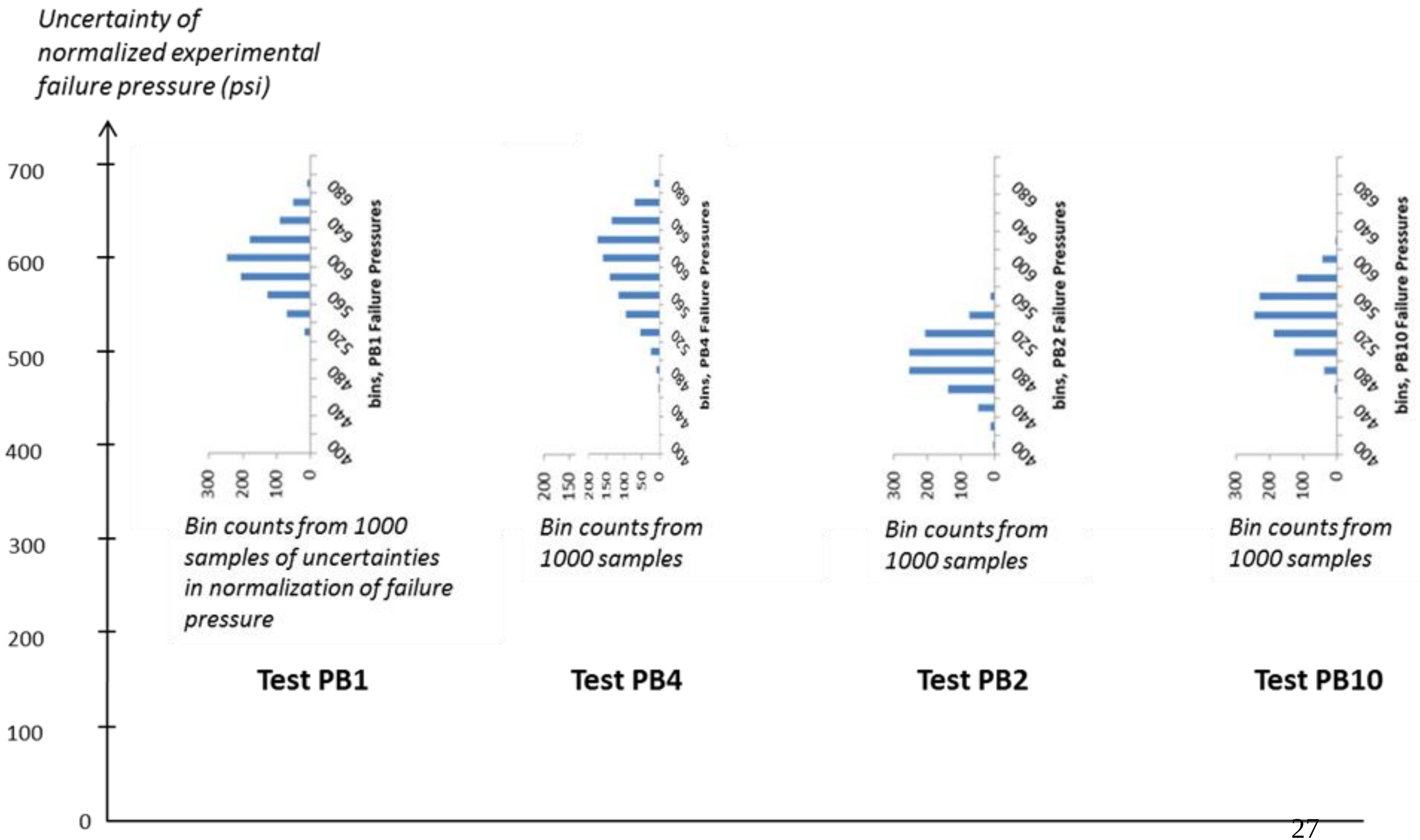
Systematic uncertainties correlated with uncers. in same columns of the spreadsheets of the other 3 experiments

- **Account for random and systematic errors/uncertainties in measurement/ processing/inference of experimental <u>input</u> and <u>output</u> quantities**

- **Normalize for:**
  - **nominal (measured) differences in experimental <u>inputs</u> in the replicate tests**

realization j	$\Delta Pfail_{measPB4,j}$ = A2j, systematic betw. PB1 & PB4	$w_{actPB4,j}$ = [0.02, 0.024] inches	$\Delta w_{PB4,j} = w_{nomPB4} - w_{actPB4,j}$ = 0.02" – B3	$\left(\frac{\partial(Pfail_{PB4})}{\partial(w)}\right)_j$ = A5j, systematic betw. PB1 & PB4	= (B4*B5)$_j$ psi	$\Delta T_{meas\text{-}TC/DAQ,j}$ = [−0.0025*711, +0.0025*711] C	$\Delta T_{meas\text{-}contact,j}$ = A8j, systematic betw. PB1 & PB4	$\Delta T_{TC4location,j}$ = [−15, 15] C	$\left(\frac{\partial(Pfail_{PB4})}{\partial(T@fail\_point)}\right)_j$ = A10j, systematic betw. PB1 & PB4	= (B7 + B8 + B9)$_j$ *B10$_j$	$[Pfail_{model}(\vec{x}_{nomPB1}) - Pfail_{model}(\vec{x}_{nomPB4})]$	= 655 psi + (B2 + B6 + B11 + B12)$_j$ psi = $Pfail_{PB4}(\vec{x}_{nomPB1})_j$
B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13
1												
j	B2=A2, sys	B3=PB4wall	B4=Δ0.02"	B5=A5, sys	B6 = B4*B5	B7=ΔTC_DA	B8=A8, sys.	B9=ΔTC_loca	B10=A10, sy	B11=B10*(B7	B12=PfPB1-	B13=655+B2+
1	7.76	0.02266	-0.00266	30701.34	-81.65	-1.39	0.52	12.84	-2.07	-24.83	-8.00	548.29
2	-5.88	0.02327	-0.00327	37837.13	-123.76	0.91	1.18	-11.81	-1.87	18.17	-8.00	535.53
3	-0.69	0.02195	-0.00195	26116.40	-51.05	0.07	1.61	-6.42	-1.83	8.66	-8.00	603.93
999	-8.55	0.02399	-0.00399	37867.63	-150.97	0.67	0.10	-14.21	-2.15	28.95	-8.00	516.43
1000	6.28	0.02353	-0.00353	29062.56	-102.57	-0.85	0.06	2.18	-1.99	-2.78	-8.00	547.94
	avg	avg	avg	avg	avg	avg	avg	avg	avg	avg	avg	avg
	0.00	0.02195	-0.00195	32361.71	-62.83	-0.05	0.91	-0.39	-1.94	-0.96	-8.00	583.21
	stdev				stdev					stdev		stdev
	5.76				39.06					17.02		42.97

Normalized Failure Pressures accounting for Experimental Uncertainties



UQ Roll Up for Experiments

Uncertainty of 0.025 & 0.975 percentiles of Failure Pressure

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

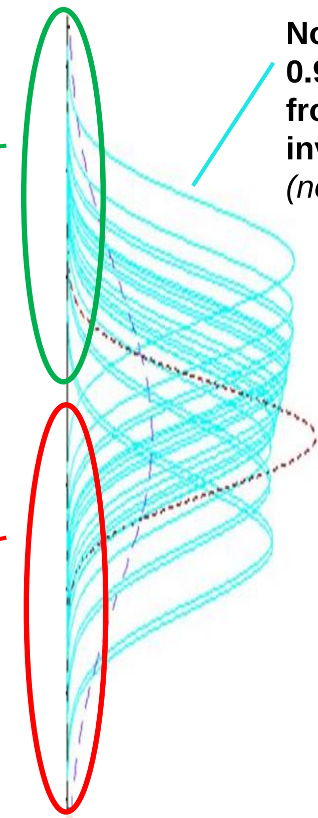
assoc. w/ <u>experimental factors</u> in the tests:
- *uncertainties in measurement and estimation of test conditions, responses, and normalization quantities*

assoc. w/ <u># of tests</u>

assoc. w/ response variability attributed to <u>stochastic elements/ behaviors in systems</u> tested

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

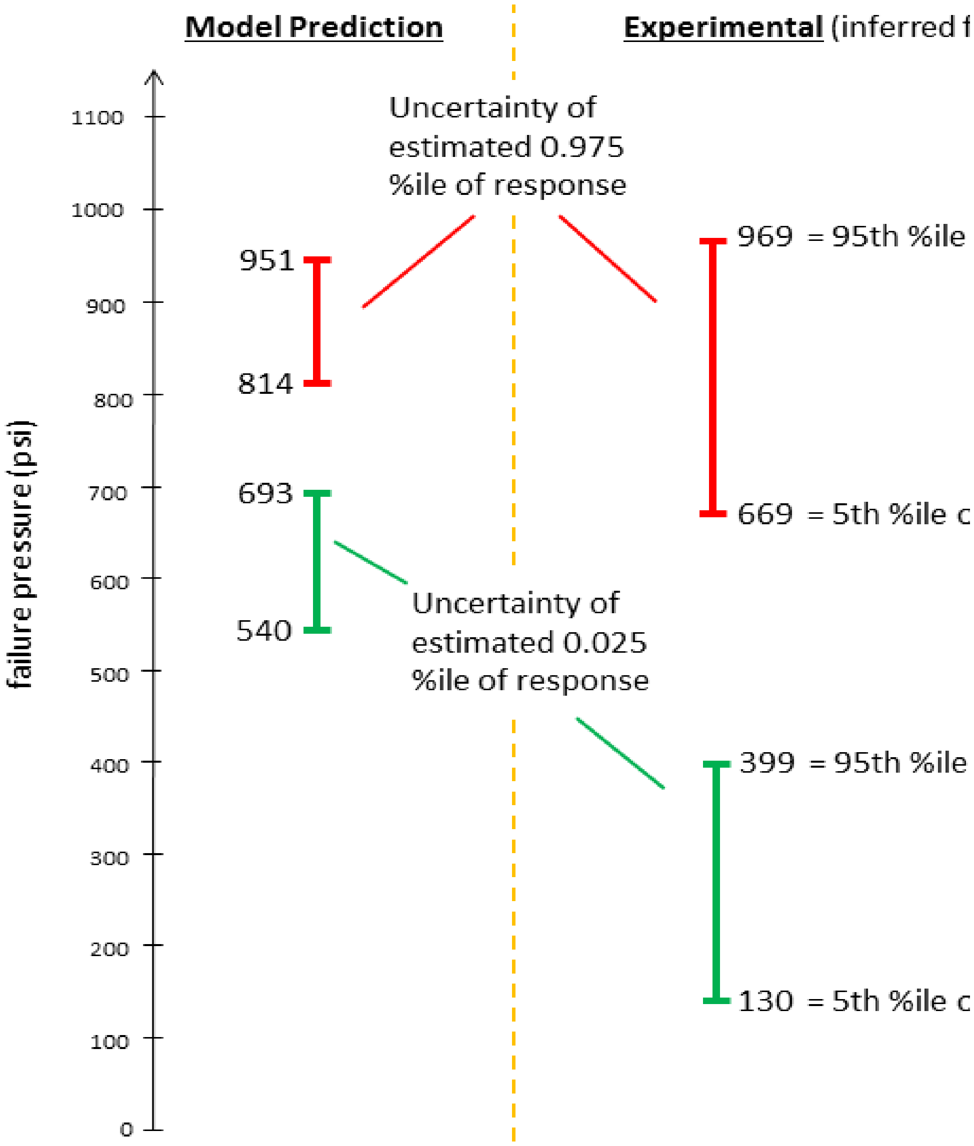
Uncertainty of 90% conf. lower bound on 0.025 percentile of experimental response *(failure pressure)*

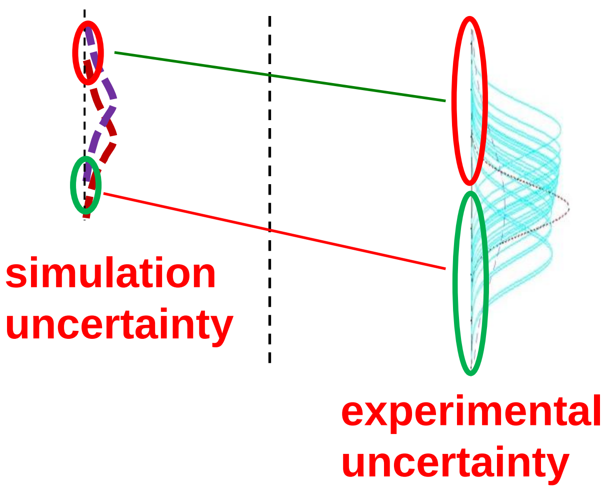


Normal PDFs fit to 0.95/0.90 Tolerance Intervals from Small # of Tests involving uncertainty *(notional PDFs for illustration)*

Results of Percentile Comparisons:

*Lower Percentile of Predicted Failure Pressure is **NonConservative** for Intended Model Use*





Closing Remarks

- **The Real Space validation methodology is versatile and practical, geared for:**
  - expensive computational models (economical in # of simulations)
  - stochastic phenomena and models
  - multiple replicate experiments with random and systematic uncers.
  - few replicates (sparse experimental data)
  - appropriate representation and roll up of various types, sources, and representations of uncertainty
    - aleatory and epistemic
    - probabilistic, interval, and discrete variables and functions

- **Real Space Validation results are:**
  - relatively straightforward to interpret
  - especially relevant for assessing models/quantities to be used in the analysis of performance and safety margins for design and risk assessment