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Perspectives from Applied Model Verification and Validation

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Nuclear Energy Safety Technol. (6230)
UQ and SA Training Class
Sandia-Albuquerque, April 22-23, 2014

What are Verification and Validation (V&V)?

<u>Code Verification</u> (not covered in this talk)

- As time and space discretizations are refined subject to appropriate constraints, do computed results converge to ***exact analytic solutions*** at the rate of the ***formal order*** of the mathematical discretization scheme?

<u>"Solution" or "Calculation" Verification</u>

- In applying the model to real problems, determine the ***empirical*** rate of convergence with appropriate discretization refinement, and from this **estimate the solution error** and uncertainty thereof.

<u>Model Validation</u>

- **How well do model results match reality for relevant quantities of interest?**
- **Is the model "*<u>good enough</u>*" for defined use purposes of the model (e.g., specific design, analysis, or decision-making purposes)?**

About this talk…

- **Shortened version of fall 2011 3hr. class:**

  Advanced Topics in Model Validation

- Introduce concepts, issues, lessons from recent and ongoing activities and developments in UQ and V&V pertaining to:
  - **Experiments**
  - **Mod/Sim**

  → **Best Estimate Predictions + Uncertainty**

- **Caveat – one particular view of things**
  - **UQ and V&V methods are still being actively researched, developed, debated, and refined in the experimental, V&V, and M&S communities**
  - **The "Real Space" model validation approach presented here is one particular approach among many, and is still under development—still evolving**
    - developed over many years, based on many diverse experiences with industrial scale applications

Outline

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- Introduce the "Real Space" approach to model validation

  + some considerations underlying it

- Survey some model V&V/UQ applications at Sandia and present an in-depth case study from a recent thermal-mechanical application

MOTIVATION for Model Validation

As an example, consider a finite-element model of a device or system

- **Let all model inputs like material properties and boundary conditions be crisp values**
- **All these crisp inputs will have some amount of error**
  - even if all model inputs are actually measured, measurement error will exist
  - majority of inputs for material properties and model parameters typically come from catalogued values determined elsewhere, under different conditions
- **Model-form error will also exist** – *all model conceptions are simplified abstractions of reality; no conception is exact*
- **The numerous errors in the model (each hopefully "small") add to an unknown discrepancy between model predictions and "reality"**

➡ *Hypothesis tests for whether the model is different from the data are improperly posed, skewed toward rejecting the more reasonable alternative hypothesis that a difference between model and reality exists*

Model Validation

- **How well do model results match reality for relevant quantities of interest?**
- **Is the model "*good enough*" for defined use purposes of the model? (e.g., specific design, analysis, or decision-making purposes)**

Observation: a model that is "Consistent" with the Data is Not Necessarily Accurate or Adequate

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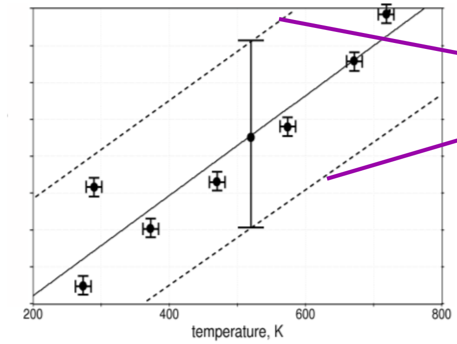
Example:
measured material property data as a function of temperature

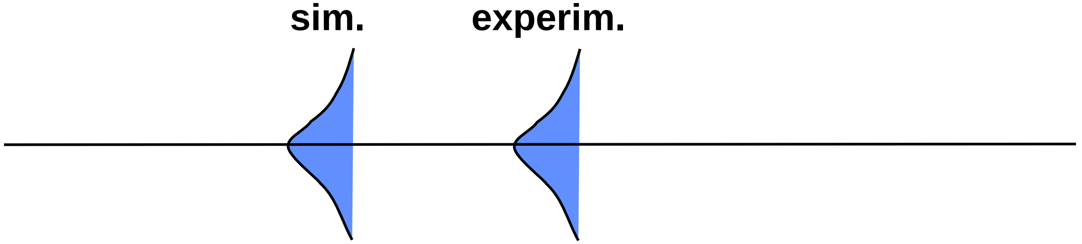


Total uncertainty associated with set of measurements (our best perception of where reality lies)

- The solid black line is a Least-Squares best-fit regression line through the data
- Regression line not an accurate model for material prop. value vs. temperature
  - Some validation paradigms would categorize the model as "consistent" with the data and therefore would accept it (➡ poses "Model User's Risk")
  - model too precise, not representative of real property variability
    - Under-predicted uncertainty could lead to trouble in downstream uses of model
  - model better characterized as: "not fully consistent" or "not inconsistent" with data
- Also demonstrates why popular validation criterion of "means matching" (does mean of sim. = mean of data?) is not an effective test for model accuracy

The Significance of Aleatory vs. Epistemic uncertainty in model validation

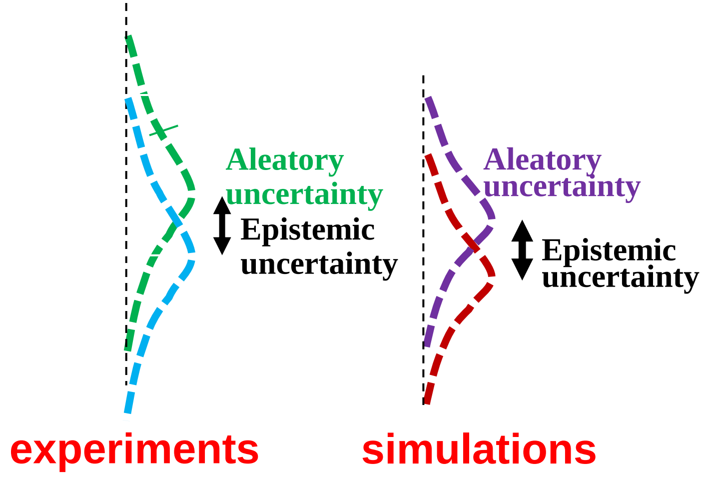
Given this uncertainty, is this model prediction perfect or likely biased?



- **Answer**: **it depends pivotally on the nature of the uncertainty represented by the PDFs**
  - Perfect model if the PDFs represent populations of results from a stochastic system tested multiple times w/ no other uncer. in the tests (aleatory uncertainty only)
  - Model likely has error if the PDFs represent only epistemic uncertainty (lack of knowledge) regarding the response of a non-stochastic system

Treatment of Aleatory and Epistemic Uncertainties

- **Both types of uncertainty are significant in many (most?) validation problems**
- **Real Space model validation framework is built to address this**
  - **segregated representation and propagation of aleatory and epistemic uncertainties**
  - **modified "Probability Box" representation of Ferson & Ginzburg**



Treatment of Aleatory and Epistemic Uncertainties in model validation

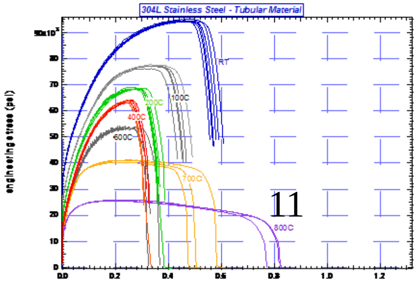
- **Real Space approach is a <u>hybrid</u> (in this regard) of other developed frameworks:**
  - **ASME V&V20 2009 *Standard for V&V in CFD and Heat Transfer***
    - geared for validation of non-stochastic systems
    - no aleatory-epistemic segregation
    - equivalent to Real Space for non-stoch. sys. and probabilistic UQ
  - **ASME V&V10 2012 *Supplement for V&V in Computational Solid Mechanics***
    - uses Ferson & Oberkampf validation metric (CDF mismatch)
    - built for validation of stochastic systems
    - segregates aleatory and epistemic uncertainties (Probability Box)
    - incurs risk of "Type X" validation error by ignoring some important sources of epistemic uncertainty in experiments that ASME VV20 and Real Space include

Other Differentiating Features of the Real Space methodology

- **Real Space method has a different comparison approach and validation metric for comparing experimental vs. simulation results**
- **Compares <u>percentiles</u> of response (experimental vs. simulation) instead of assessing at a whole-distribution level**
- **Provides a <u>more granular</u> look at how the model is doing**
- **Enables validation assessment of models to be used in the analysis of upper and/or lower performance and safety <u>margins</u>**
- **Doesn’t cost extra for the finer granularity, just requires a different way of processing the experimental and simulation results**

Other Differentiating Features of the Real Space methodology

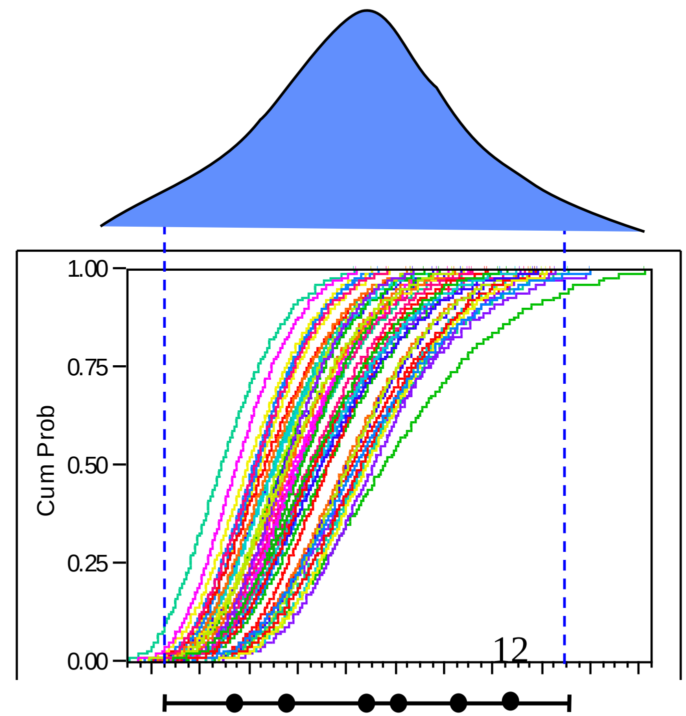
- **Explicitly accounts for epistemic uncertainty arising from small sample sizes (limited numbers of replicate tests) in experimental characterization of mtls., systems**
  - a dominant or significant uncertainty in many cases
- **The RS framework has demonstrated protocols for treatment of the following representations of uncertainty, individually and in combination:**
  - **Interval**
  - **Distributional (probability density functions, PDFs)**
  - **Discrete (non-parametric)**
    - e.g. discrete turbulence model forms and discrete stress-strain curves (data)

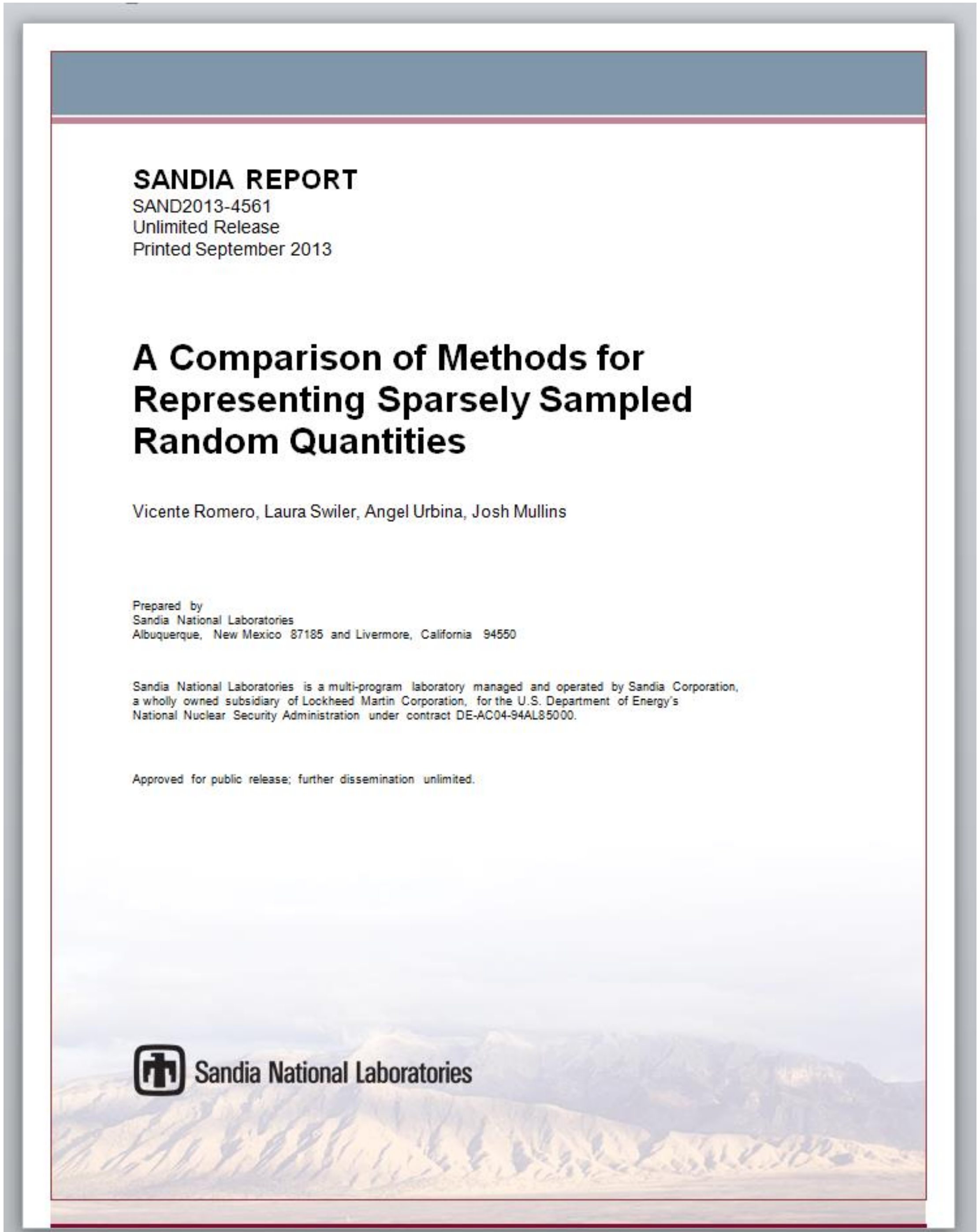


A Key Element of the Real Space validation methodology is the use of classical statistical Tolerance Intervals to deal with Sparse Data

Vs. other methods evaluated,
Tolerance Intervals significantly reduce the complexity and expense of adequately representing, propagating, and aggregating Aleatory + Epistemic uncertainties due to Sparse Data

From sparse data use 0.90/0.95 tolerance intervals to define a central 95th percentile range of a *Normal* distribution that has approx. 90% odds that its central 95 percentile range contains the 95 percentile range of the true PDF




SANDIA REPORT
SAND2013-4561
Unlimited Release
Printed September 2013

A Comparison of Methods for Representing Sparsely Sampled Random Quantities

Vicente Romero, Laura Swiler, Angel Urbina, Josh Mullins

Prepared by
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Albuquerque, New Mexico 87185 and Livermore, California 94550

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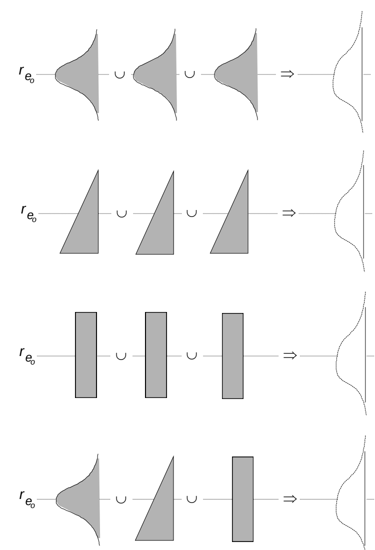
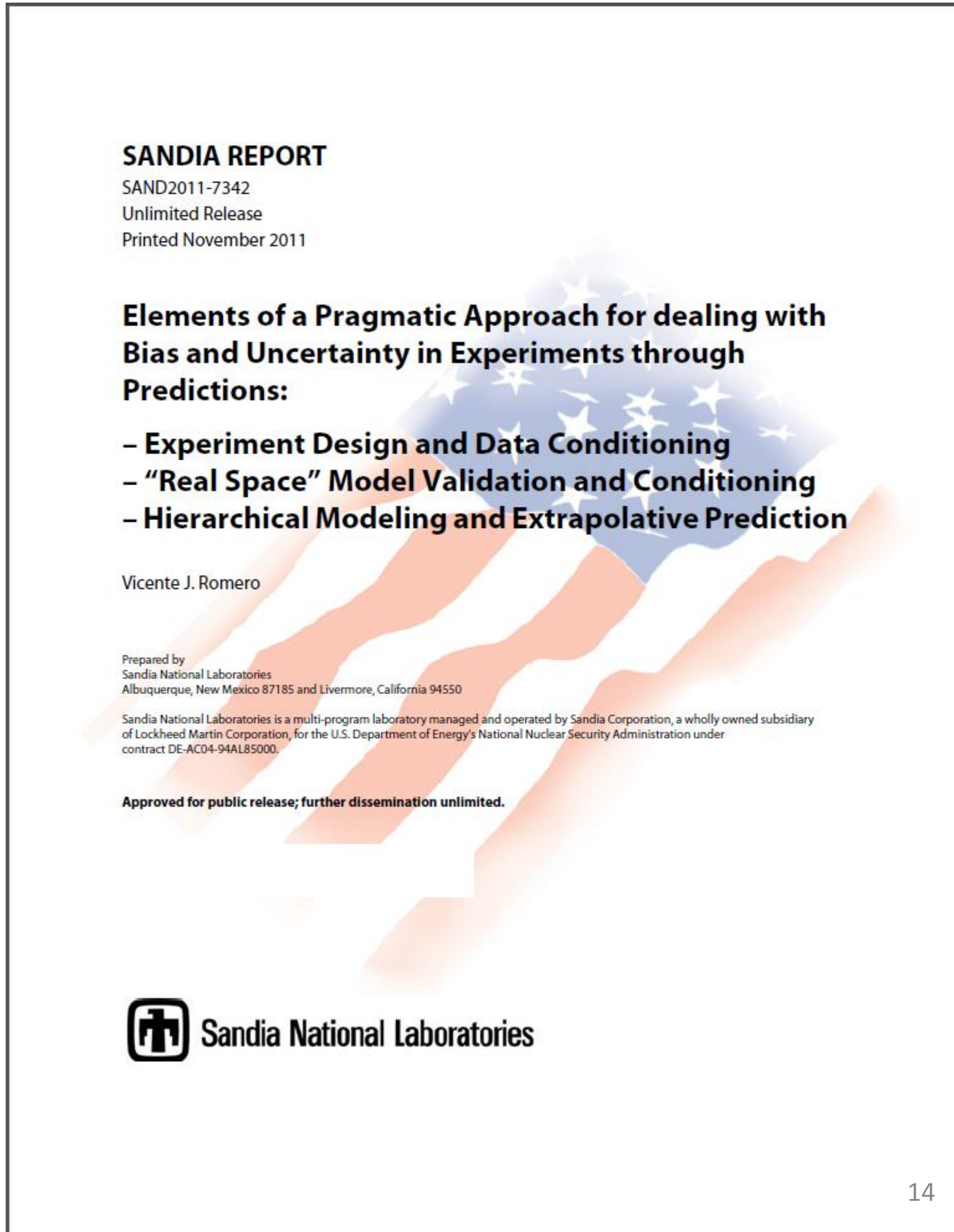
- 5 methods assessed on 21 test problems



See this report for more observations, considerations, and philosophy underlying the Real Space model validation approach and comparison to other validation approaches



SANDIA REPORT
SAND2011-7342
Unlimited Release
Printed November 2011

Elements of a Pragmatic Approach for dealing with Bias and Uncertainty in Experiments through Predictions:

– Experiment Design and Data Conditioning
– "Real Space" Model Validation and Conditioning
– Hierarchical Modeling and Extrapolative Prediction

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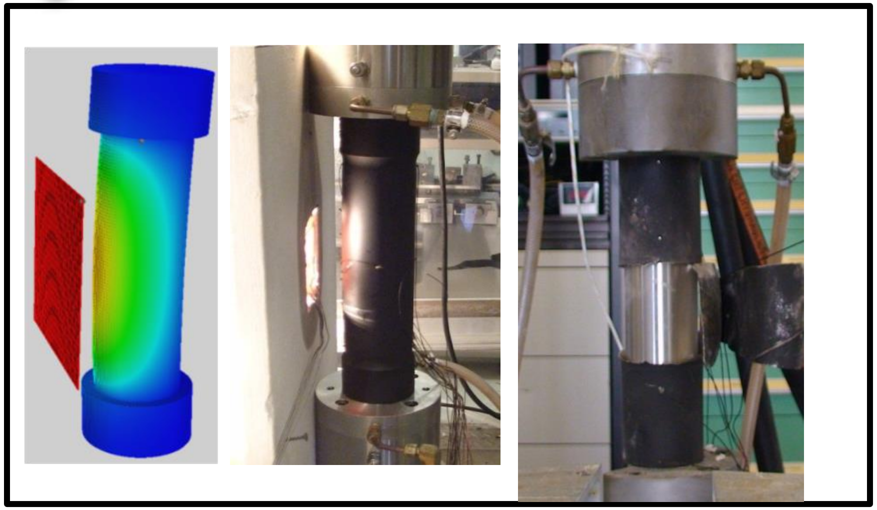
"Pipe Bomb" V&V/UQ Case Study



Pipe Bomb simulations and experiments

Experiments
- Bonnie Antoun (8256)
- Kevin Connelly (8256)

Models and Simulations
- Frank Dempsey –PI (1526)
- Jerry Wellman (retired)

V&V/UQ Methodology and Analysis
- Vicente Romero (1544)

Funding Source: ASC abnormal thermal-mechanical

Project Description and Challenge

Perform V&V assessment of a high-temperature stainless steel elastic-plastic constitutive model tested in heated pipes pressurized to failure.

SANDIA REPORT
SAND2014-YYYY
Unlimited Release
Printed April 2014

UQ and V&V Techniques applied to Experiments and Simulations of Heated Pipes Pressurized to Failure

Vicente Romero, J. Franklin Dempsey, Bonnie Antoun

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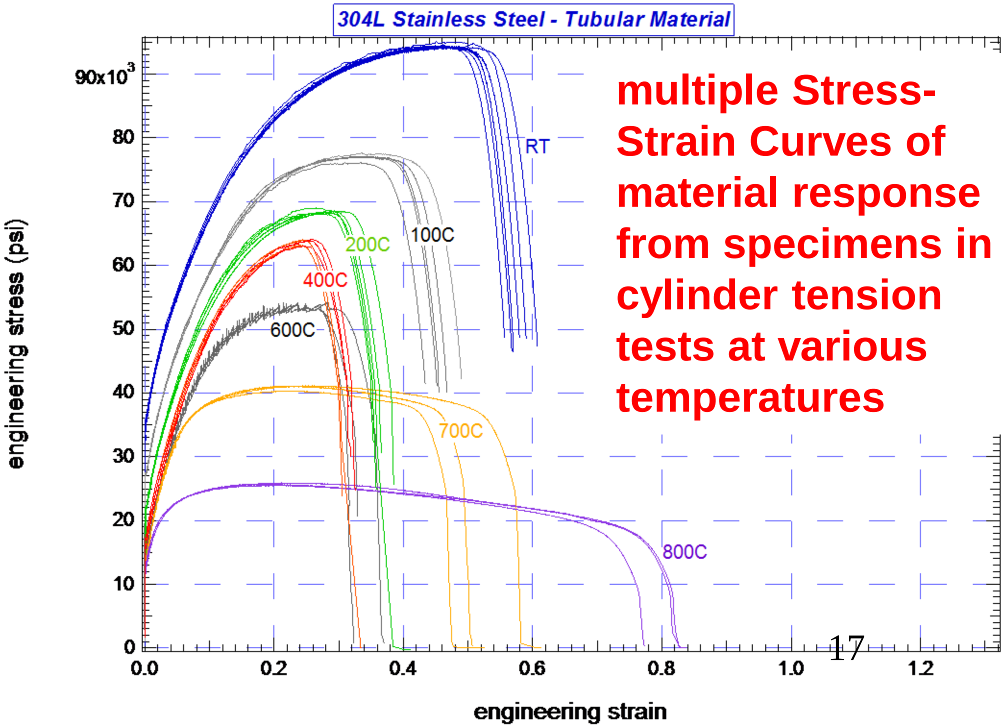
Material Characterization:

Aleatory and Epistemic uncertainties from Sparse Samples of Discrete Random Functions

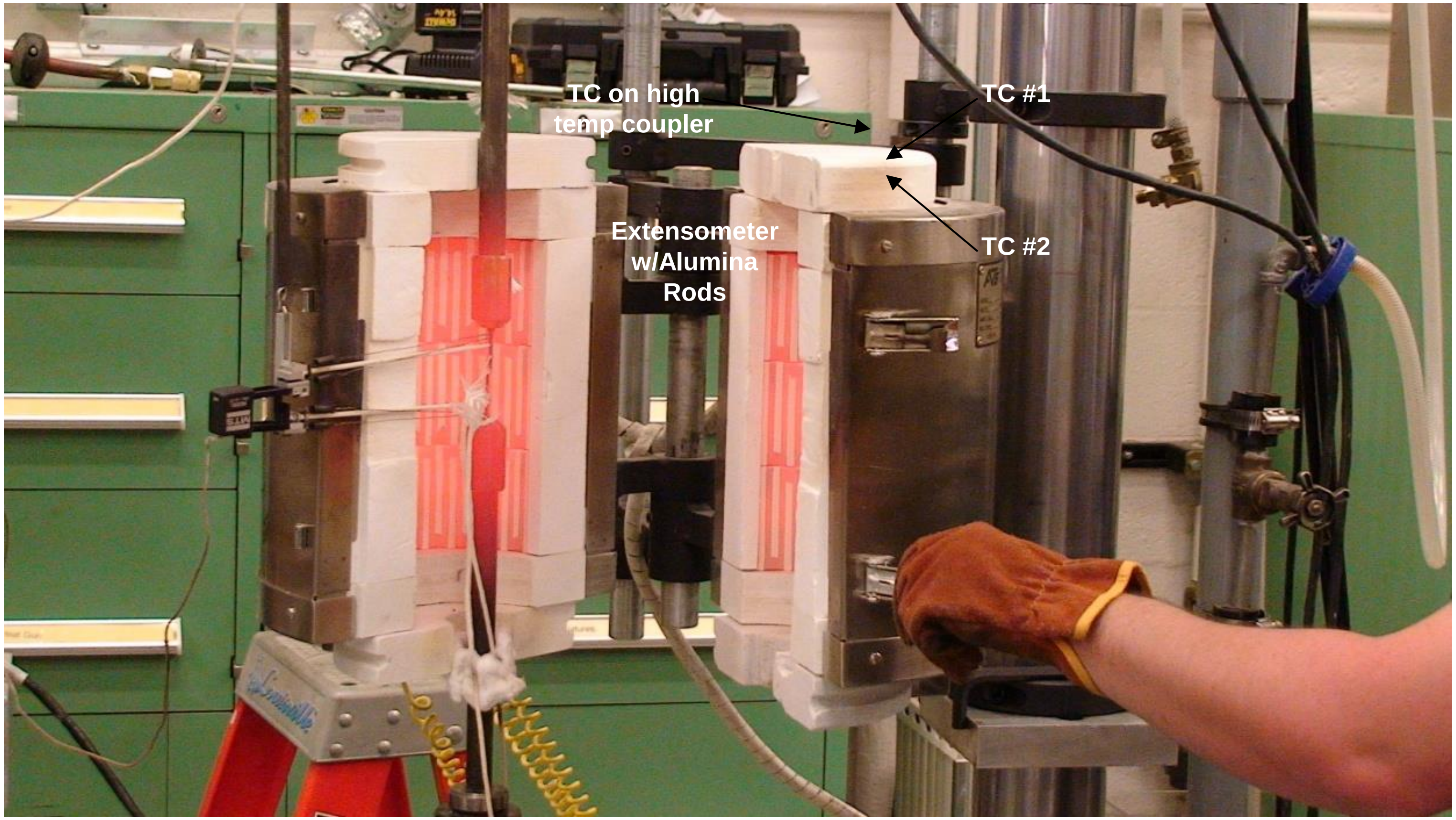
- **Here: multiple Stress-Strain Curves of material variability in calibration of constitutive model**
- **QASPR: similar issues in electronics modeling**
  –calibrations to experimental response curves yield discrete parameter sets considered non-interpolable in between

cylinder Tension-test specimens



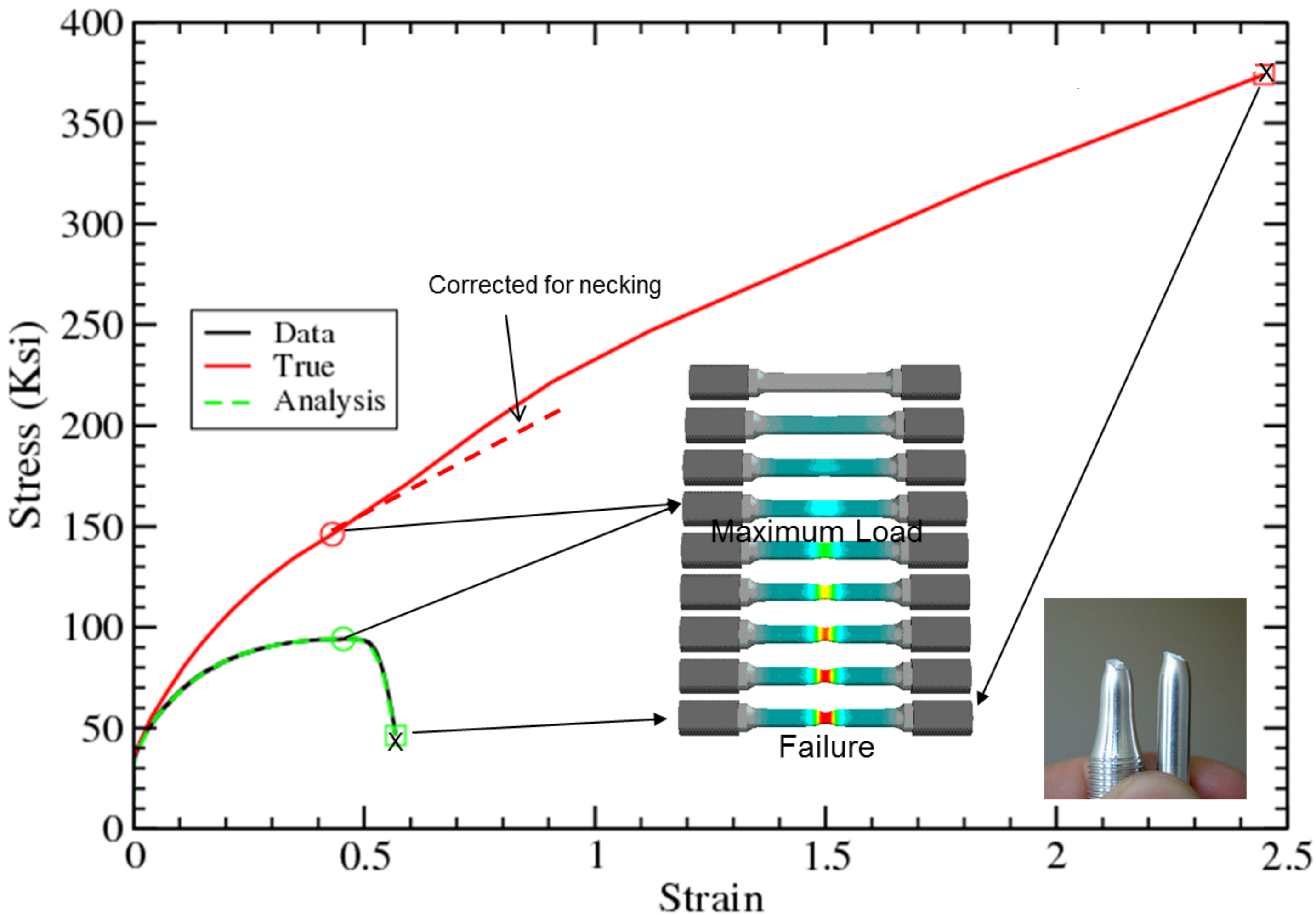
multiple Stress-Strain Curves of material response from specimens in cylinder tension tests at various temperatures

Cylinder Material Specimen Tension Test at 800C



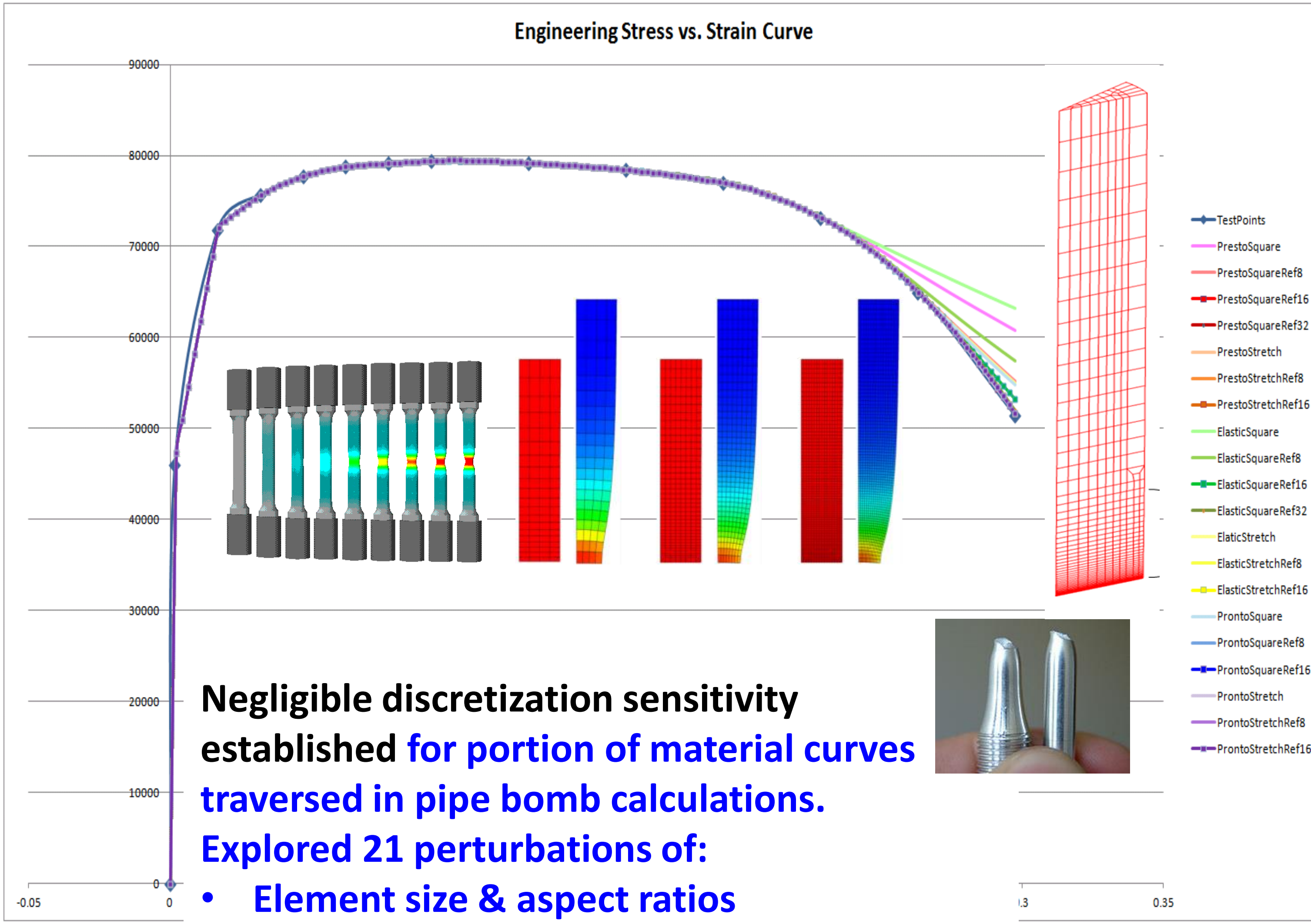
Inversion Procedure to extract Cauchy-Stress/Logarithmic-Strain from Experimental Stress-Strain Curves (Adagio)

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



"Eliminate" Mesh and Solver Effects

in modeling necking/failure in material characterization tests



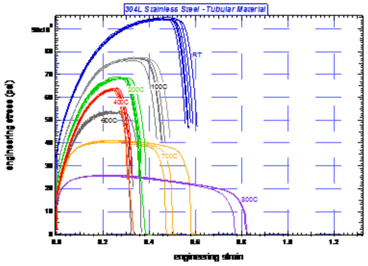
Negligible discretization sensitivity established for portion of material curves traversed in pipe bomb calculations.

Explored 21 perturbations of:

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

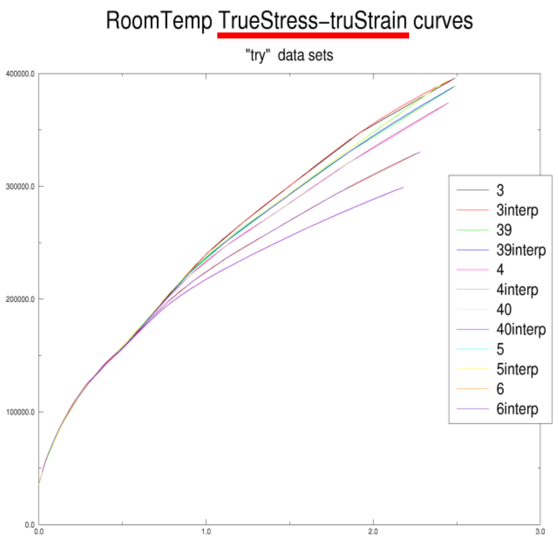
UQ – Characterize Material Strength Variability from Small # of Stress-Strain Curves – a False Start

Generate synthetic ±2σ uncertainty bounds from 6 discrete stress-strain curves

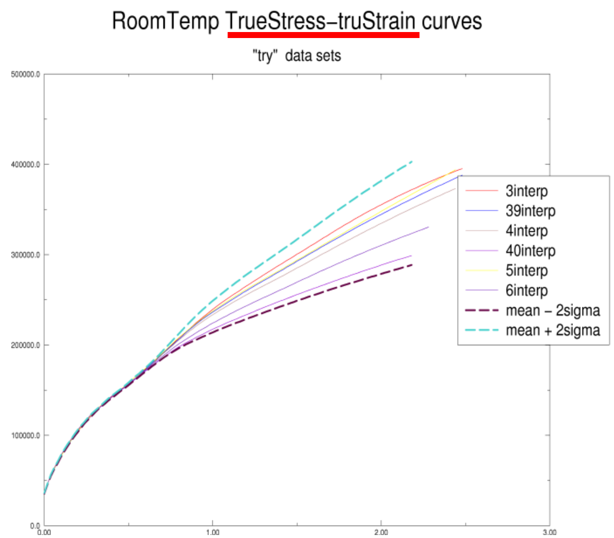


- **Room Temperature Data – 25C**
  --worked OK for this case and for data at some other temperatures

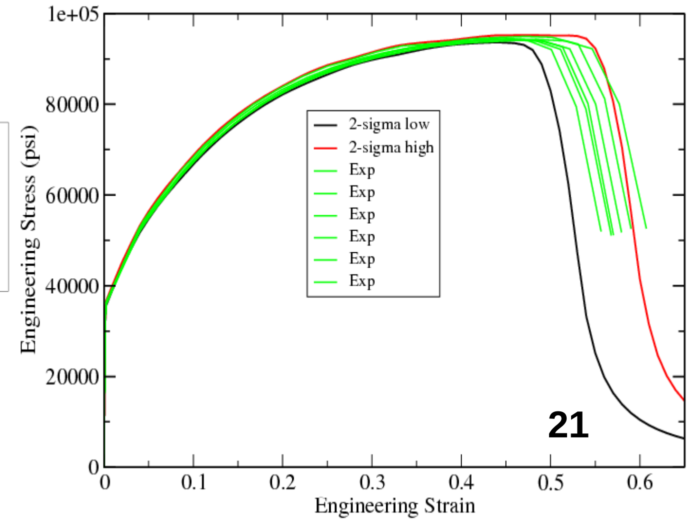
Original data and data interpolated onto standard increments of 0.02 strain



Mean ± 2σ (μ ± 2σ) curves calculated from interpolated data (σ = 1 standard deviation)



μ ± 2σ curves from *True Strain-Stress* space *mapped to Engr. Stress-Strain* for sanity check



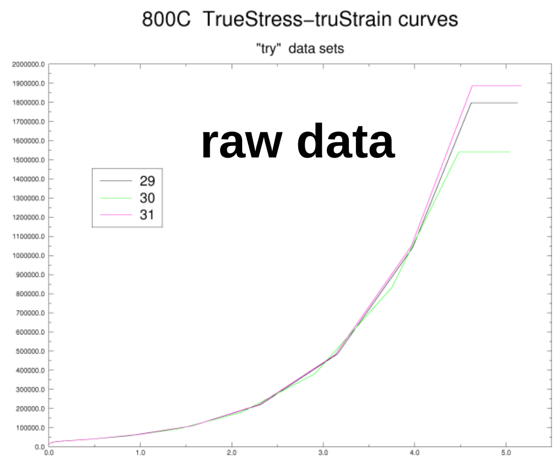
Generation of synthetic ±2σ uncertainty bounds from 3 discrete stress-strain curves

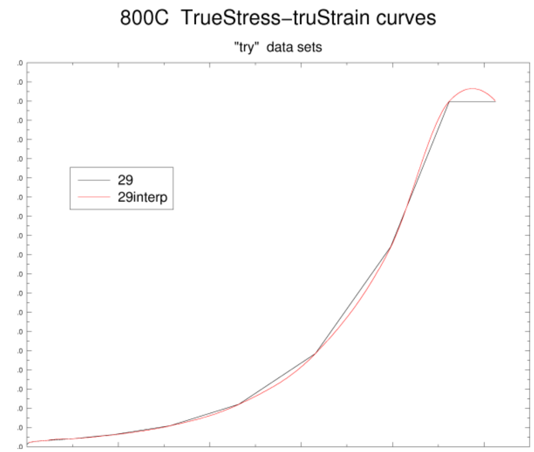
–didn't work for this case or for data at some other temperatures

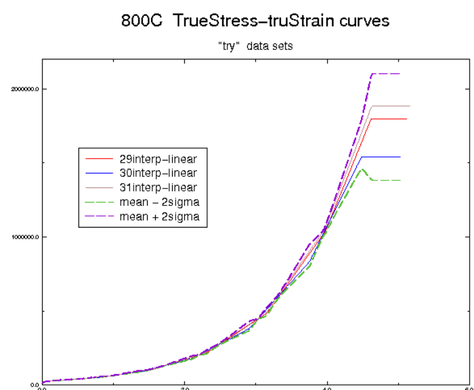
- **800C data**

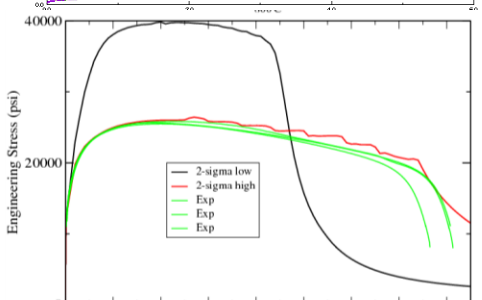
Cubic Interpolation "bubbling" and "curve crossing" problems

raw data

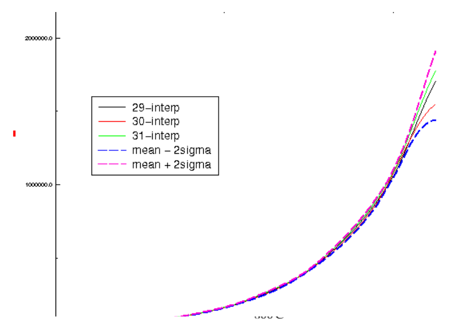


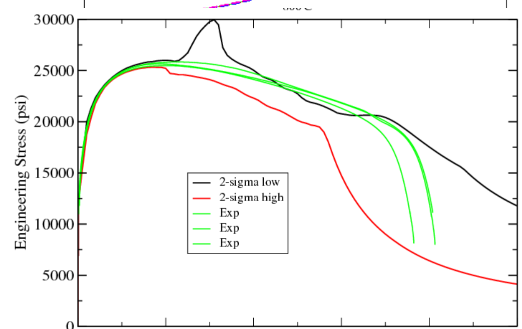




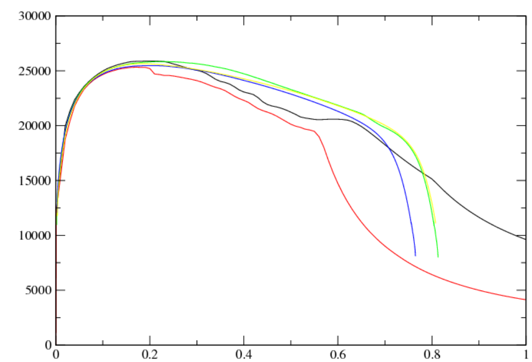


try with linear interp.





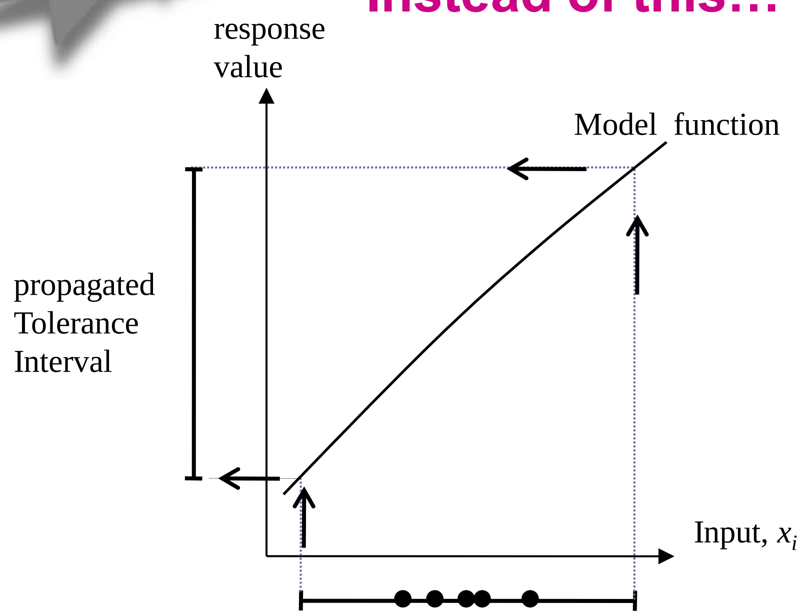
Cub. Interp. & truncated



Wellman further smoothed

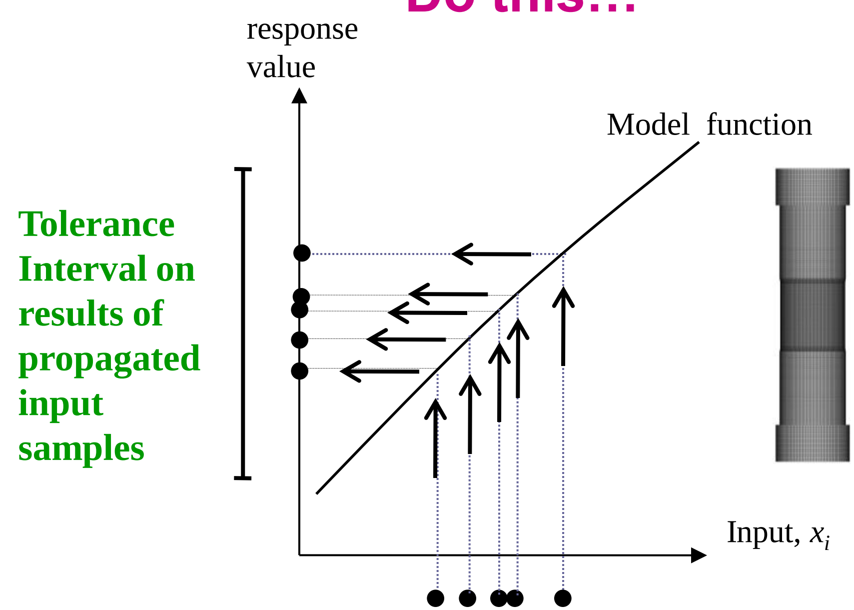
Another way…

Instead of this…

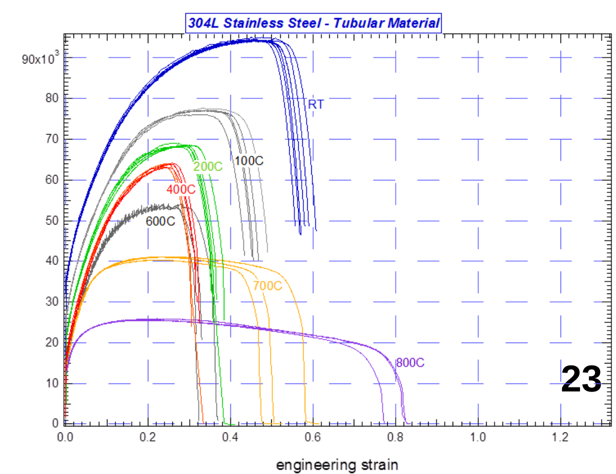


Parameterize input variability, then propagate represented variability

Do this…

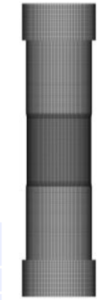


Propagate realizations of input variability, then form Tol Intvl. on realizations of response

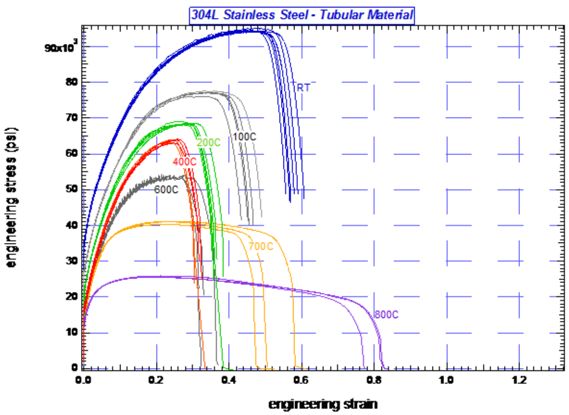


Predicted Variability of Pipe-Bomb Failure Pressures due to Variability of Material Stress-Strain Curves

(Each curve ➡ a run of isothermal pipe bomb model)



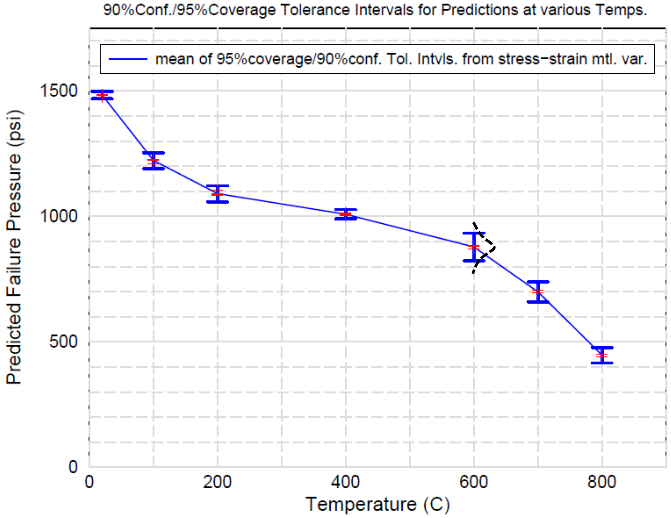
Discrete Random Functions representing material variability



Sparse-Data Tolerance Intervals

Predicted Failure Pressure vs. Temperature

90%Conf./95%Coverage Tolerance Intervals for Predictions at various Temps.



Case	T_max	P_max (psi)	dt (sec)	EQPS_max *	Status	# Procs	cpu-hrs	res	Adaptive
try3-rt	20	1484.5	1.60E-11	0.601		192	0.368	1.00E-06	feti
try4-rt	20	1482.8	9.00E-13	0.571		192	0.308	1.00E-06	feti
try5-rt	20	1485.2	9.00E-13	0.575	high	192	0.324	1.00E-06	feti
try6-rt	20	1485	9.00E-13	0.549		192	0.348	1.00E-06	feti
try39-rt	20	1483.9	9.00E-13	0.587		192	0.402	1.00E-06	feti
try40-rt	20	1474.8	9.00E-13	0.555	Low	192	0.309	1.00E-06	feti
try14-100	100	1227.1	1.00E-11	0.586	High	192	0.441	1.00E-06	feti
try15-100	100	1208.7	9.00E-13	0.528	Low	192	0.546	1.00E-06	feti
try16-100	100	1225.3	9.00E-13	0.561		192	0.31	1.00E-06	feti
try36-100	100	1226.3	8.60E-12	0.559		192	0.335	1.00E-06	feti
try37-100	100	1222.9	1.60E-08	0.549		192	0.284	1.00E-06	feti
try11-200	200	1102.1	1.70E-09	0.529	High	192	0.335	1.00E-06	feti
try12-200	200	1085.8	9.00E-13	0.426		192	2.62	1.00E-06	feti
try13-200	200	1088.6	1.30E-06	0.469		192	2.26	1.00E-06	feti
try34-200	200	1089.9	9.00E-13	0.442		192	0.453	1.00E-06	feti
try35-200	200	1081.7	9.00E-13	0.402	Low	192	0.342	1.00E-06	feti
try17-400	400	1010.3	1.00E-12	0.394		192	0.393	1.00E-06	feti
try18-400	400	1007.2	1.00E-12	0.386		192	0.325	1.00E-06	feti
try19-400	400	1005.7	3.00E-09	0.432		192	0.312	1.00E-06	feti
try32-400	400	1001.9	1.00E-12	0.373	Low	192	2.479	1.00E-06	feti
try33-400	400	1014	1.00E-12	0.384	High	192	0.369	1.00E-06	feti
try22-600	600	869.2	1.00E-12	0.409	Low	192	0.361	1.00E-06	feti
try23-600	600	880.1	4.00E-07	0.49		192	2.54	1.00E-06	feti
try24-600	600	884.7	1.20E-09	0.523	High	192	0.359	1.00E-06	feti
try25-700	700	705.1	1.00E-12	0.617	High	192	0.431	1.00E-06	feti
try26-700	700	694.8	1.00E-12	0.605	Low	192	0.431	1.00E-06	feti
try27-700	700	695.5	1.00E-12	0.606		192	0.443	1.00E-06	feti
try29-800	800	448	3.50E-11	0.501		192	0.476	1.00E-06	feti
try30-800	800	440.8	1.00E-12	0.632	Low	192	0.431	1.00E-06	feti
try31-800	800	448.8	1.00E-12	0.645	High	192	0.414	1.00E-06	feti

Key Assumption for Computational UQ Feasibility

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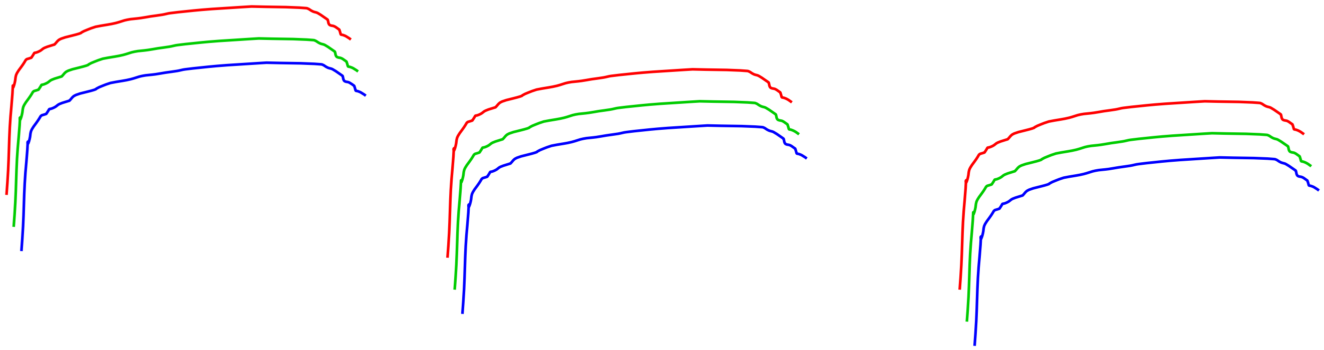
Assume material strength is strongly correlated over temperature, e.g.,

600C **700C** **800C**



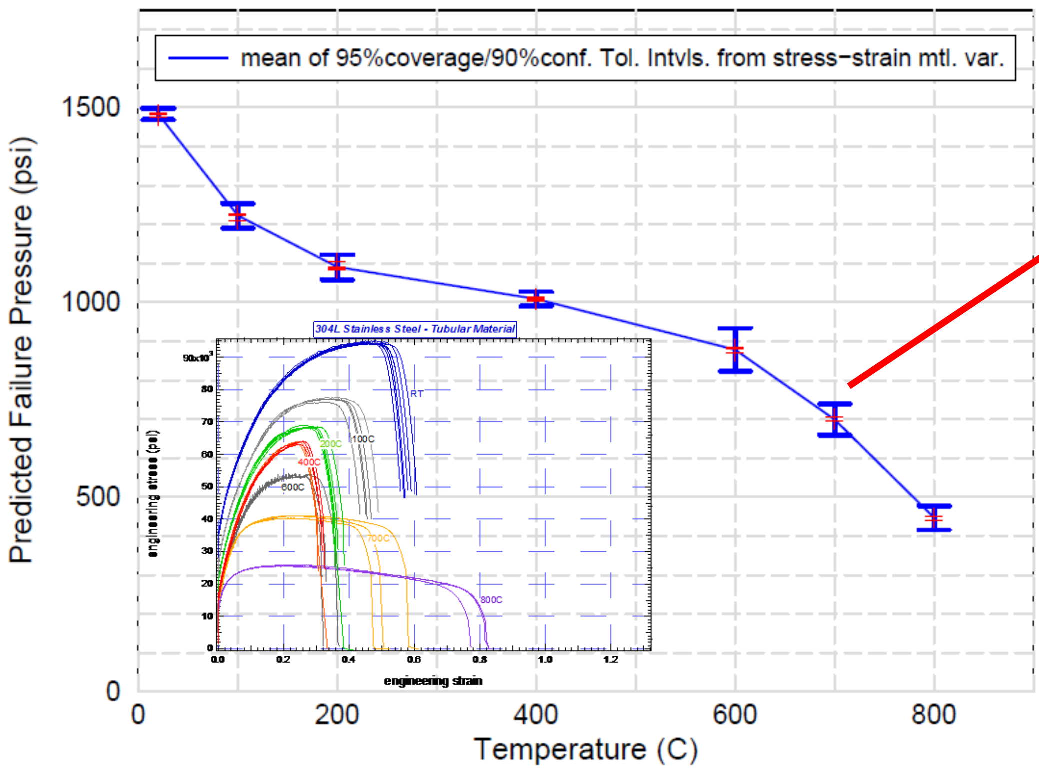
Red curves = high strength (HS) σ-ε curve set over temperatures

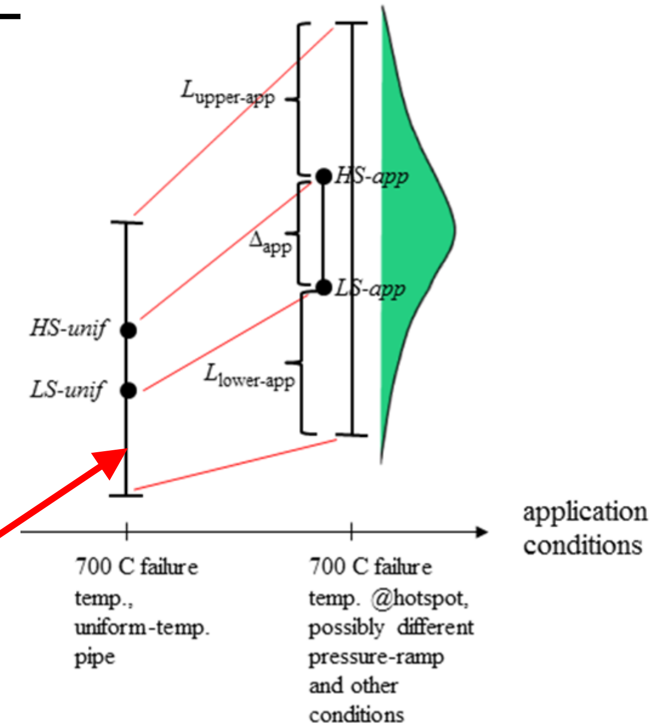
Green curves = medium strength (MS) set over temperatures

Blue curves = low strength (LS) set over temperatures

Economical Parameterization of TIs via 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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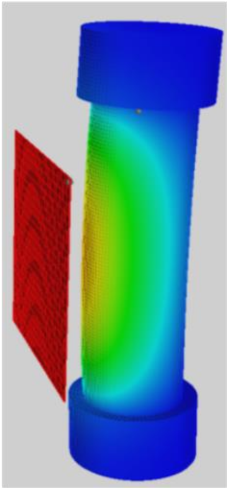
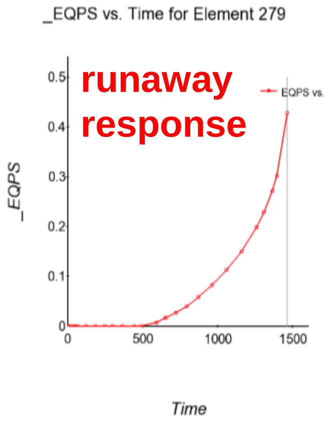
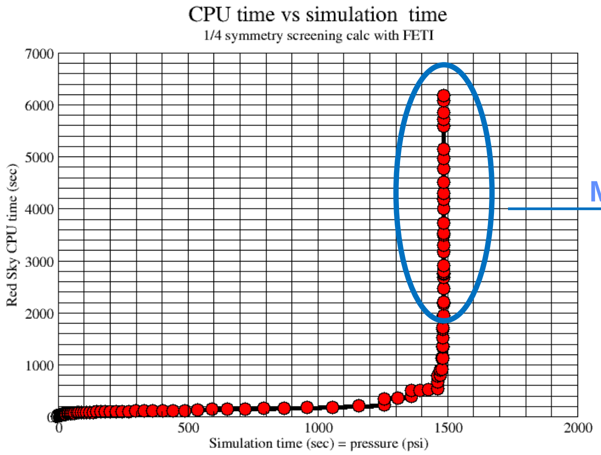
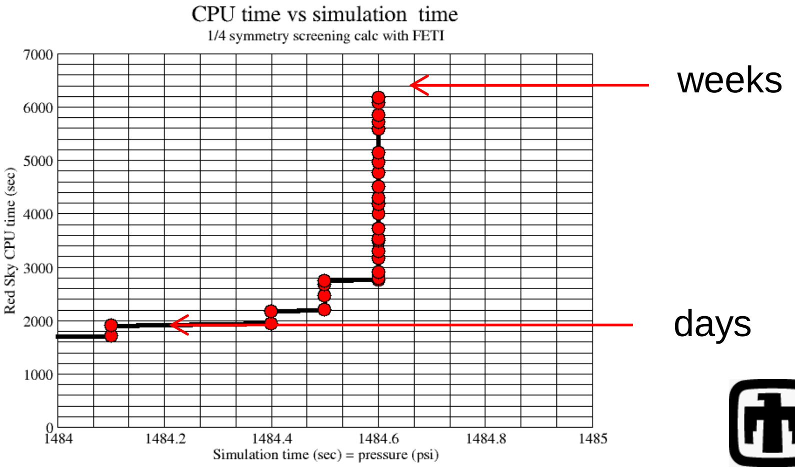
Pipe Response Simulation Difficulty: *creep up to a physical instability point*

- **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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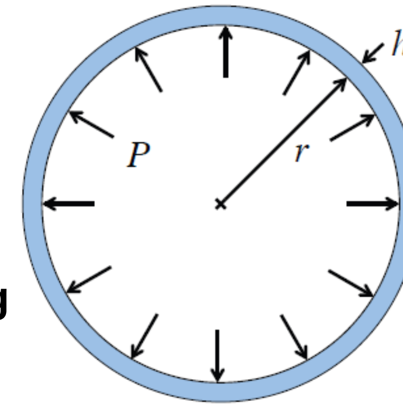
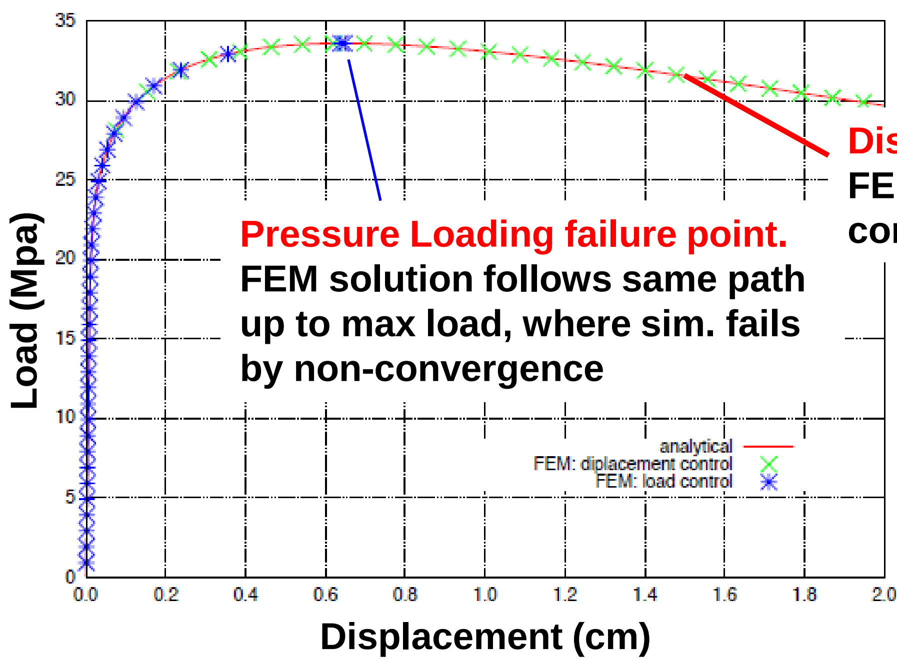
Calculation Instability marking Structural Failure confirmed for analytic "nearby problem" by Bill Scherzinger (1524)

- **Test Problem:**
  - **Ring internally loaded to failure (plain strain)**
  - **Two types of loading:**
    - ***displacement controlled* — radial displacement loading**
    - ***load controlled* — internal pressurization**





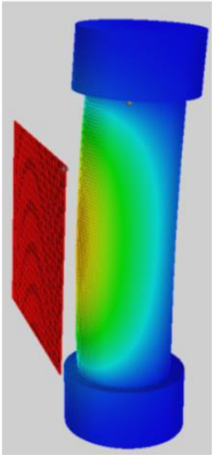
Solver Accuracy and Speed Assessment for Accurate Curve "Strength" Rankings

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)

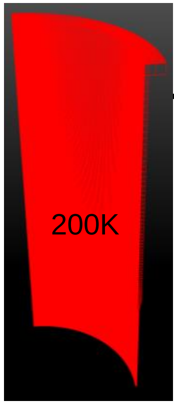
* CPU times reported in Adagio output file via global output variable *cpu_time*. CG and FETI sims. were run on 192 processors of Red Sky

- **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**



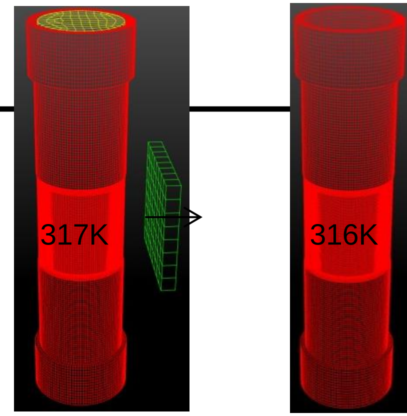
Models used for UQ



4tt

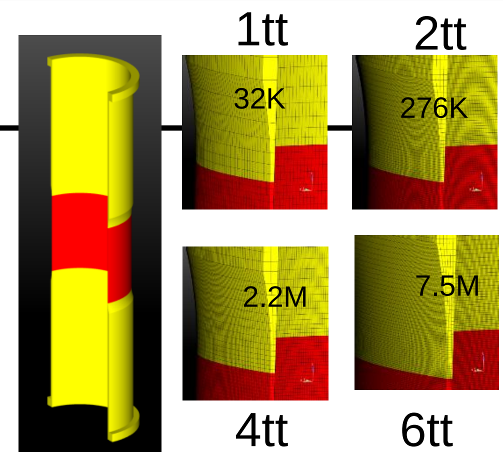
High-Low materials study
Isothermal - 1/8 symmetry

4tt

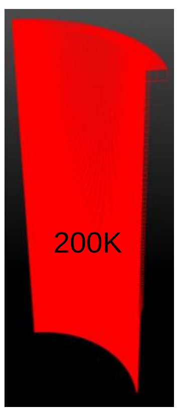


4tt

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



Mesh convergence
¼ symmetry



4tt

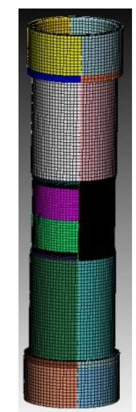
Solver parameters study
Isothermal - 1/8 symmetry

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

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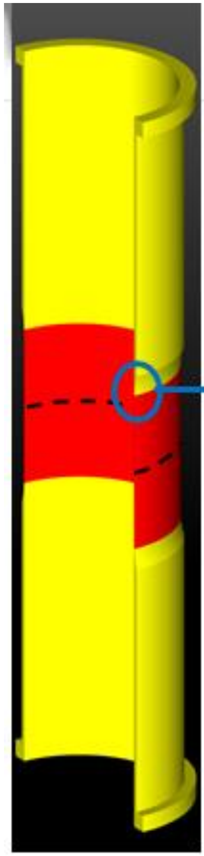
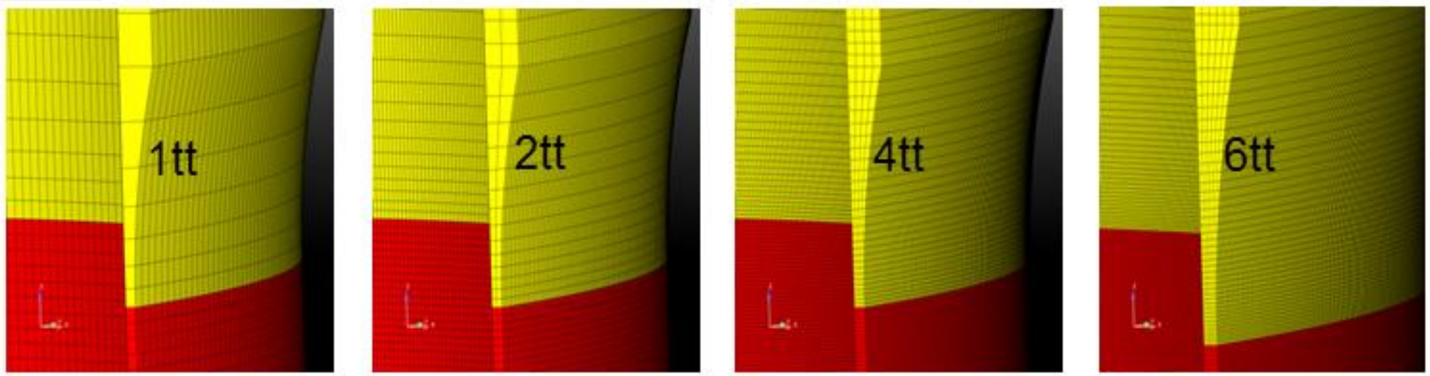
Pipe Bomb Calculation Verification
Mesh Refinement Studies



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)

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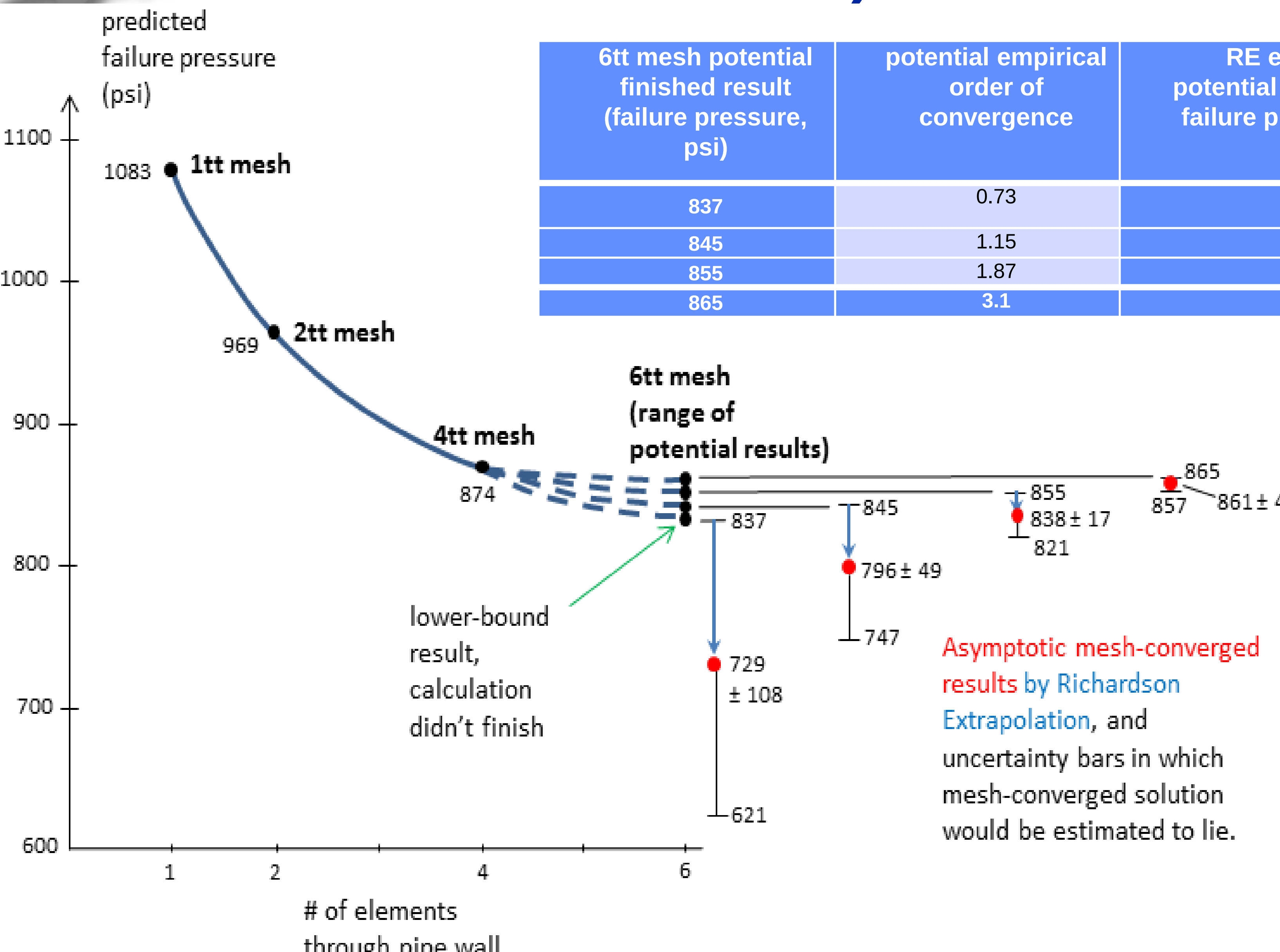
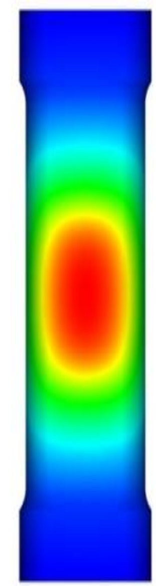
Calculation Verification
Mesh Study Results

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.



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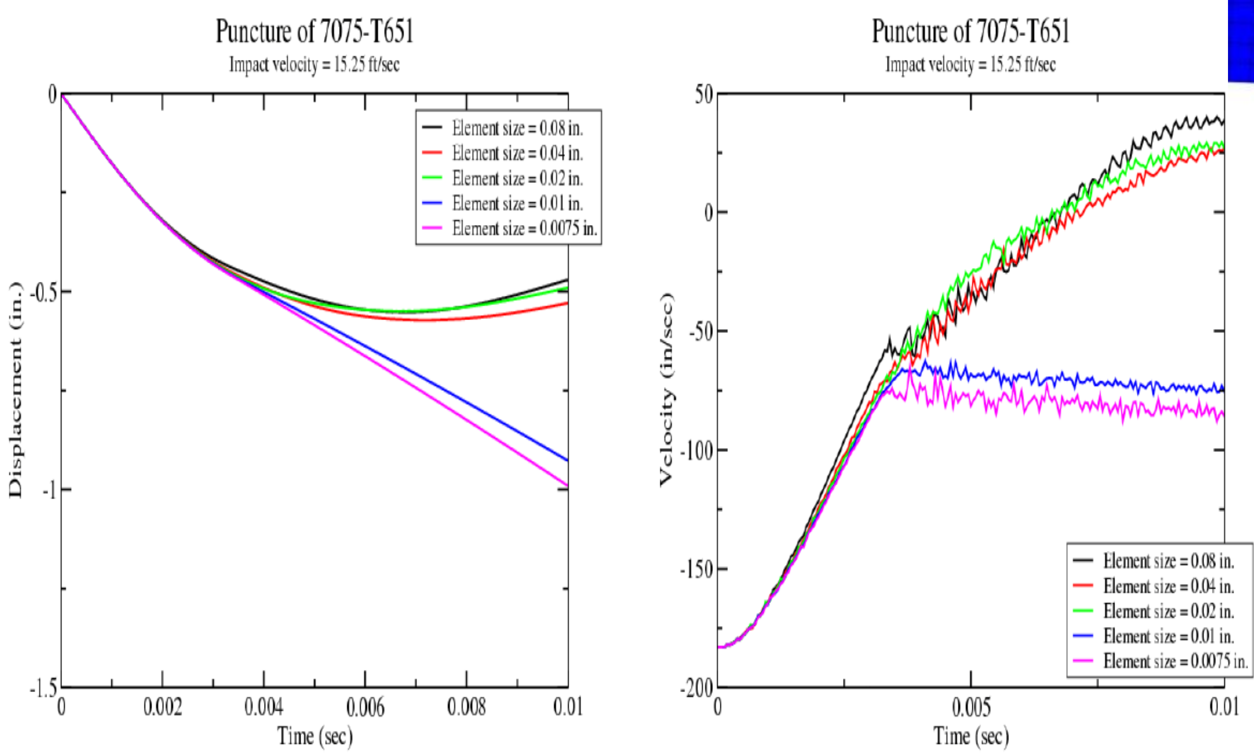
Aim for at least 4 suitably refined meshes

Example of divergent behavior between coarse-group and fine-group meshes….Keep Refining!

- In this case we see completely different behavior from coarse meshes (1-3) and fine meshes (4-5).



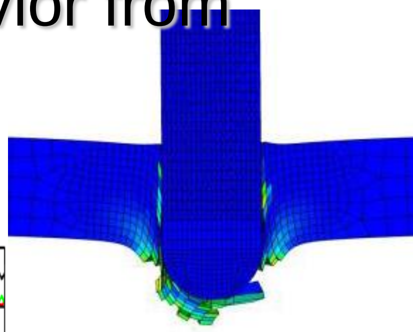


Plate Puncture

Displacement/velocity histories (15.25 ft/s).

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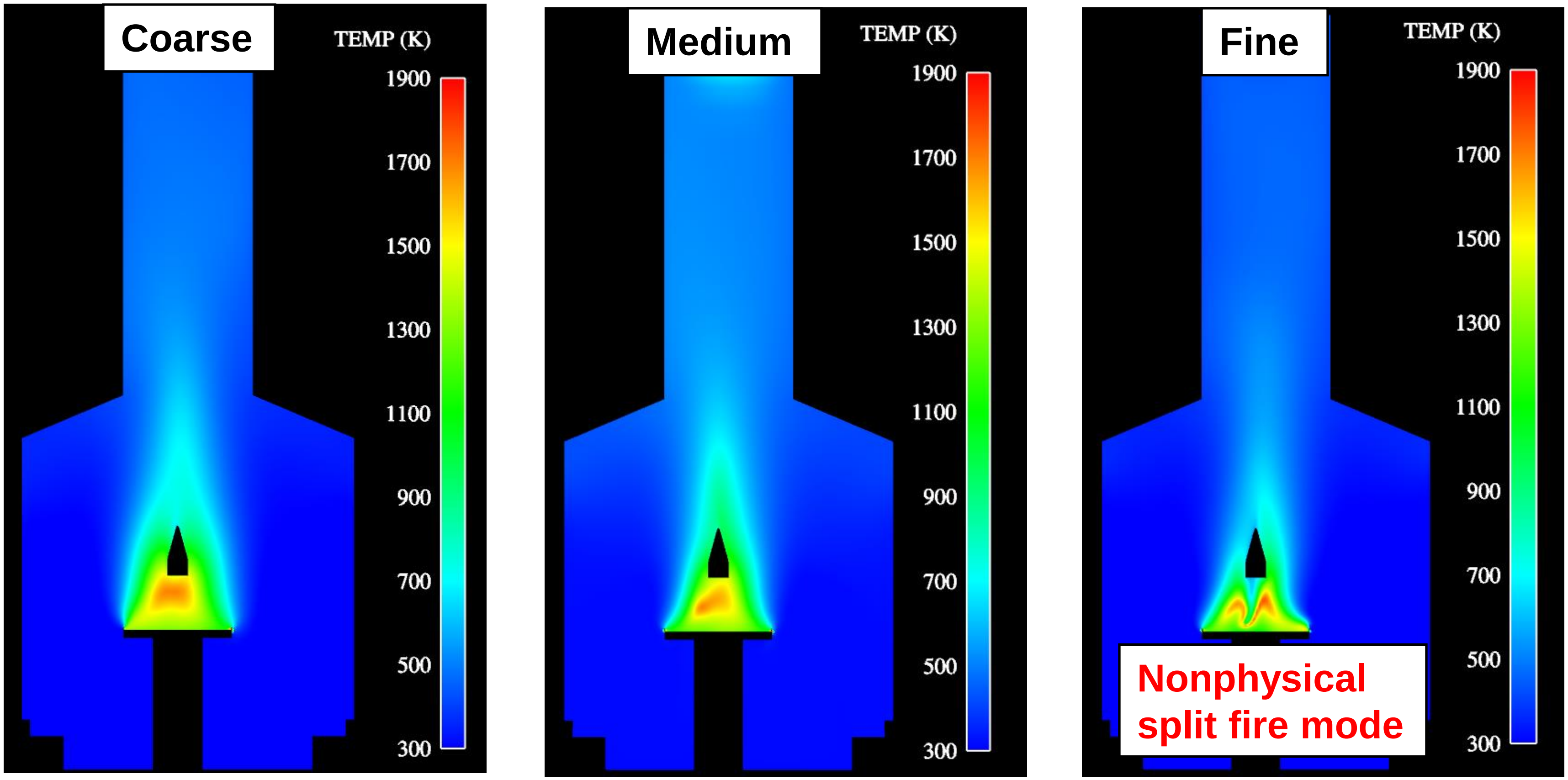
BEWARE! — Some formulations aren't meant to converge with continued mesh refinement



- fire CFD with **BVG RANS** turbulence model (spatial filtering below a certain length scale)
- fixed spatial filtering length scale not consistent with continued grid refinement

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

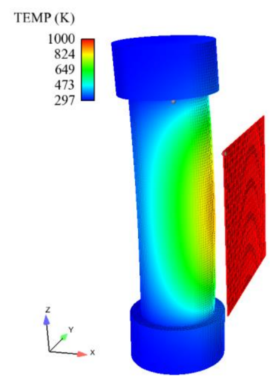
Model

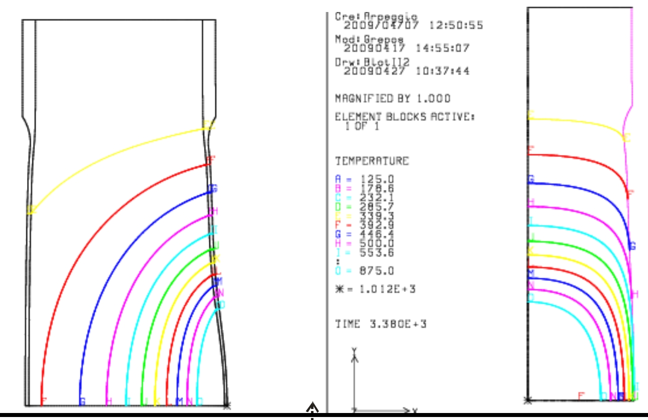
- Pipe radiatively heated by plate
- Convection neglected
- Viewfactors change as pipe bulges toward plate at hot spot

Temperature Contours

Side view, top half of pipe

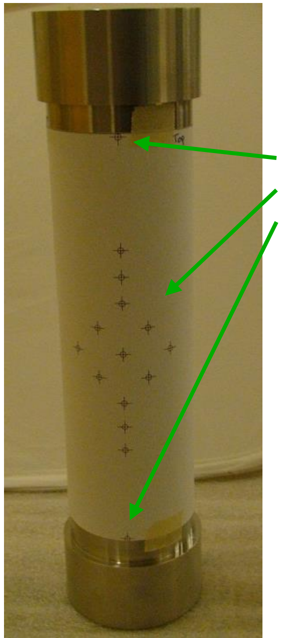
Front view, ¼ symmetry





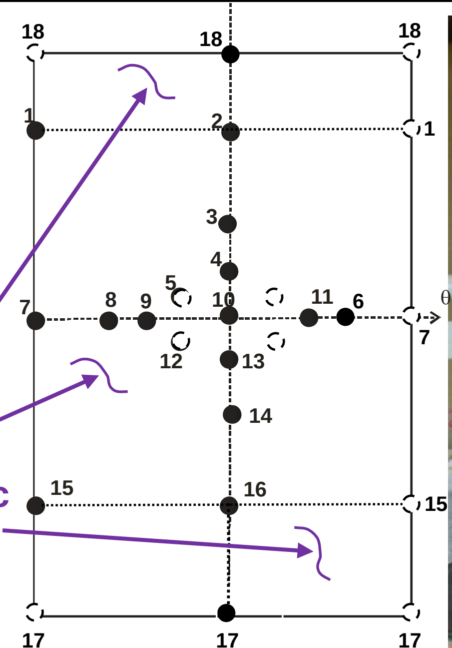
Experiment Design Quantities

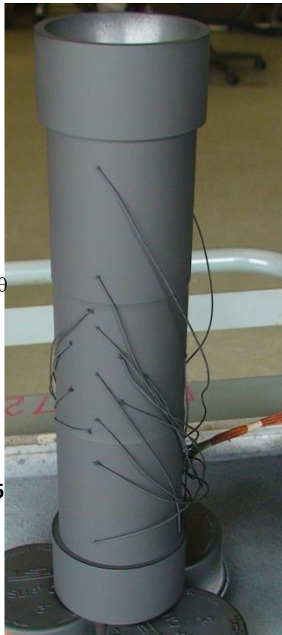
- Size & location of plate relative to pipe
- # of thermocouples and locations to adequately reproduce temperature field on pipe surface
- in conjunction with design of interpolation method



Thermocouples (23 total, front & back)

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





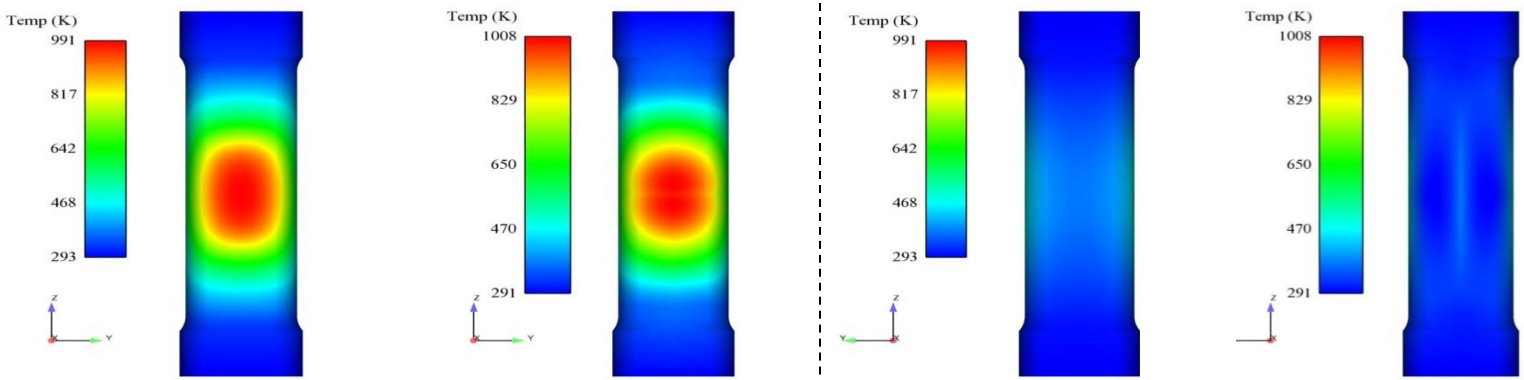
TC Temperature Field Mapping/Interpolation Error

Exact Temperature Field
Front view, 3390sec.

Interp. Temperature Field
Front view, 3386 sec.

Exact Temperature Field,
Back view, 3390sec.

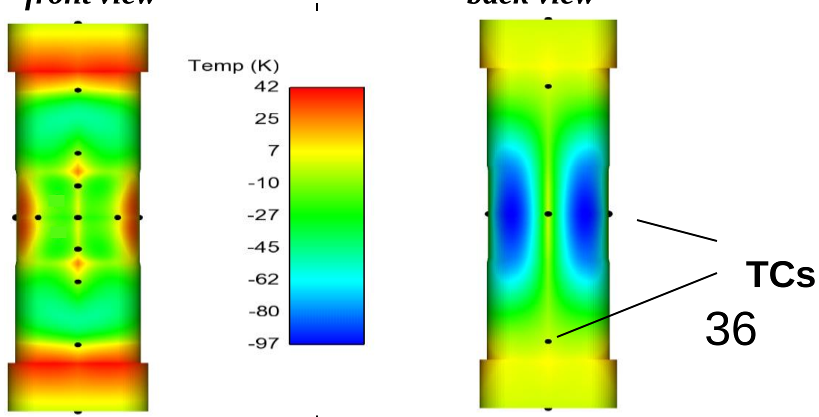
Interp. Temp. Field
Back view,3386sec.



Difference (error) Plots

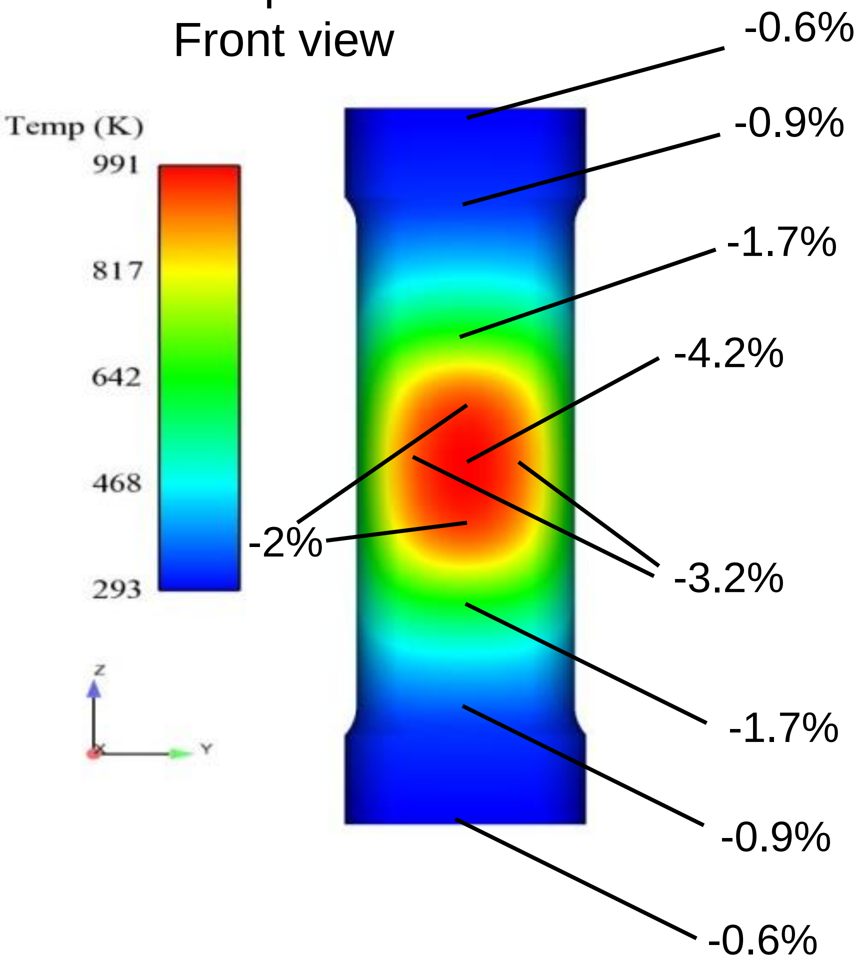
- **temperature interpolation error is characterized and corrected for validation predictions**
- **a ~4% (35 PSI) error in predicted failure pressure if not corrected for interp. error**

front view *back view*

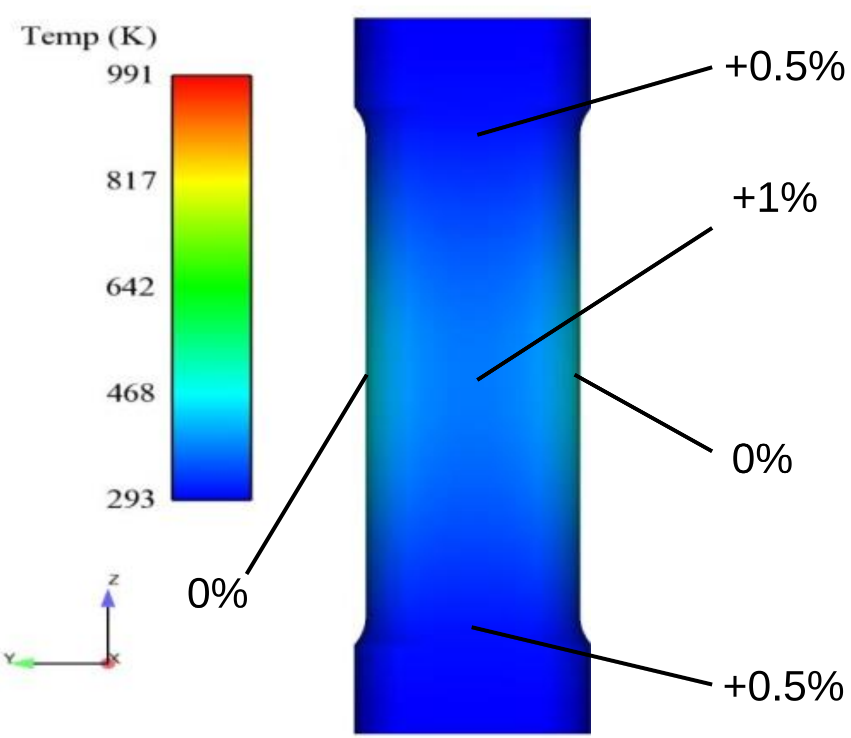


Bias Correction of TC Temperatures for Contact Resistance and Fin Effects

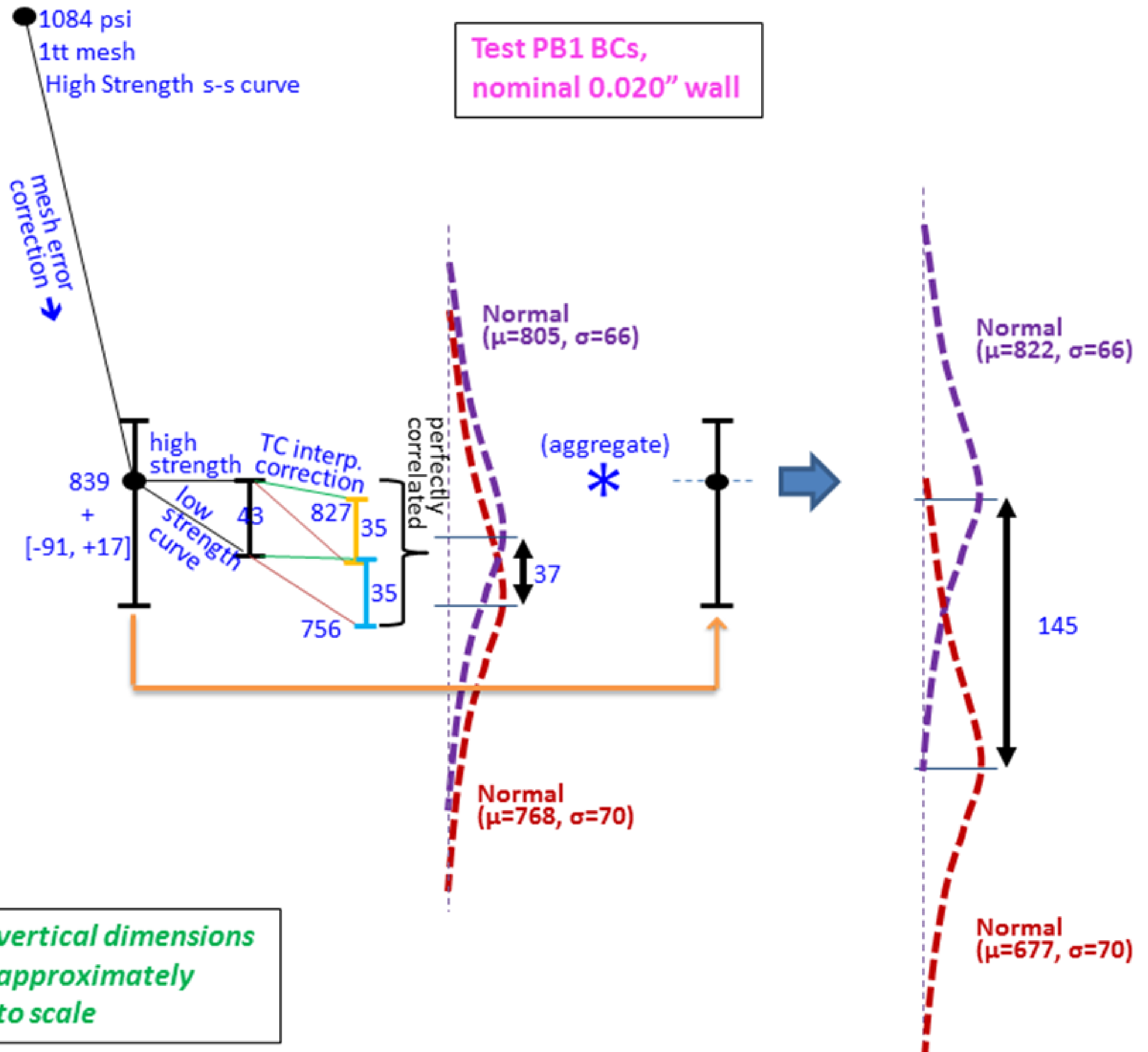
Temperature Field
Front view



Temperature Field
Back view

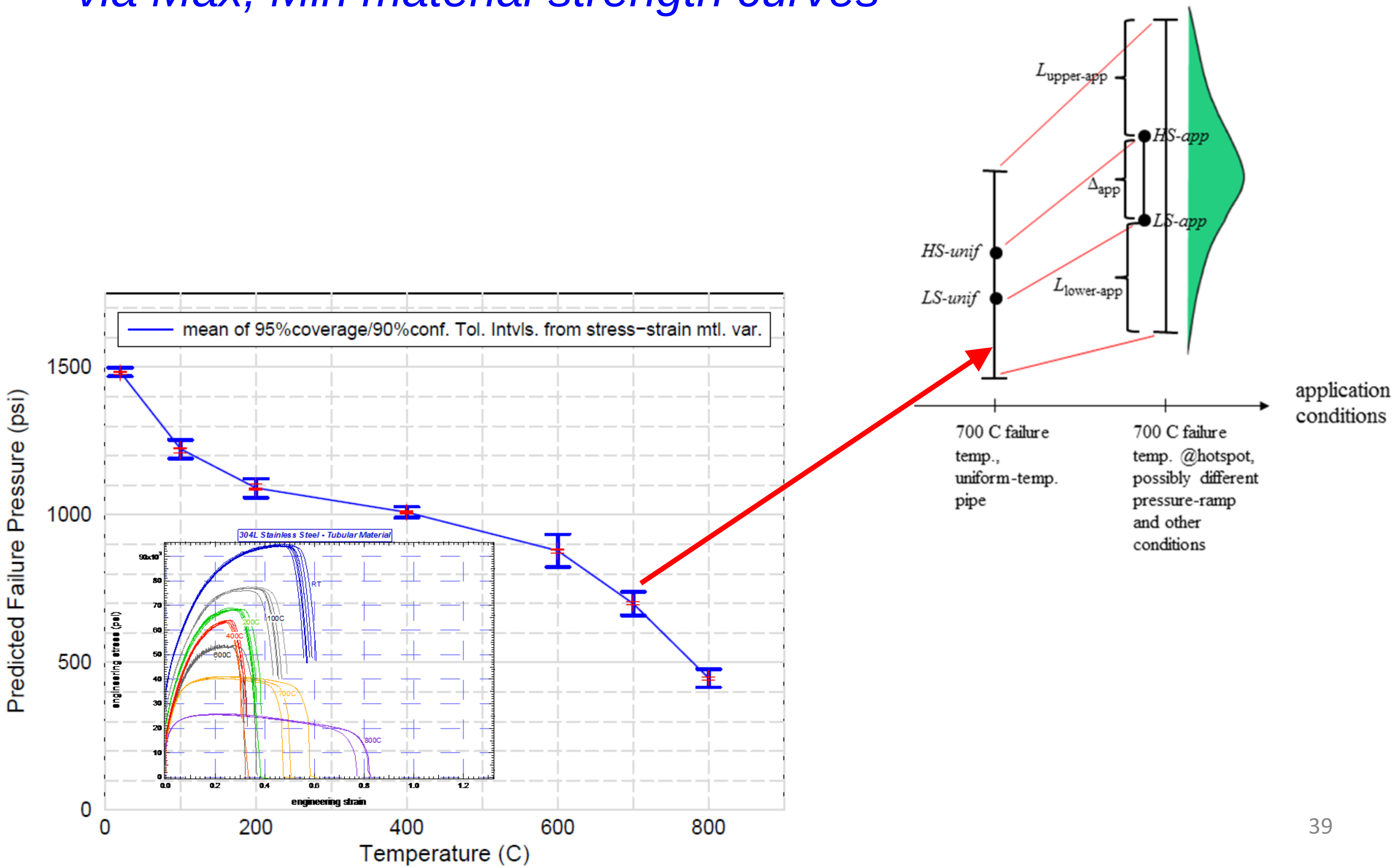


Simulation UQ Rollup



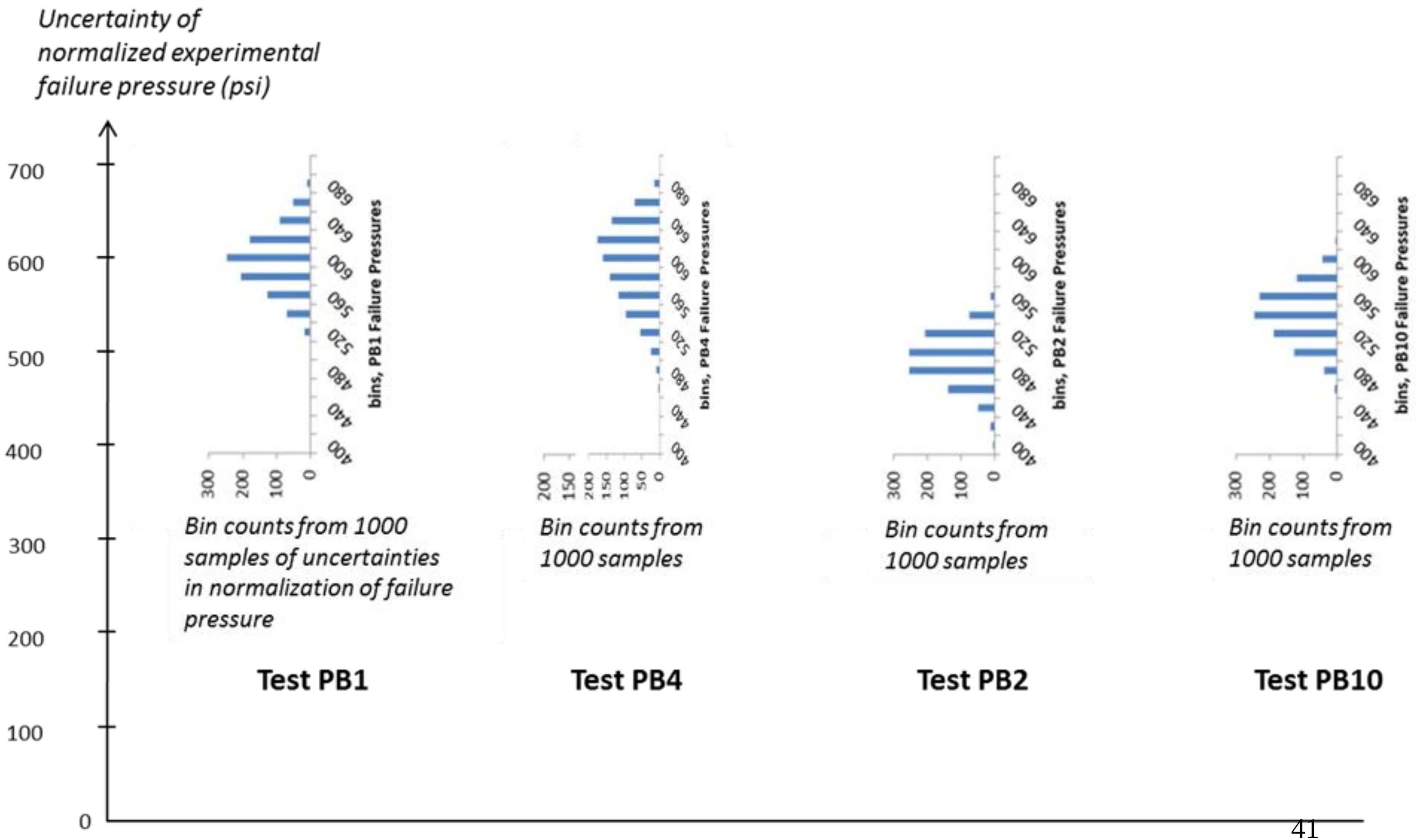
vertical dimensions approximately to scale

Tolerance Intervals/Normal PDFs on previous slide by Scaling of Failure Pressure Variability via Max, Min material strength curves



Processing of Experimental Failure Pressures

Normalized Failure Pressures accounting for Experimental Uncertainties



Spreadsheet propagation of Experimental Uncertainties

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

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

random and systematic uncertainties of experimental inputs & outputs

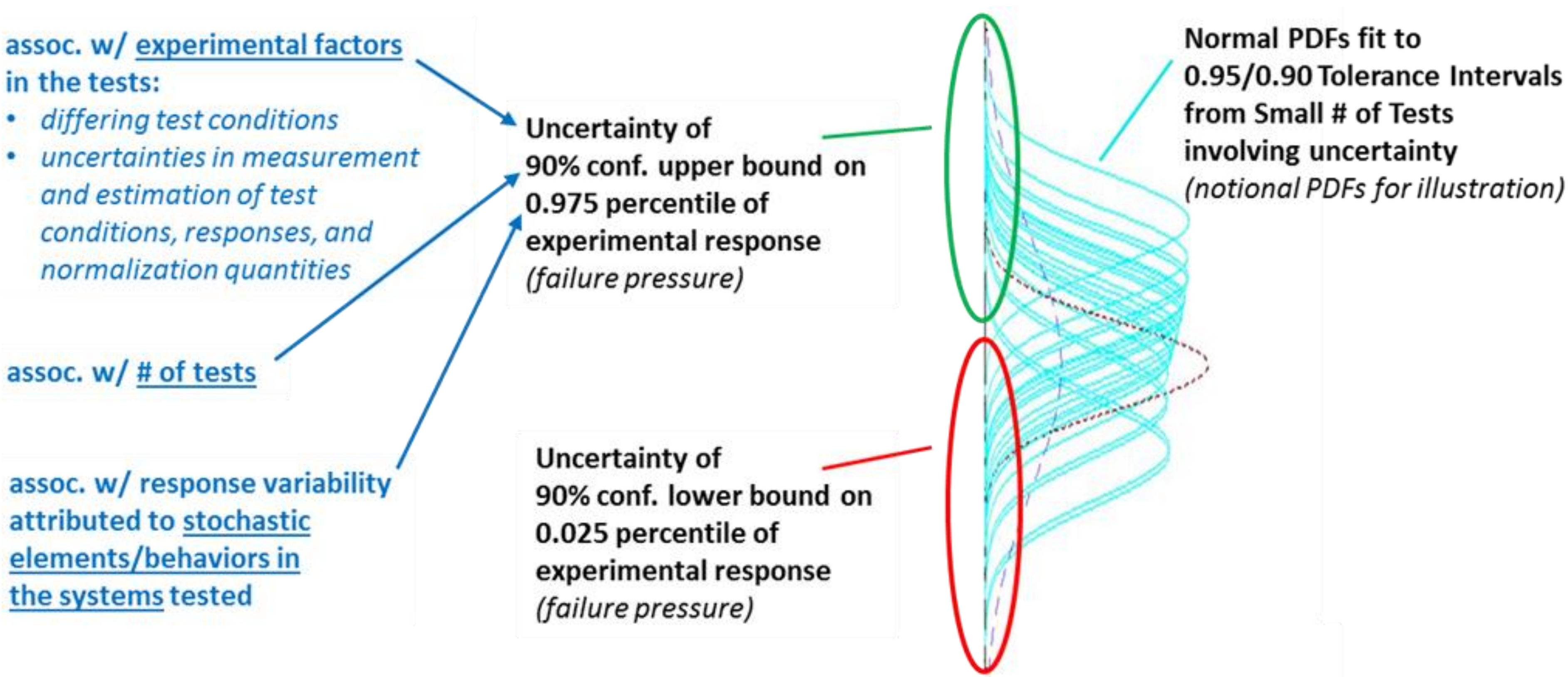
B1	realization j
B2	$\Delta Pfail_{measPB4,j}$ = A2j, systematic betw. PB1 & PB4
B3	$w_{actPB4,j}$ = [0.02, 0.024] inches
B4	$\Delta w_{PB4,j} = w_{nomPB4} - w_{actPB4,j}$ = 0.02" − B3
B5	$\left(\frac{\partial(Pfail_{PB4})}{\partial(w)}\right)_j$ = A5j, systematic betw. PB1 & PB4
B6	= (B4*B5)$_j$ psi
B7	$\Delta T_{meas\text{-}TC/DAQ,j}$ = [−0.0025*711, +0.0025*711] C
B8	$\Delta T_{meas\text{-}contact,j}$ = A8j, systematic betw. PB1 & PB4
B9	$\Delta T_{TC4location,j}$ = [−15, 15] C
B10	$\left(\frac{\partial(Pfail_{PB4})}{\partial(T@fail\_point)}\right)_j$ = A10j, systematic betw. PB1 & PB4
B11	= (B7 + B8 + B9)$_j$ *B10$_j$
B12	$[Pfail_{model}(\vec{x}_{nomPB1}) - Pfail_{model}(\vec{x}_{nomPB4})]$
B13	= 655 psi + (B2 + B6 + B11 + B12)$_j$ psi = $Pfail_{PB4}(\vec{x}_{nomPB1})_j$

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

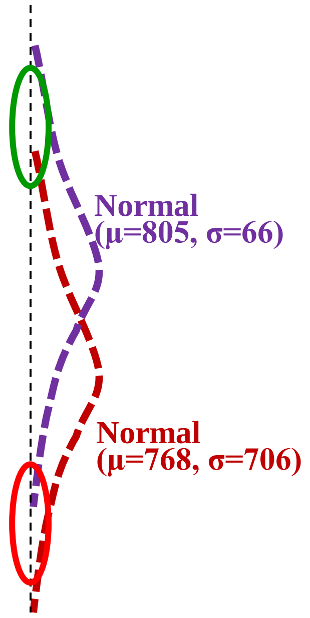
UQ Rollup for Experiments

Uncertainty of 0.025 & 0.975 percentiles of Failure Pressure

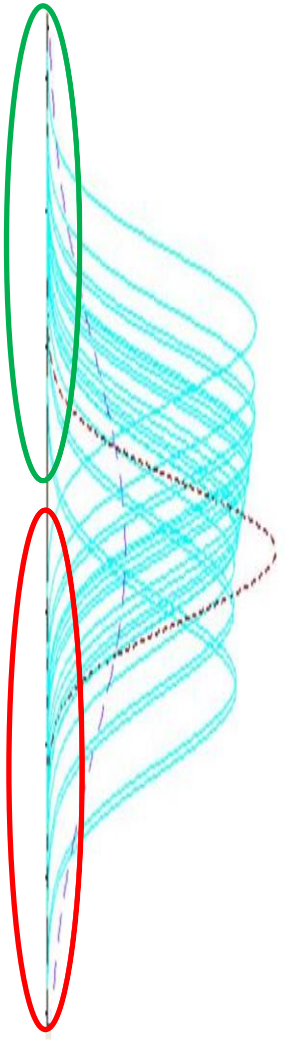
- these %iles combine uncertainties in both mean & variance of response



Comparison of Processed Experimental and Simulation Percentiles

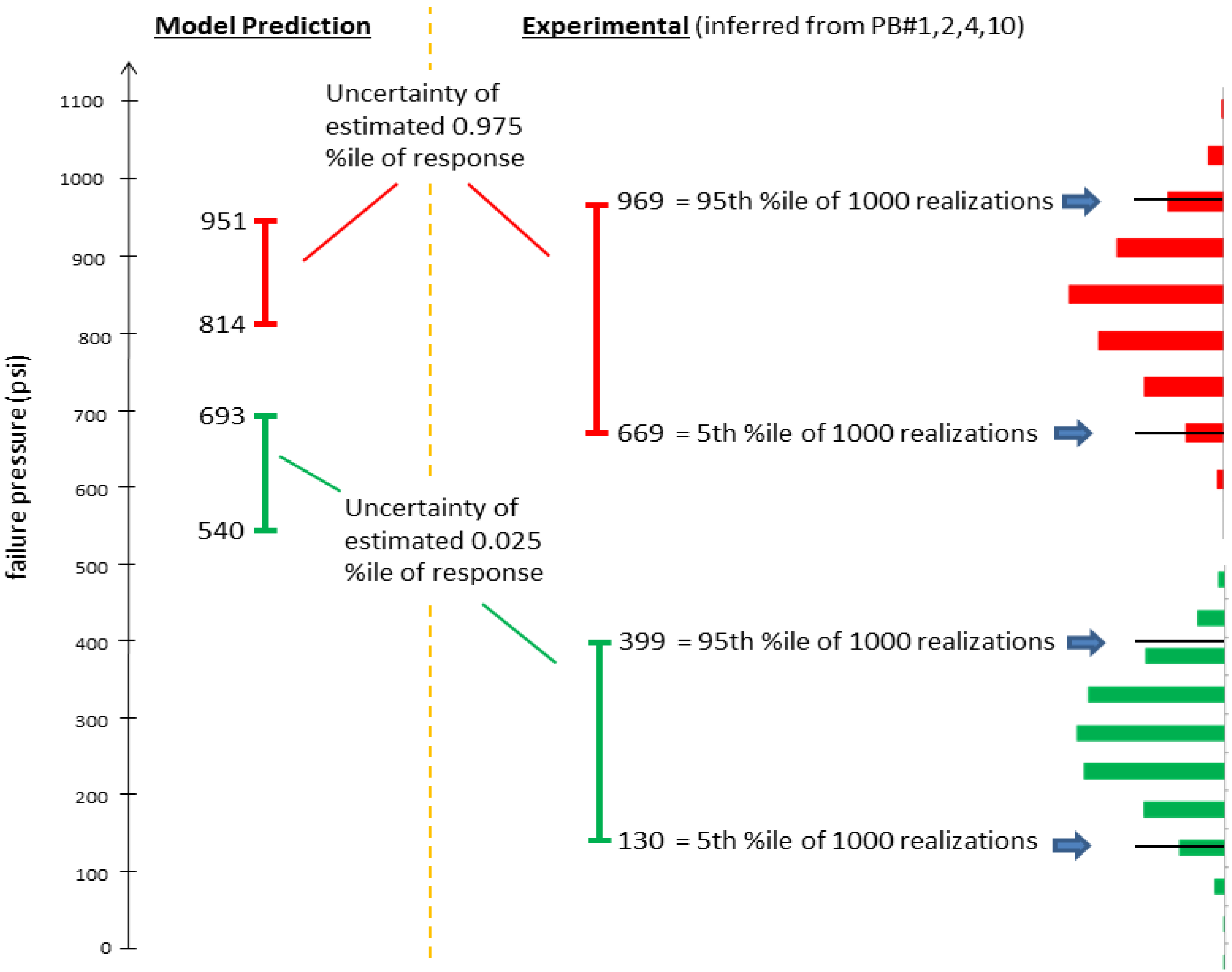


Net simulation uncertainty



Net experimental uncertainty

<u>Lower</u> Percentile of Predicted Failure Pressure is ***NonConservative*** *for Intended Model Use*



Remarks

- **"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)
  - Quantification and economical management of model discretization effects
  - Rollup of various types, sources, and representations of uncertainty
  - Sparse experimental data
  - Multiple replicate experiments
  - Stochastic phenomena and models

Real Space Framework has evolved from working many <u>diverse</u> and <u>challenging</u> applications

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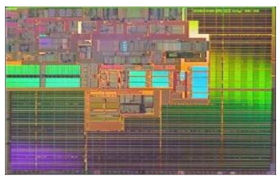
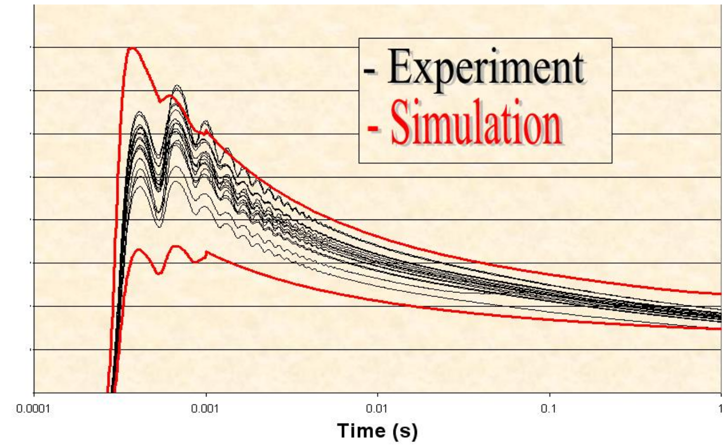
- **QASPR - radiation-damaged devices and circuits**
  - **model calibration & validation**

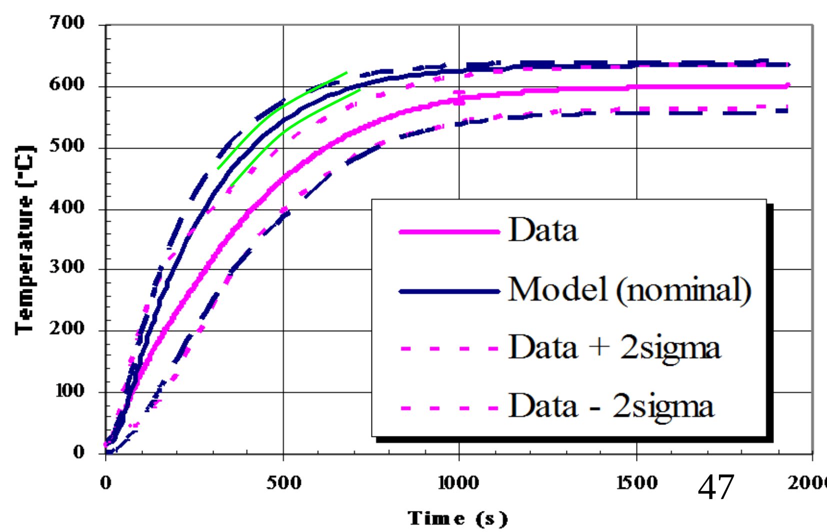
neutrons
x-rays
γ-rays
radiation damage



<u>Device</u> effects (transistor, diode, etc.) and <u>circuit</u> effects



- **Temperature response of weapon components**
  - **stronglinks**
  - **weaklinks**



Validation/Conditioning of Foam Thermal Transport Model at Elevated Temperatures

(thermal conductivity with radiation enhancement term)

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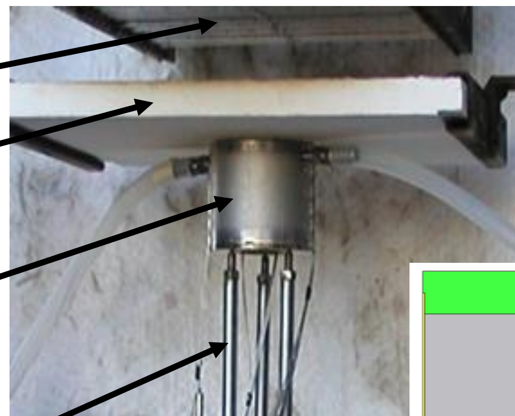
Experiments

quartz heating lamps

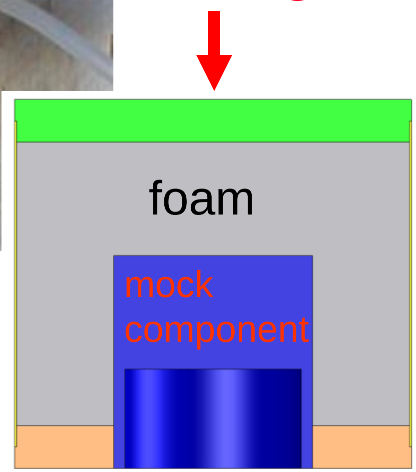
insulation board

24 thermocouples on and inside canister

pointed low-thermal-contact holding posts

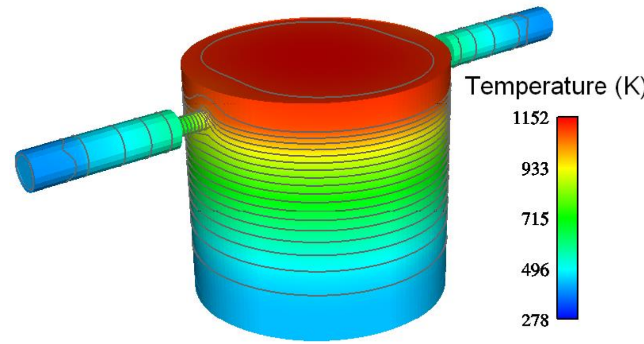


Applied heating



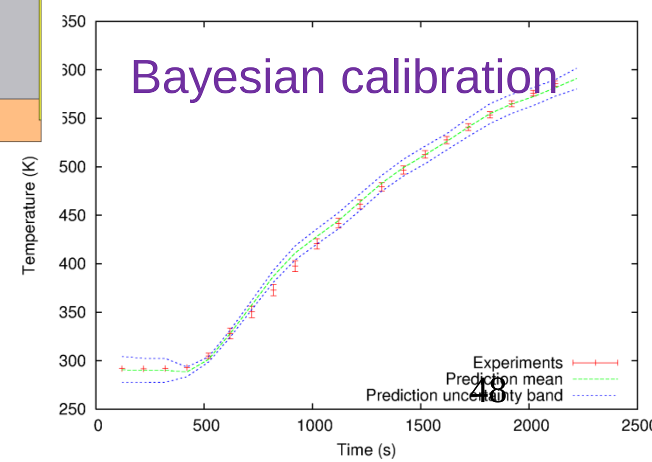
decomposed foam char matrix

Simulations



FE Thermal Model:

- **Conduction,**
- **Convection**
- **Radiation**



Applications worked…

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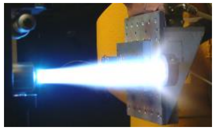
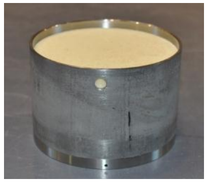
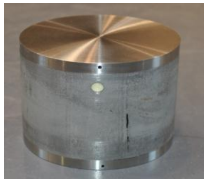
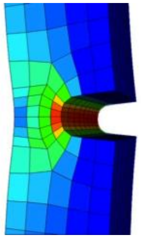
- Validation of Propellant Fire Models



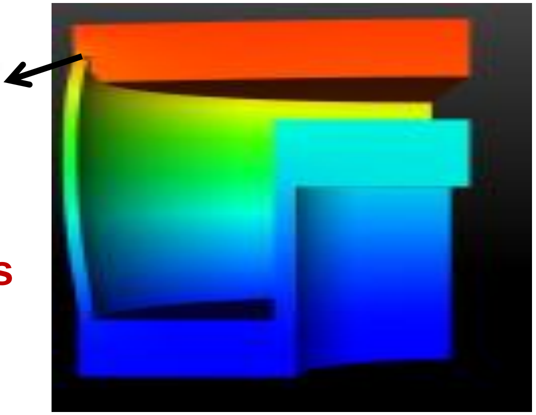
- <u>PCAP project</u>
- heat → foam decomp. → internal pressurization → container-deformation → eventual failure at lid welds

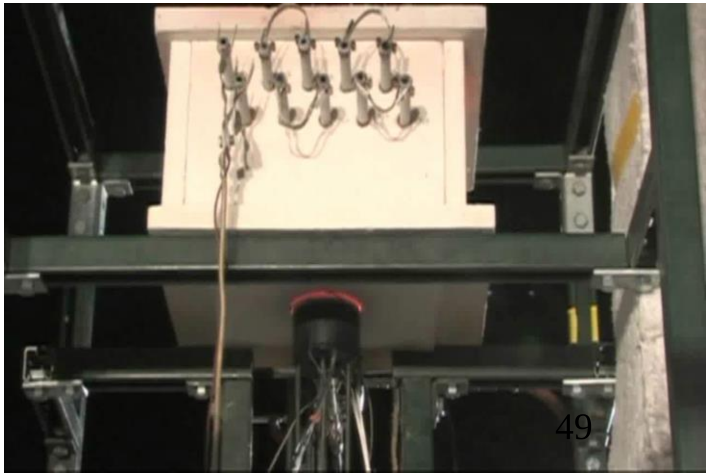






stress
at welds





Sandia Thermal Test Complex

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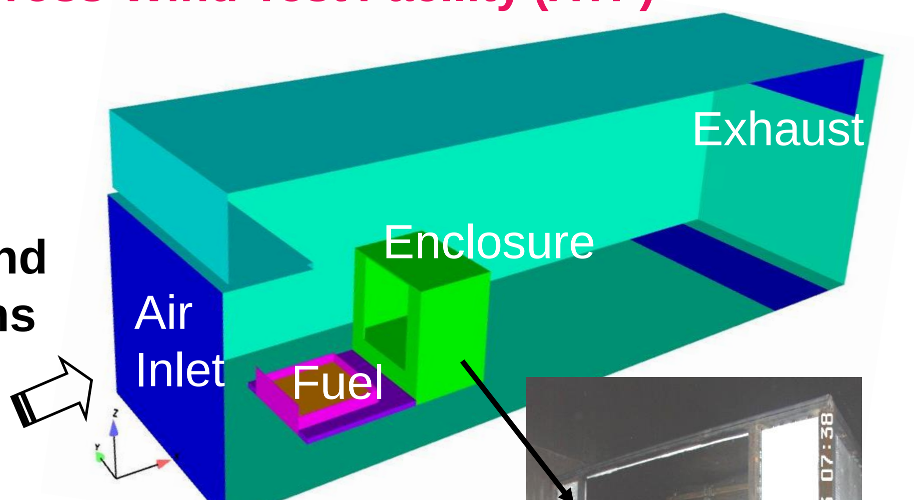
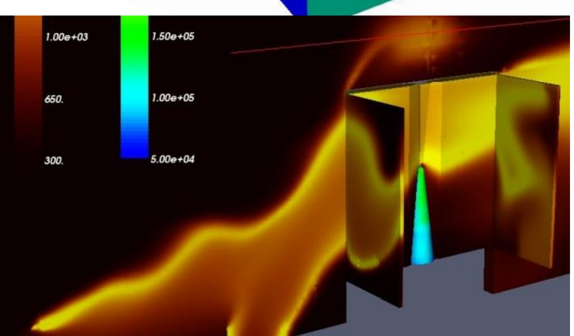
Validation of Fire CFD sims.

- **Validate fire CFD simulations of radiative and convective heating of a weapon-like calorimeter in wind-driven fire.**

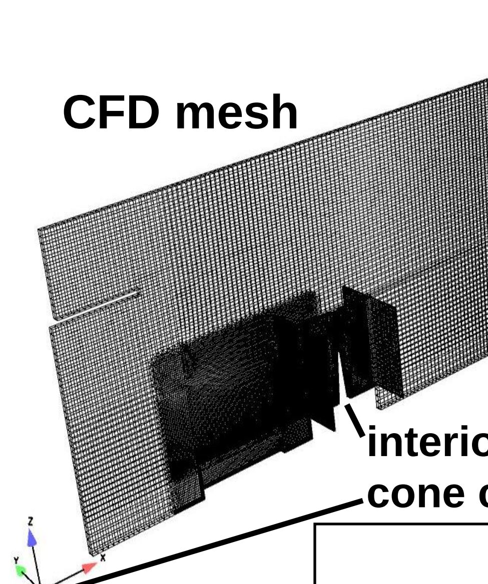
Cross-Wind Test Facility (XTF)

wind fans

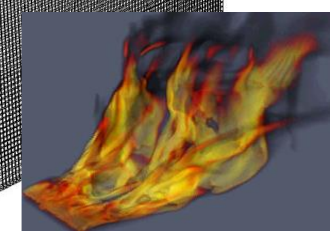




CFD mesh

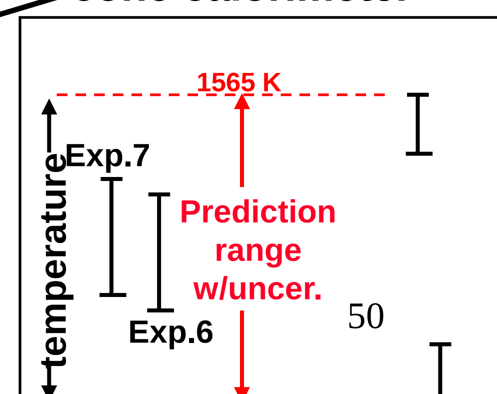


movie



interior of cone calorimeter

Calorimeter Response at location 10



Closing Remarks

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- Model validation is somewhat complex -- philosophically, conceptually, and procedurally
- Many different conceptions, approaches, and frameworks exist and the area is still rapidly evolving
- The Real Space validation approach has been developed and implemented on a number of diverse and challenging Sandia applications, subject to pragmatic cost and resource constraints in industrial-scale applications
- …but is itself still evolving and is just one option among several validation approaches that 1544 is evaluating under various problem characteristics and project needs & constraints

Backup Slides

Real Space vs. Transform Space Representations of Model Discrepancy

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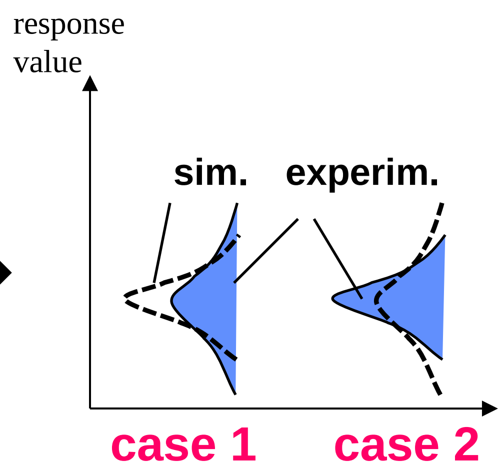
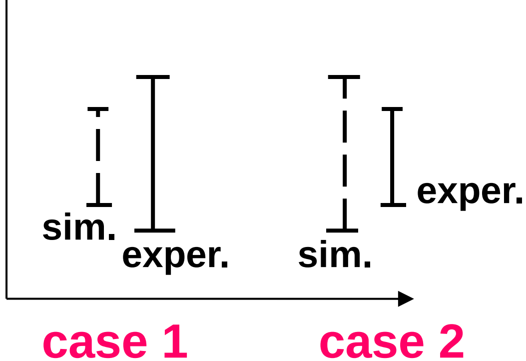
Consider two cases where relative uncertainties in experiment and simulation results are very different



- The transform-space validation metrics below have non-unique mappings from real space to transform space
- This can hide prediction risk and undermine metric use for extrapolation

Real Space representation

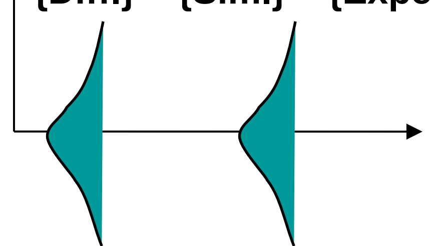
- reveals different prediction risks in the two cases above



ASME V&V20 Sub-tractive Diff. Metric

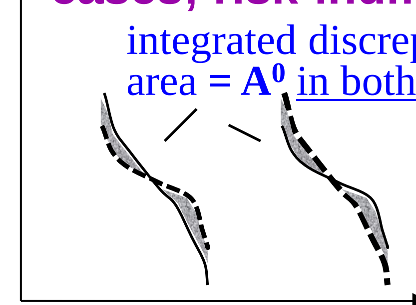
- same result both cases; no indication of differing risk

{Diff.} = {Sim.} – {Exper.}



Roy/Oberk. Area Metric

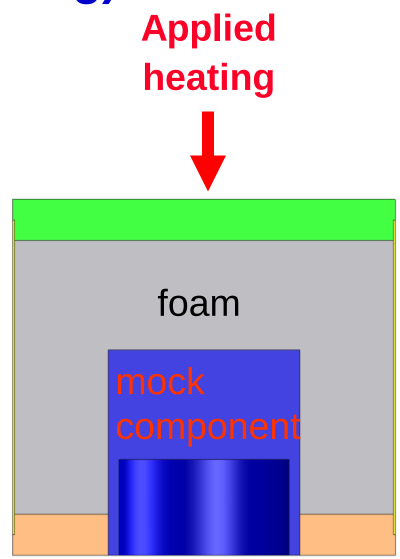
- same area value both cases; risk-indifferent

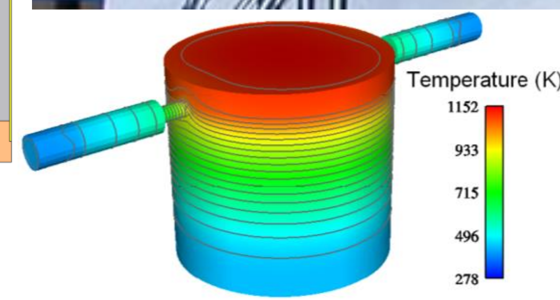


Concept of “Traveling” and “Non-Traveling” portions of the Experiment Model (E Model)

☞ **connectivity to Downstream predictions (extrapolation, incl. hierarchical modeling)**

- **E.g., E model (at right) is the model that participates in the val. or calibration activity**
- **Foam behavioral model (vaporization & altered heat transfer) is object of val. or cal.:**
  - **is the only <u>traveling</u> portion of E model**
- **Everything else in E model does <u>not travel</u> to downstream use:**
  - canister, vents, and slug
  - BC models of heating loads and radiative and convective cooling





Uncertainties are treated in the Framework according to whether they are affiliated with traveling or non-traveling aspects of E model

Real Space Accuracy/Discrepancy measure and "Zero-order" Model Adequacy Criterion

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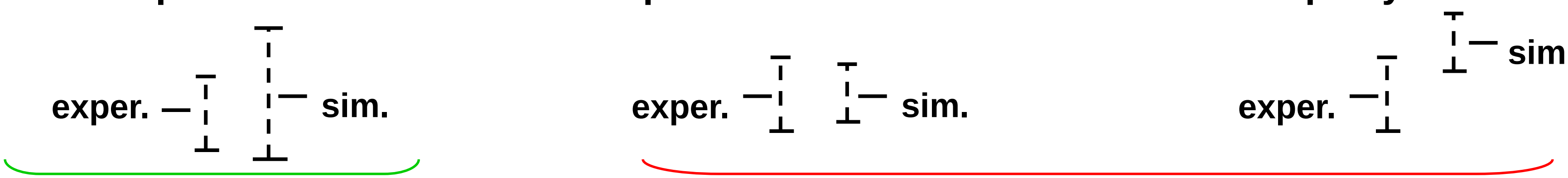
- "Real Space" – **involves no subtractive difference of simulation and experiment results, or other transform discrepancy measures**
- **Simple intuitive criterion for a provisional indication of model adequacy**



This case meets "Zero-order" conditions for model adequacy

- **model prediction bounds experimental uncertainty bar** (as the best available evidence of where "reality" lies)
- **If the data/model relationship remains consistent in extrapolation (*the hope in all modeling*), the predictions will bound reality in the extrapolation conditions**

☑**Reality lying w/in the predictions is what a designer or decision maker wants***

*assuming non-excessive (acceptable) sim. uncer. range as assessed by propagation to system level

Greater prediction risk in above cases

– **much of reality lies outside the model predictions**

– **If data/model relationship remains consistent in extrapolation then much of reality will lie outside predictions**

Adequacy in any of the 3 cases shown above can be assessed more definitively if can propagate errors to system level & assess whether errors are acceptably small (jointly, for all lower-level validation results considered together)

– Requires system-level model & parametric map to "traveling model" at validation setting

Thorny Issue of <u>Pre-Specified</u> Accuracy Requirements for Model Adequacy

(paradigm of ASME V&V-10 Computational Solid Mech., & many others)

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- **In hierarchical validation projects difficulties exist with Top-Down parsing of acceptable error tolerances to the various submodeling activities (difficult inverse problem + non-uniqueness)**

- **In “isolated” phenominological model development & validation work, e.g. turbulence or constitutive model development at a university, there is no project-level accuracy requirement in the first place (to parse downward)**

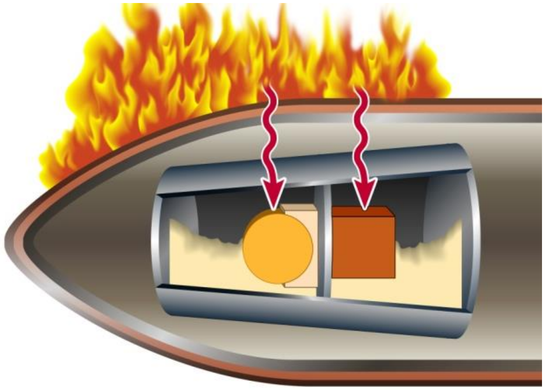
- **Potential constraint violation of pre-specified accuracy requirements:**

  ➡ <u>Experimental uncer. sets limit</u> on the validation accuracy (and any assoc. rqmts.) that can be achieved by a model

  – *this limit not known until <u>after</u> the experiments performed and processed*

☞ **<u>bottom line</u>: not a viable approach**

System-Level risk analysis — Weapon in a Fire



Multiple underlying submodels:

Fire model for heat load BCs
\+
Heat Transfer models (mult. modes)
\+
Mtl. behavior & transformation models
\+
Component response & failure models
+…+…+…

Real Space vs. Transform Space —*Support for Extrapolation*

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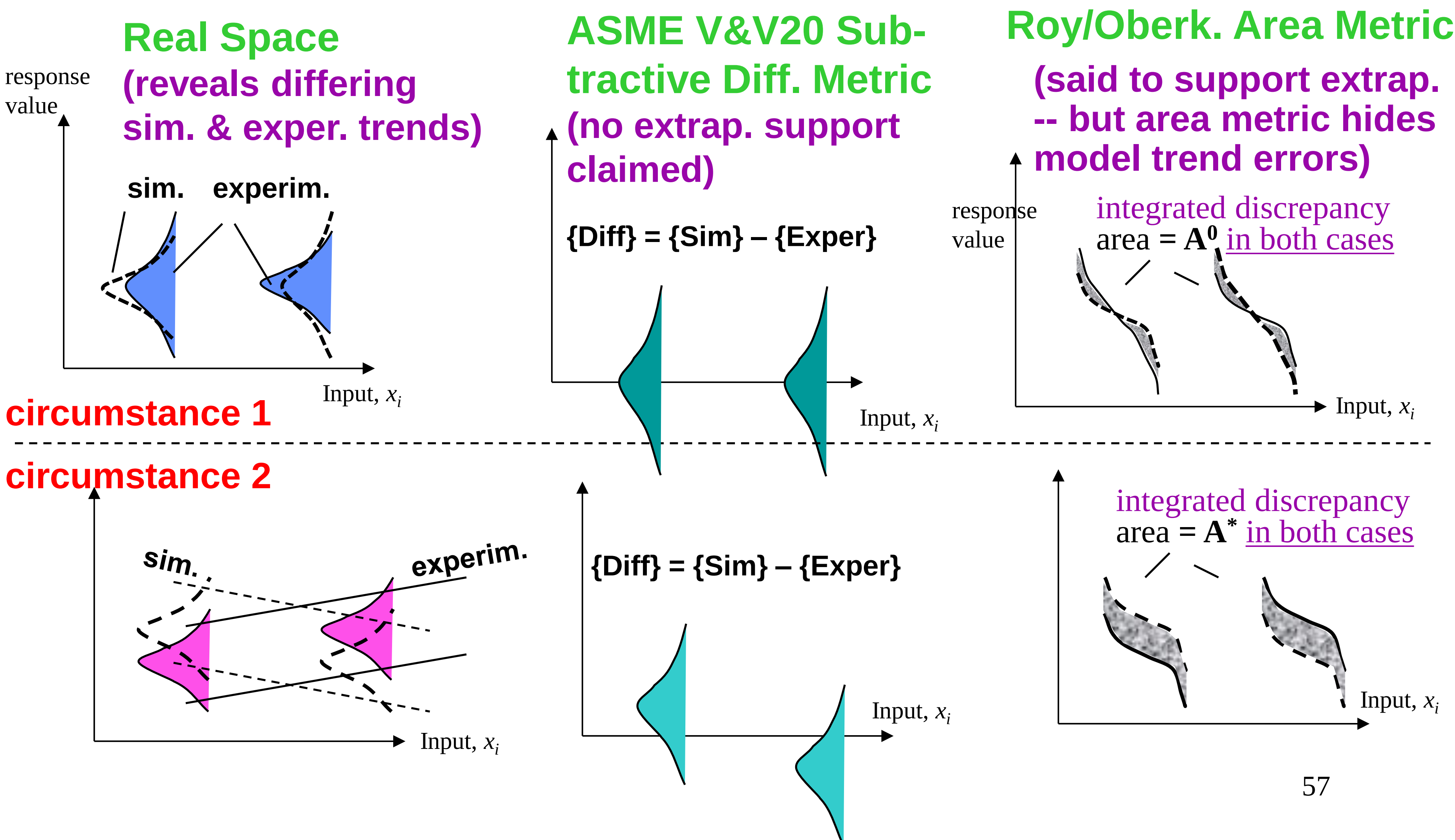

Subtraction Metric prevents proper handling of some types of Random Variability in a population of repeat experiments

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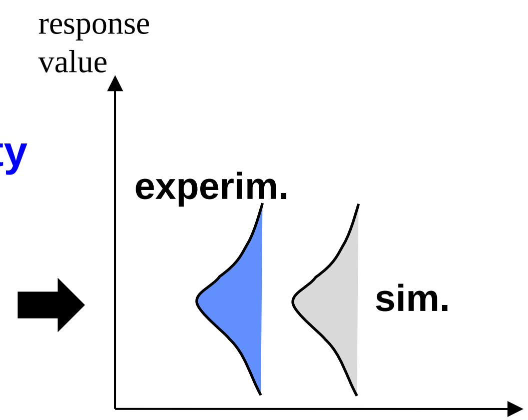
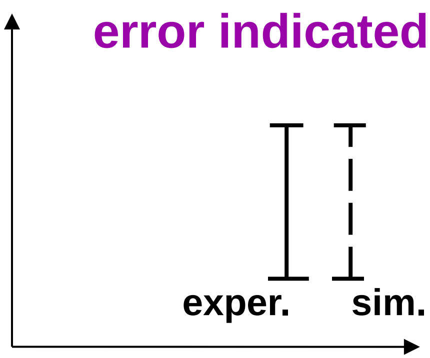
E.g., let simulated stochastic variability of system exactly equal variability of real system tested many times



- Conditions: no measurement errors in the experiments; and "large" # of tests
- Observed response variability is due to unit-to-unit stochastic variability of the tested systems
- and/or due to variability of experimental input conditions
- variability sources independently characterized for simulations, and play out consistently in experims.

Real Space approach

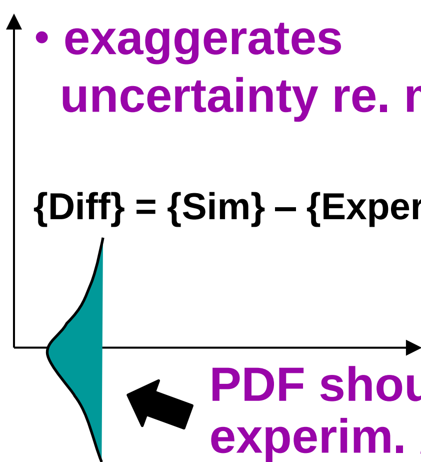
✓ works; no model error indicated



ASME V&V20 Sub-tractive Diff. Metric

- exaggerates uncertainty re. model bias

{Diff} = {Sim} – {Exper}



PDF should have zero width for exact experim. / sim. variability match above

Roy/Oberk. Area Metric

✓ works; no model error indicated

- **The Real Space validation approach is the featured approach in:**

Joint Army/Navy/NASA/Air Force (JANNAF)
Guide to V&V, UQ, and Simulation Credibility in Continuum Physics Applications