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SAND2007-0753C

Verification & Validation:

Measured Credibility, on Demand, for Stockpile Applications

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Validation and Uncertainty Quantification, 1544

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Presentation for:
FAA William J. Hughes Technical Center
Albuquerque, New Mexico
February 6, 2007

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

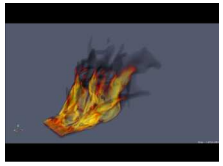
We Need V&V Because We Care!

- **Stockpile Applications**
  - There *is* a decision context: High consequence design and decision making associated with nuclear weapons
- **On Demand**
  - Agility and responsiveness are critical to the nuclear weapons complex of the future
- **Measured Credibility**
  - What's the "certificate of credibility" that accompanies M&S results

M&S Increasingly Contributes to *Risk-Informed Decisions* at Sandia

Stockpile Lifecycle Risk-Informed Decisions:
Assertion-Based and Challenged via Peer Review

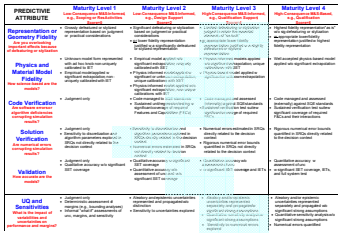
Testing



Play Movie

CF=M/U

PCMM



DECISION SUPPORT

C³:
- Conservative Requirements
- Conservative Scenarios
- Conservative Assessments

Decision Paradigm Change

QMU:
Quantified Margins and Uncertainties BE+U

Test/Experiment
Relevant Physical Data

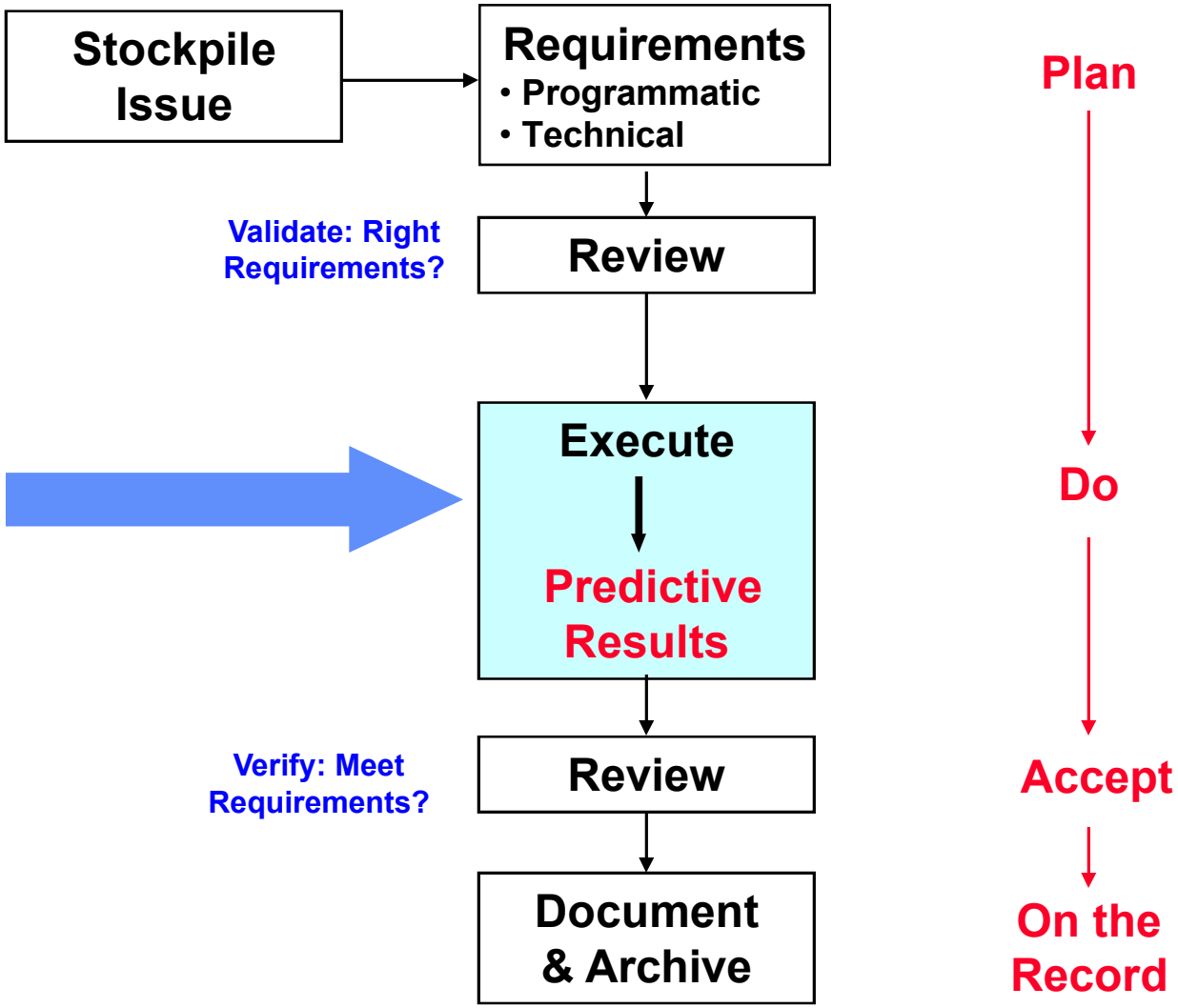
M&S
Predictive Capability

CREDIBILITY
Of Models and Experiments

For improved technical basis, communication, decisions

High Consequence Issues Demand Predictive Capability

Concepts of Stockpile Computing: SAND2004-2479



We Demand *Predictive Capability* Here

What Does it Mean "to Predict"?

American Heritage Dictionary:

- **Predict: To state, tell about, or make known in advance, especially on the basis of *special knowledge**

What *special knowledge* do we demand of M&S to assert a predictive capability and how do we communicate it?

You Can't Measure and Communicate "it" Unless You Know What "it" Is

- Some Attributes of Predictive Capability
  - Representation or geometric fidelity
  - Physics and material model fidelity (predictive science)
  - Code verification
  - Solution verification
  - Validated models
  - Uncertainty quantification with sensitivity analysis

How Much is Enough?

- Sufficiency can only be discussed in an application context
- Graded approach
  - Maturity Level 1:
    - Low-consequence, M&S-informed (e.g., scoping studies)
  - Maturity Level 2:
    - Low-consequence, M&S-informed (e.g., design support)
  - Maturity Level 3:
    - High-consequence, M&S-informed (e.g., qual support)
  - Maturity Level 4:
    - High-consequence, M&S-based (e.g., qualification)
- Negotiate expectations for future work or communicate maturity for work already done

Increasing Rigor Expected

This is Where We Are Going
Predictive Capability Maturity Model (PCMM)

PREDICTIVIE ATTRIBUTE	Maturity Level 1 Low-Consequence M&S-Informed, e.g., Scoping or Res Activities Score=0	Maturity Level 2 Low-Consequence M&S-Informed, e.g., Design Support Score=2	Maturity Level 3 High-Consequence M&S-Informed, e.g., Qualification Support, Score=4	Maturity Level 4 High-Consequence M&S-Based, e.g., Qualification Score=6
Representation or Geometry Fidelity Are you overlooking important effects because of defeaturing or stylization	• Grossly defeatured or stylized representation based on judgment or practical considerations	• Significant defeaturing or stylization based on judgment or practical considerations • or lower fidelity representation justified w a significantly defeatured or stylized representation	• Limited defeaturing or stylization judged to retain the essential elements of "as built" • or appropriate lower fidelity representation justified w a slightly defeatured or stylized representation	• Highest fidelity representation "as is" w/o sig defeaturing or stylization • or appropriate lower fidelity representation justified w highest fidelity representation
Physics and Material Model Fidelity How science-based are the models?	• Unknown model form represented with ad hoc knob non-uniquely calibrated to IET • Empirical model applied w significant extrapolation, non-uniquely calibrated with IET	• Empirical model applied w/o significant extrapolation, uniquely calibrated with SET • Physics informed model applied w significant or unknown extrapolation, unique calibrations with SET • Physics-informed model applied w/o significant extrapolation, non-unique calibrations with IET	• Physics informed models applied w/o significant extrapolation, unique calibrations with SET • Physics-based model applied w significant or unknown extrapolation	• Well accepted physics-based model applied w/o significant extrapolation
Code Verification Are software errors or algorithm deficiencies corrupting simulation results?	• Judgment only	• Code managed to SQE standards • Sustained unit/regression testing w significant coverage of required Features and Capabilities (F&Cs)	• Code managed and assessed (internally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs	• Code managed and assessed (externally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs and their interactions
Solution Verification Are numerical errors corrupting simulation results?	• Judgment only • Sensitivity to discretization and algorithm parameters explored in SRQs not directly related to the decision context	• Sensitivity to discretization and algorithm parameters explored in SRQs directly related to the decision context • Numerical errors estimated in SRQs not directly related to decision context	• Numerical errors estimated in SRQs directly related to the decision context • Rigorous numerical error bounds quantified in SRQs not directly related to the decision context	• Rigorous numerical error bounds quantified in SRQs directly related to the decision context
Validation How accurate are the models?	• Judgment only • Qualitative accuracy w/o significant SET coverage	• Qualitative accuracy w significant SET coverage • Quantitative accuracy w/o assessment of unc and w/o significant SET coverage	• Quantitative accuracy w/o assessment of unc • w significant SET coverage and IETs	• Quantitative accuracy w assessment of unc • w significant SET coverage, IETs, and full system test
UQ and Sensitivities What is the impact of variabilities and uncertainties on performance and margins?	• Judgment only • Deterministic assessment of margins (e.g., bounding analyses) • Informal "what if" assessments of unc, margins, and sensitivity	• Aleatory and epistemic uncertainties represented and propagated w/o distinction • Sensitivity to uncertainties explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w significant strong assumptions • Quantitative sensitivity analysis w significant strong assumptions • Sensitivity to numerical errors explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w/o significant strong assumptions • Quantitative sensitivity analysis w/o significant strong assumptions • Numerical errors quantified

Why PCMM?

- Educate the decision maker about what should be expected from M&S
- Measure/communicate process maturity (not adequacy of results) associated with M&S in a decision context
- Provide program vision so that technical and infrastructure needs can be leveraged across multiple funding lines to enhance the credibility of M&S results
- Speak to the *whats*, not dictate the *hows*

Setting the National Agenda in V&V

Representation or Geometric Fidelity

Are you overlooking important effects because of judgment-based Defeaturing or Stylization?

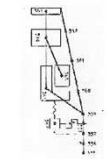
Grossly defeatured or stylized

Significant D&S based on judgment

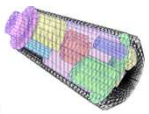
Limited D&S judged to retain the essential elements of "as built"

Highest fidelity representation "as built" w/o significant D&S

H Risk Tolerant | Risk Tolerant | Risk Adverse | H Risk Adverse

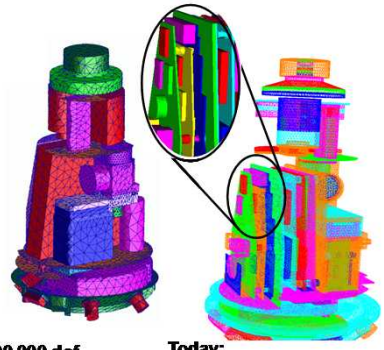


10 years ago: Shellshock 2D NASTRAN 200 dof



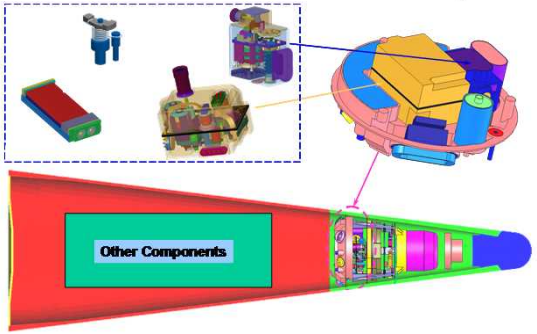
Recent Past: NASTRAN

30,000 dof



800,000 dof

Today: SALINAS MP >10M dof



Physics and Material Model Fidelity

Are the models science-based?

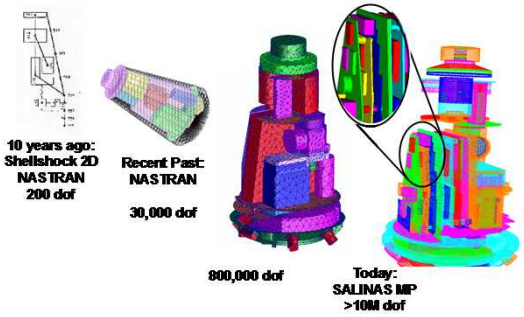
Unknown model form or empirical model form applied w sig extrap

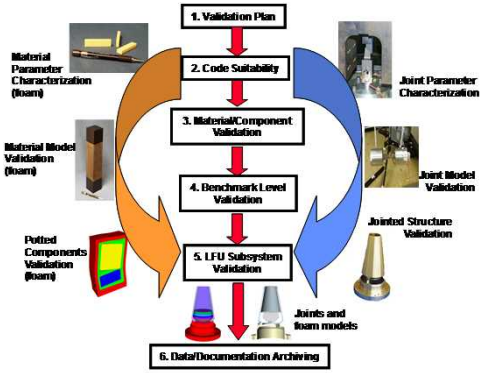
Empirical model form applied w/o sig extrap or physics informed model applied w sig/unk extrap

Physics-informed model applied w/o sig extrap or physics based model applied w sig/unk extrap

Physics-based model applied w/o sig extrap

H Risk Tolerant → **Risk Tolerant** → **Risk Adverse** → **H Risk Adverse**





Code Verification

Are software errors or algorithm deficiencies corrupting simulation results?

Judgment only

Code managed to SQE standards

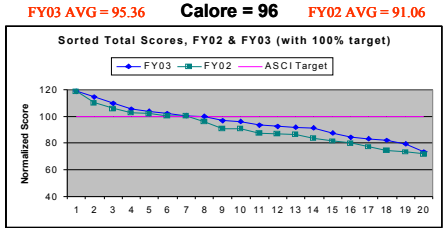
Sustained unit/regression tests w sig coverage of F&C

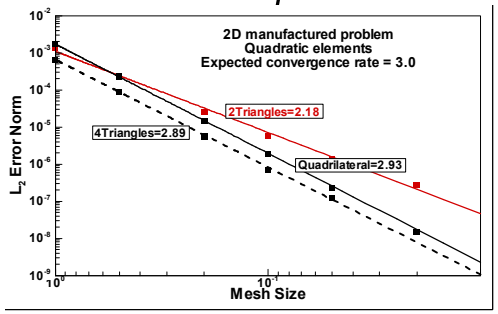
SQE +assessment + sustained VERTS w sig coverage of F&C

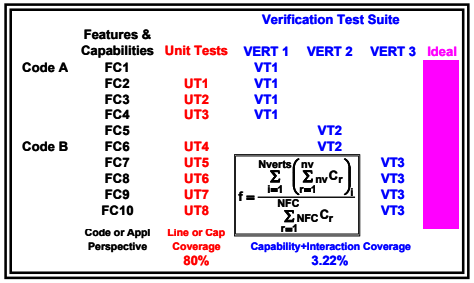
SQE(A) + VERTS w sig coverage of F&C interactions

H Risk Tolerant → **Risk Tolerant** → **Risk Adverse** → **H Risk Adverse**

Code/Code Comparisons







Solution Verification

Are numerical errors corrupting simulation results?

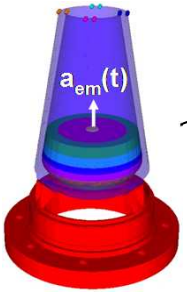
Judgment only

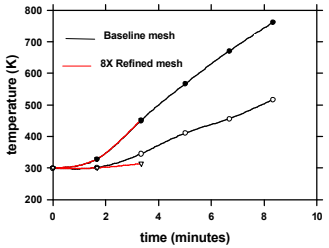
Explore sensitivity to discretization and algorithm parameters

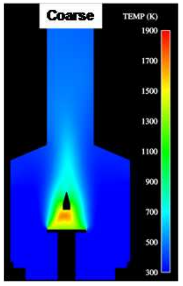
Estimate numerical errors

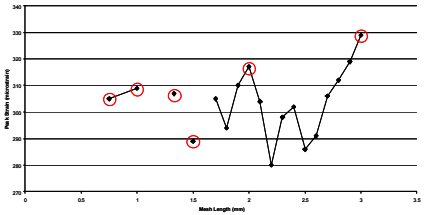
Quantify rigorous numerical error bounds

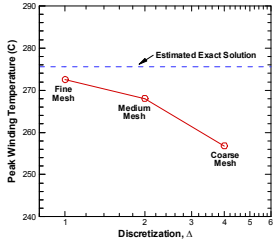
H Risk Tolerant → **Risk Tolerant** → **Risk Adverse** → **H Risk Adverse**

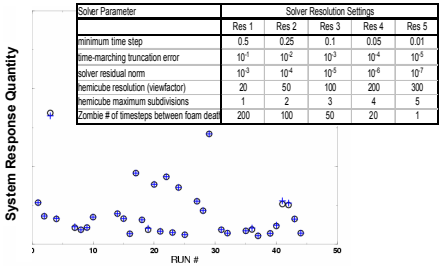


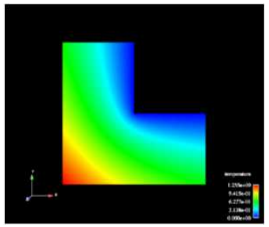










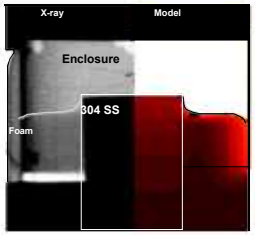


Validation

How accurate are the models?

Judgment only	Qual accuracy w SET coverage	Quantitative accuracy w/o assessment of unc *and* w SET coverage and IETs	Quantitative accuracy w assessment of unc *and* SET coverage and IETs and full system

H Risk Tolerant	Risk Tolerant	Risk Adverse	H Risk Adverse



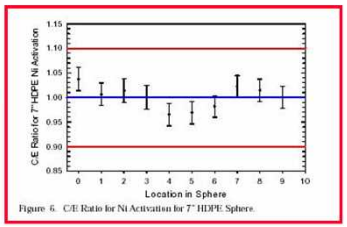


Figure 6. C/E Ratio for Ni Activation for 7" HDPE Sphere.

Uncertainty Quantification and Sensitivities

What is the impact of variabilities and uncertainties on performance and margins?

Judgment only
Deterministic assessment of margins or informal "what if" studies

Aleatory and epistemic unc represented w/o distinction

Sensitivities explored

Aleatory/epistemic unc interpreted separately w strong assumptions

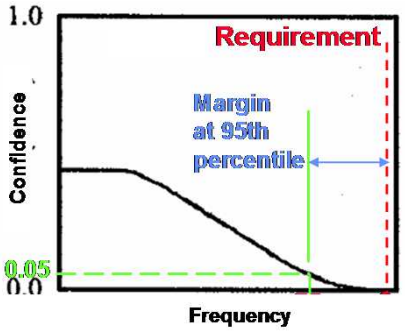
Sensitivities w strong assumptions

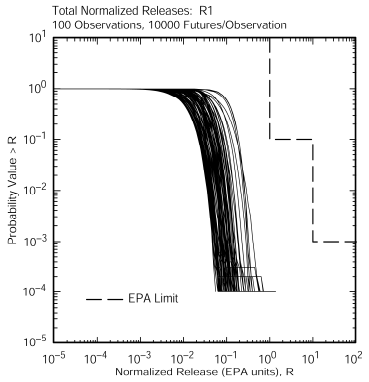
Sensitivity to numerical errors exp

Aleatory/epistemic unc interpreted separately w strong assumptions
Sensitivities w strong assumptions
Numerical errors quantified

H Risk Tolerant | **Risk Tolerant** | **Risk Adverse** | **H Risk Adverse**

DAKOTA





ASC Projects Should Map to Capability/Agility Needs

PREDICTIVIE ATTRIBUTE	Maturity Level 1 Low-Consequence M&S-Informed, e.g., Scoping or Res Activities Score=0	Maturity Level 2 Low-Consequence M&S-Informed, e.g., Design Support Score=2	Maturity Level 3 High-Consequence M&S-Informed, e.g., Qualification Support, Score=4	Maturity Level 4 High-Consequence M&S-Bas e.g., Qualification Score=6
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Code Verification Are software errors or algorithm deficiencies corrupting simulation results?	• Judgment only	• Code managed to SQE standards ned unit/regression testing cant coverage of required es and Capabilities (F&Cs	• Code managed and assessed nternally) against SQE standards stained verification test suite w gnificant coverage of required &Cs	• Code managed and assessed (externally) against SQE standa • Sustained verification test suite significant coverage of required F&Cs and their interactions
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DART

Wisdom

PEM

SQE

V&V Methods

Adaptivity

Dakota

Codes and Platforms

Predictive Capability Maturity Model (PCMM)

Communicating Credibility

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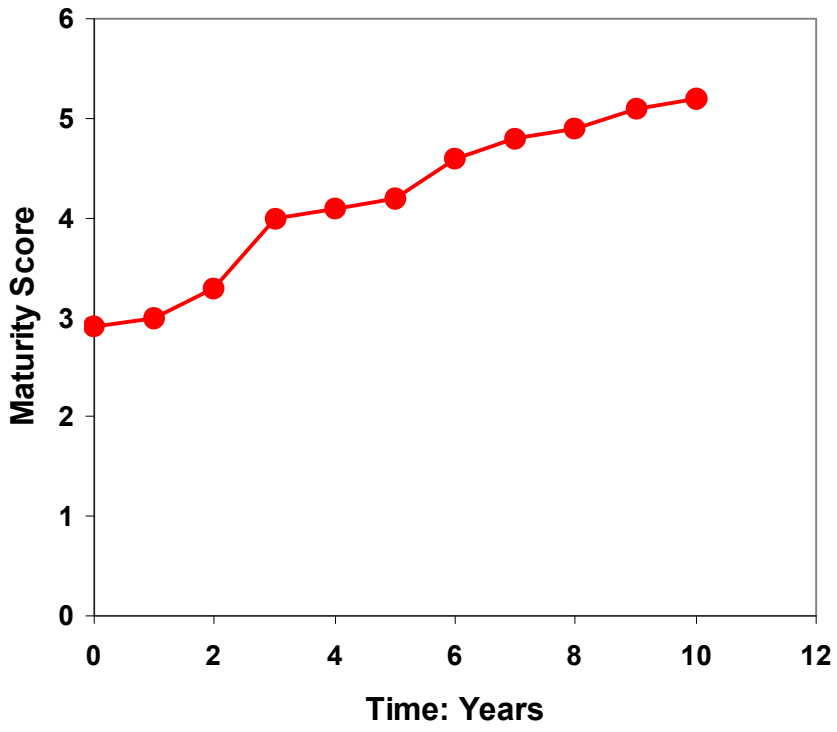
Measure Progress Over Time

Application: Legacy Weapon in Fuel Fire	Avg/Avg Score	Avg/Min Score
Rollup Scores	2.9	2.0
Representation or Geometric Fidelity	4.5	4.0
Fire Environment	4.0	
Weapon	5.0	
Physics and Material Modelel Fidelity	3.2	1.0
Fire Environment	3.0	2.0
Fuel vaporization from spill	2.0	
Fluid mechanics	4.0	
Turbulent mixing	3.0	
Combustion	4.0	
Emmission	2.0	
Radiative transport to weapon	4.0	
Convective transport to weapon	2.0	
Weapon Thermal Response	3.3	0.0
Code Verification	2.0	2.0
Fire Environment	2.0	
Weapon Thermal Response	2.0	
Solution Verification	1.5	1.0
Fire environment	1.0	
Weapon thermal response	2.0	
Validation	2.1	0.0
Fire Environment	1.6	0.0
Weapon Thermal Response	2.3	0.0
UQ/SA	4.0	4.0



Note: all scores are notional

Measured Credibility, on Demand, for Stockpile Applications

- Decision makers need to understand predictive capability in order to make informed decisions and to efficiently leverage and make use of research dollars
- Progress in predictive capability needs to be measured in each individual decision context
  - Predictive capability is more than geometric fidelity or even physics fidelity
  - There is a need to define sufficiency (or adequacy) in each attribute of predicative capability
- The Predictive Capability Maturity Model provides a graded approach to assessing and measuring predictive capability for specific applications

The Credibility of M&S is Critical

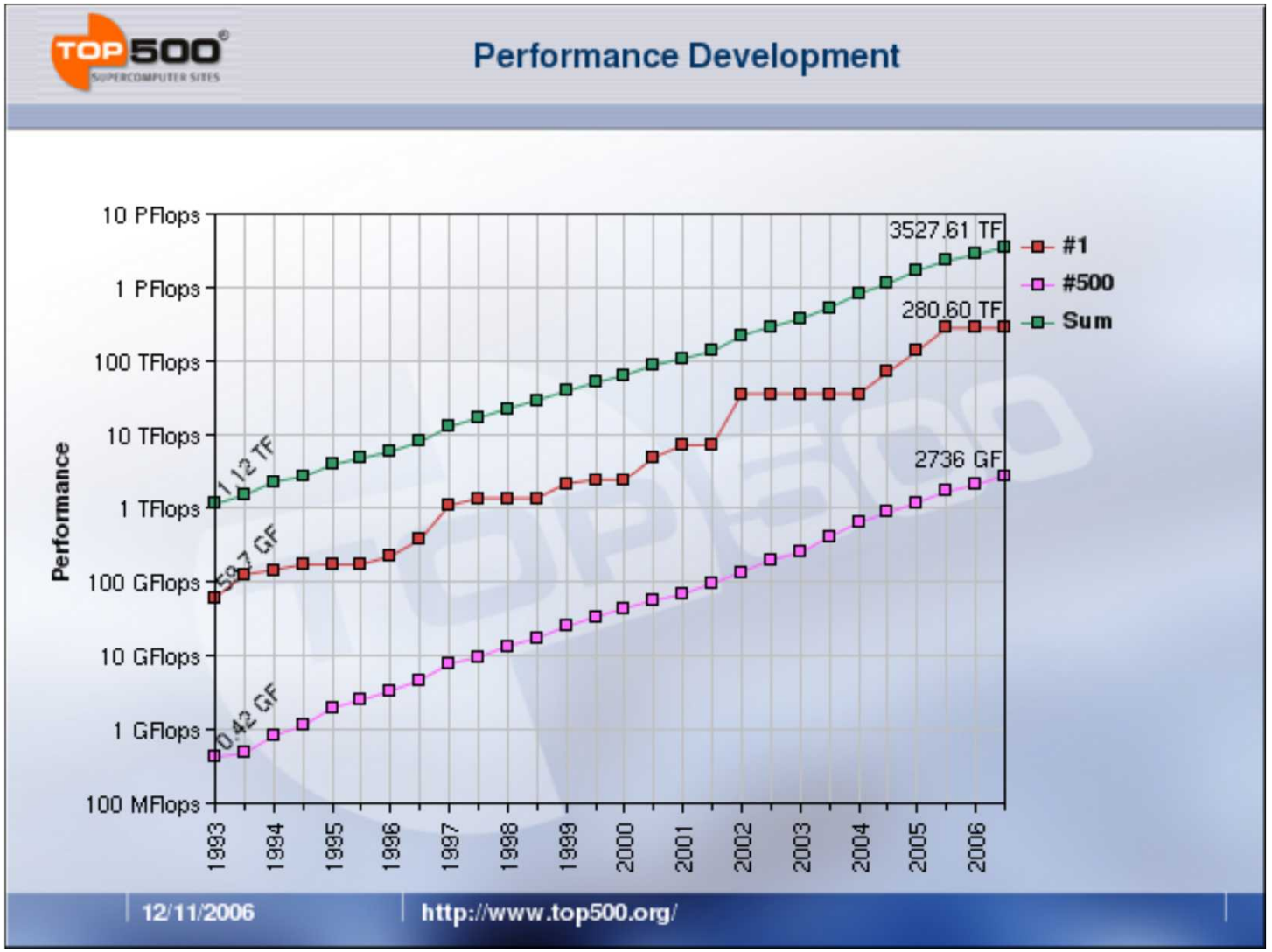
"Due diligence means asking *all* the questions, even if you don't think you'll like the answers."

Representational (Geometric) Fidelity

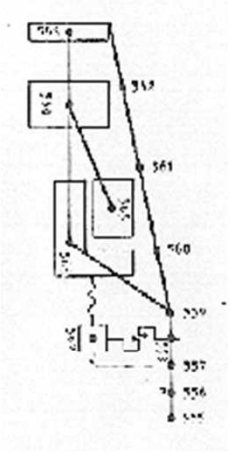
Hyperlinks

Imagine the Future!

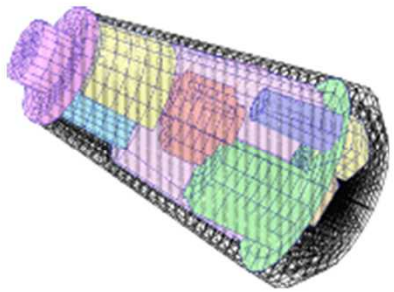
Computing Speed - Dec. 2006



Progress in Representational Fidelity in Structural Dynamics

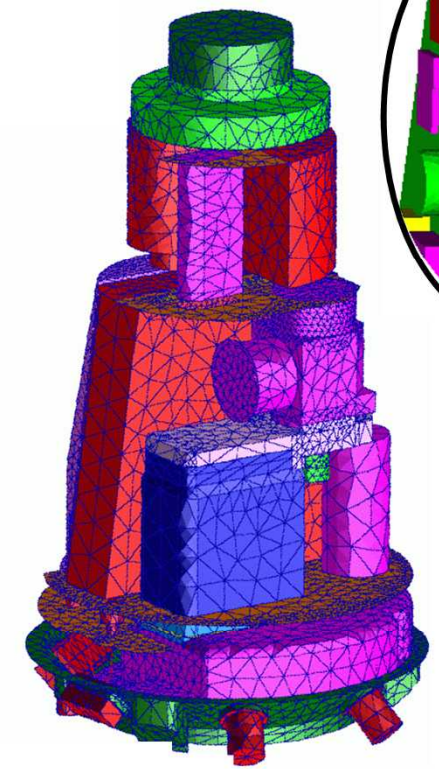


10 years ago:
Shellshock 2D
NASTRAN
200 dof

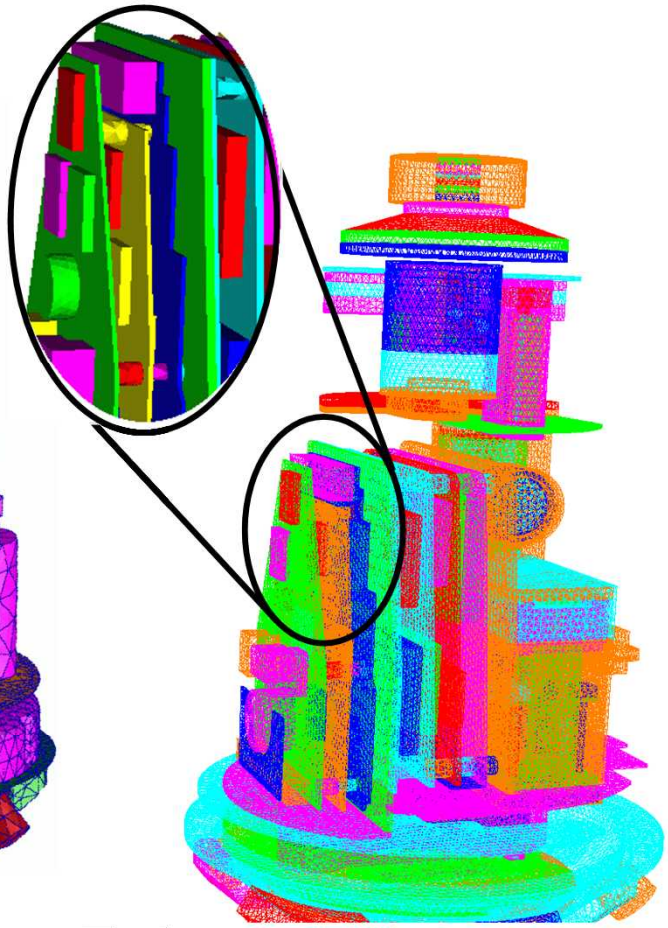


Recent Past:
NASTRAN

30,000 dof

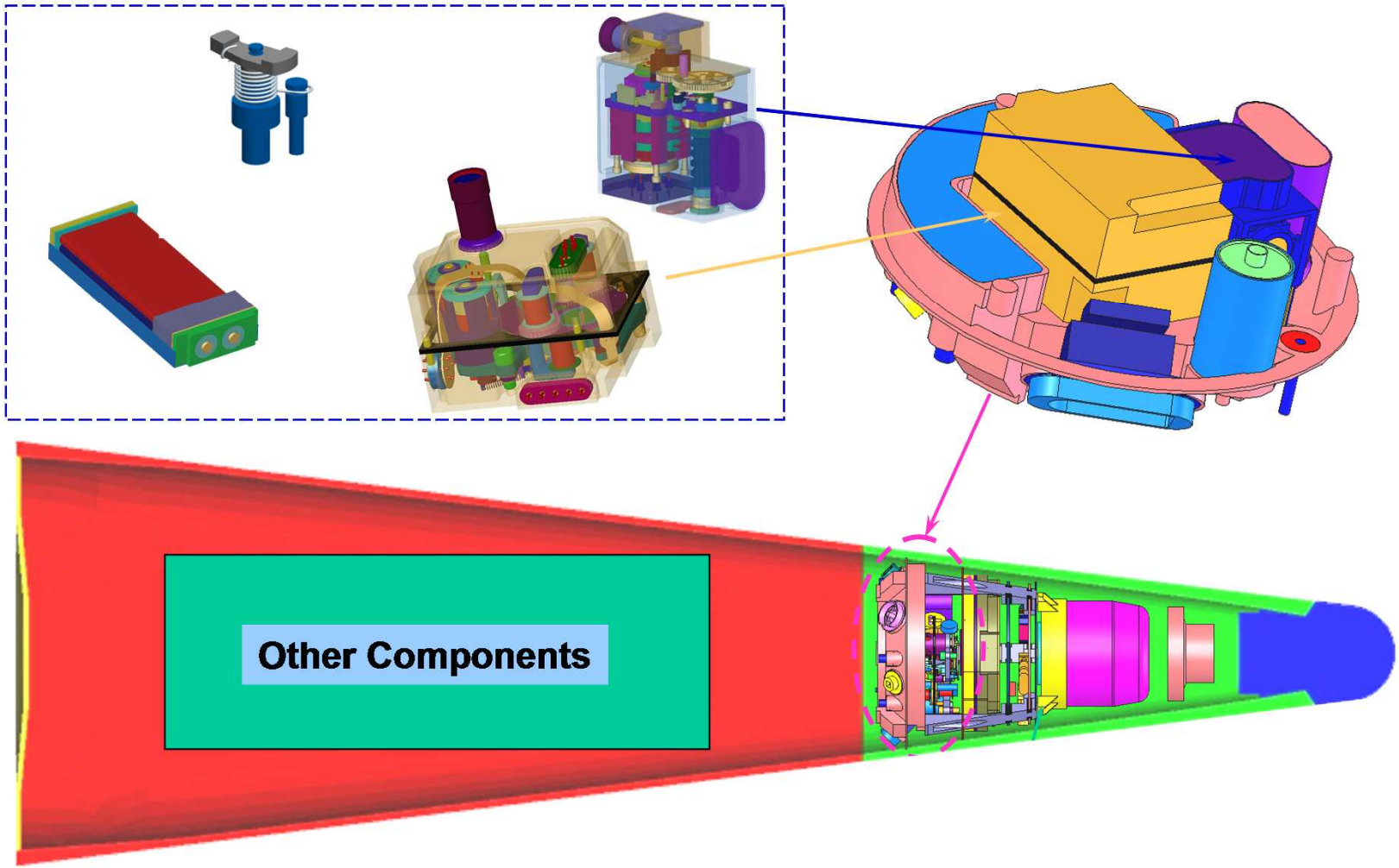


800,000 dof



Today:
SALINAS MP
>10M dof

Progress in Representational Fidelity Thermal Modeling



Physics Fidelity

Hyperlinks

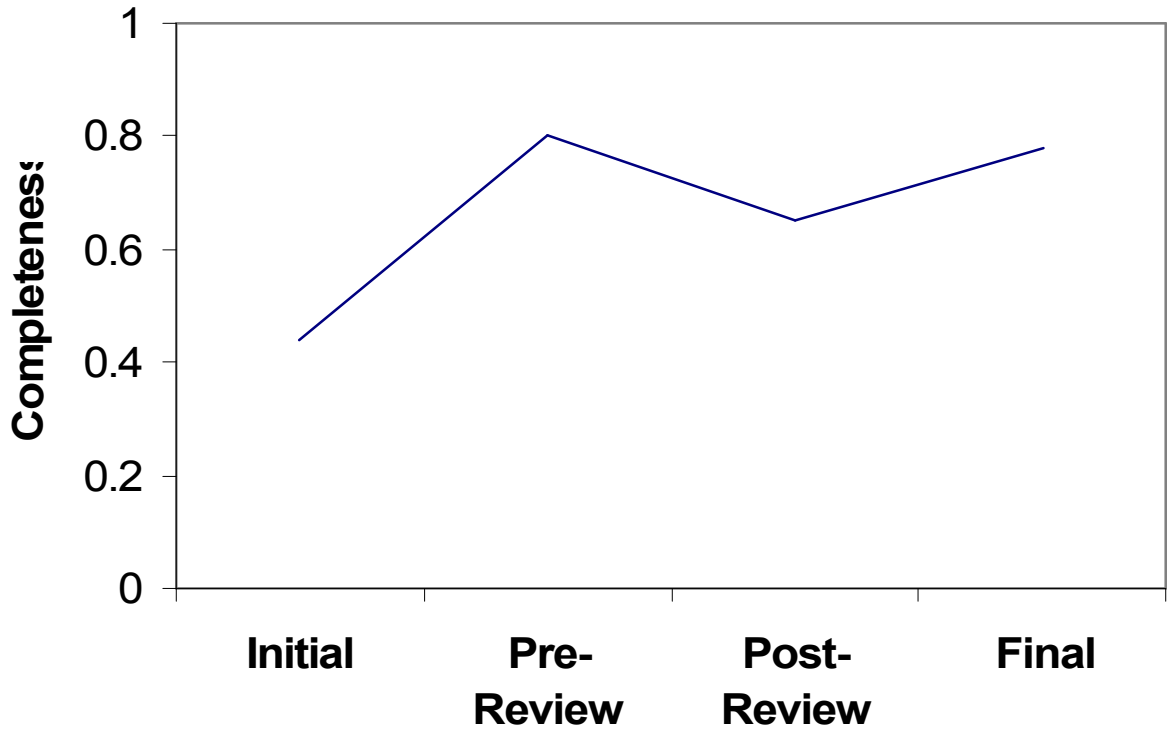
Phenomena Identification and Ranking Tables (PIRT)

Establish efficiency and sufficiency of activities

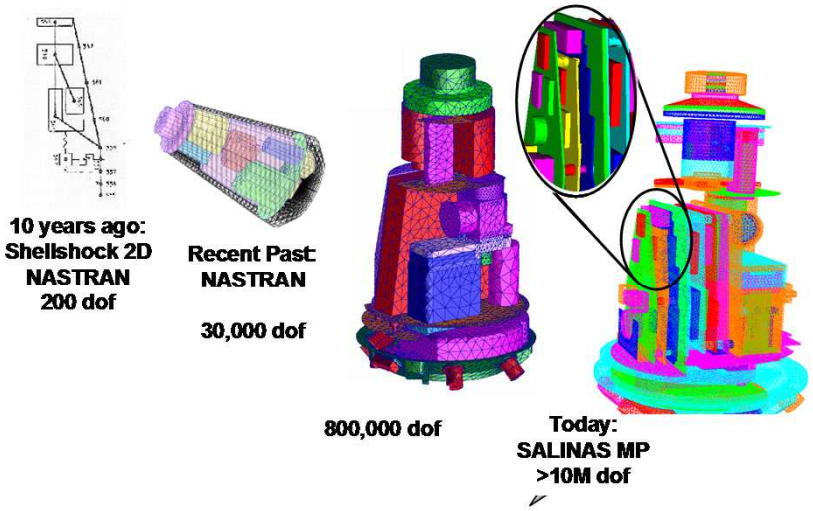
Phenomena	Importance	Adequacy: Model	Adequacy: Code	Adequacy: Validation
P1	H	H	M	L
P2	M	M	L	L
P3	L	L	L	L

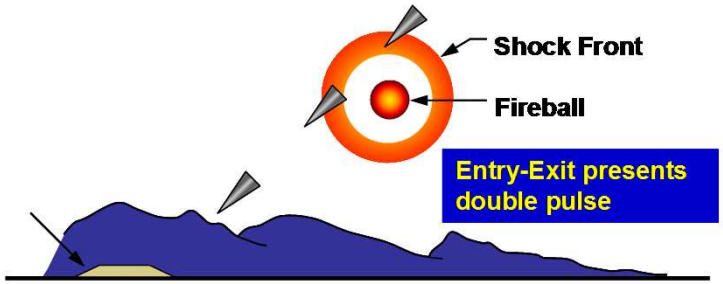
Gap = 5

Completeness = 0.44



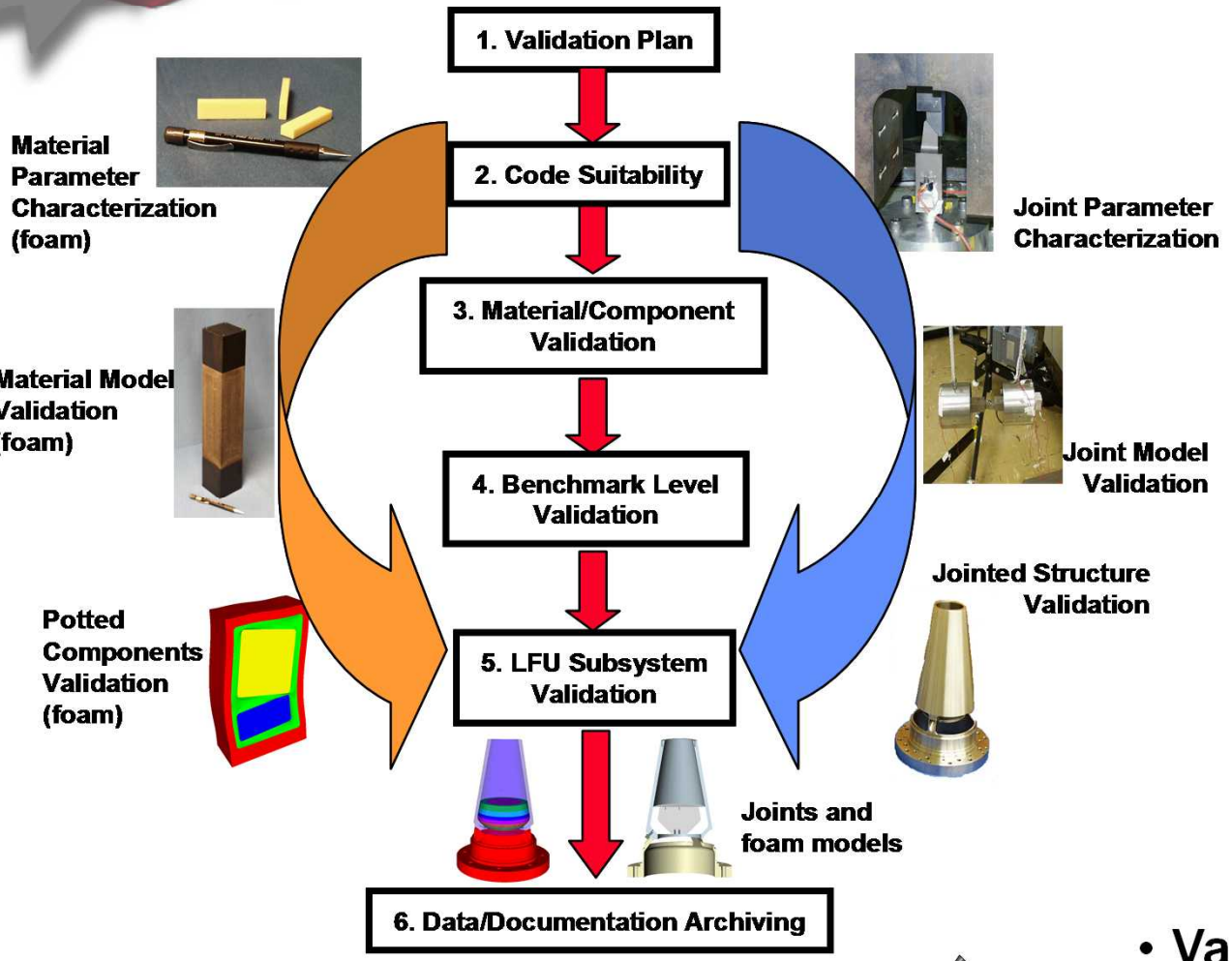
Low Physics Fidelity



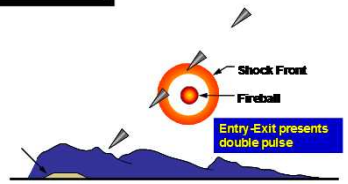


- Conduct blast test
- Calibrate model to blast test using global stiffness and damping parameters: knobs that act as surrogates for missing or unknown physics
- Use calibrated model to make prediction in tactical environments

Improving Physics Fidelity



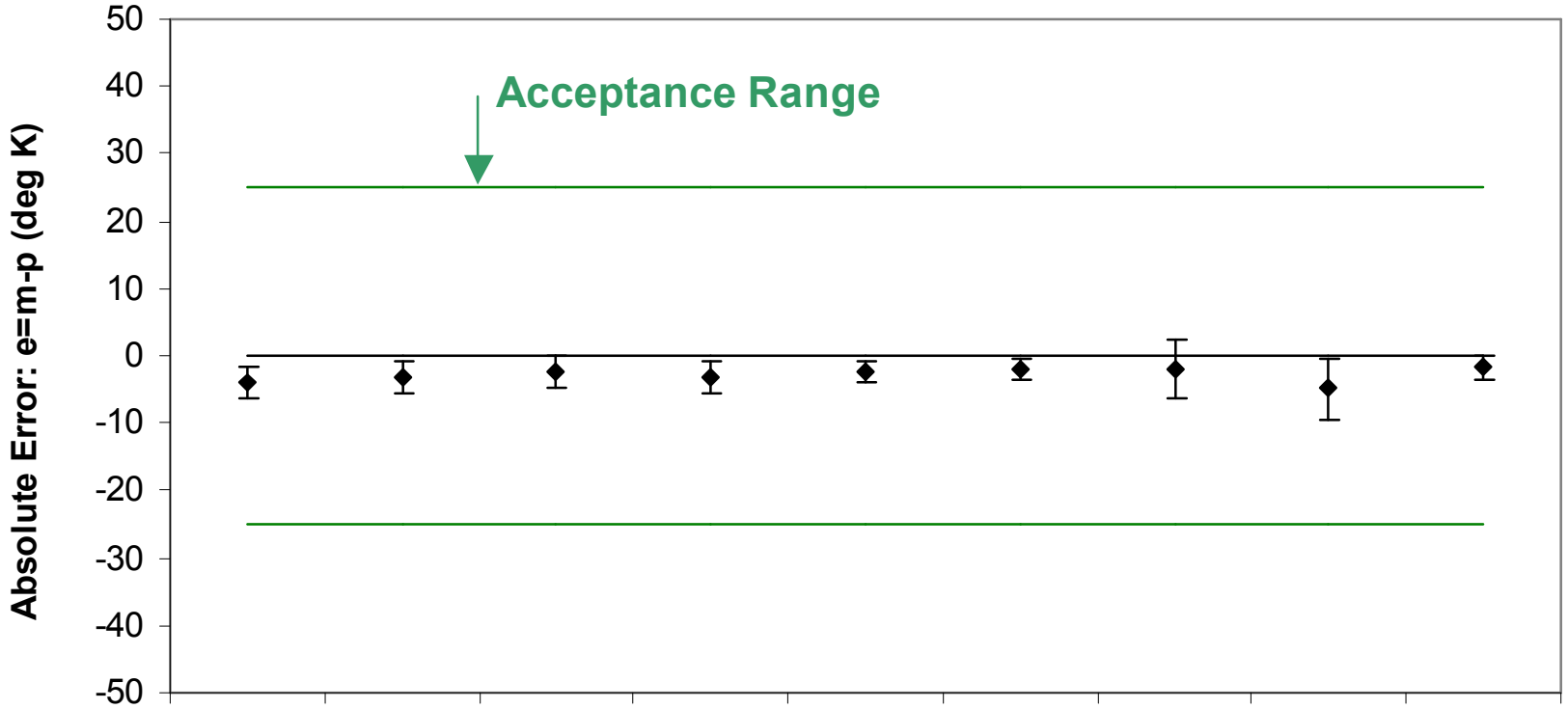
- **Physics-informed models validated against separate effects tests**



- **Validate against blast test and make prediction in tactical environments**

Well Established Physics Fidelity

e~2K for conduction



Various Locations in Test Object

Code Readiness

Hyperlinks

Attributes of Verification

Demonstrating Convergence to Correct Answer for the Intended Application

Solution Verification: Convergence for intended application, *but is it the right answer?*

• *Address adequacy of spatial AND temporal AND other discretizations AND numerical knobs*

Inference → Application

Coupled Multi-Physics Across Codes

Coupled Multi-Physics Within Code

Separate Physics

Issues: non-smooth solutions, contact, constitutive laws, internal constraints, multiscale physics, global/local norms, etc.

Inference

Regression Testing

Code Verification: Convergence to correct answer, *wrong application*

• Eliminate code bugs *AND* inadequate algorithms

SQE(A)

Code to Code Comparisons Are a Poor Substitute for Formal Verification

Code Comparison Principle (CCP)

Code 1 = assessed code Code 2 = benchmark code

$$\|\text{Code 1} - \text{Truth}\| \le \|\text{Code 1} - \text{Code 2}\| + \|\text{Code 2} - \text{Truth}\|$$

$$\therefore \|\text{Code 1} - \text{Code 2}\|$$

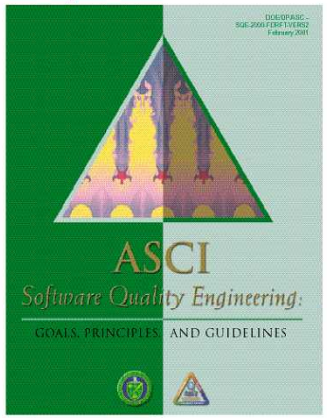
What if this term is not negligible?

- Could be that Code 1 models are different from Code 2 models
- Could be a bug in Code 1 or Code 2
- Could be an algorithm flaw in Code 1 or Code 2
- Could be that Code 1 or Code 2 model is not converged

Points to path for better code-to-code comparisons; but if Code 2 is formally verified, why not verify Code 1 to the same verification test suite? And if not, why bother with the code-to-code comparison?

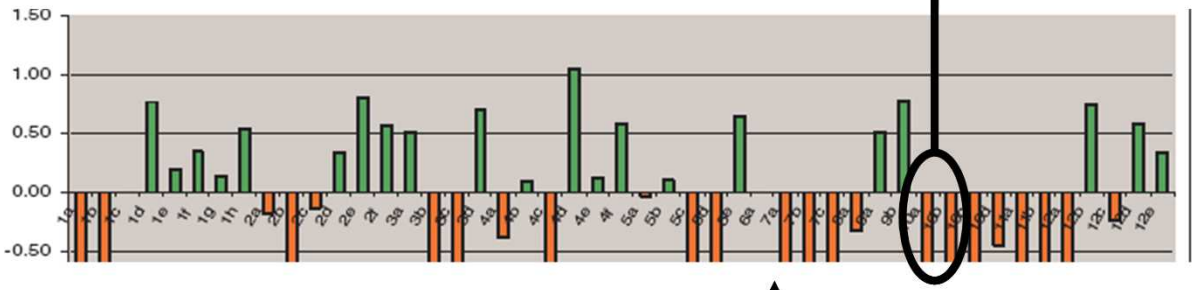
SQE(A): Demonstrated Due Diligence in the Stewardship of Codes

Requirements



SourceForge: Issue Tracking

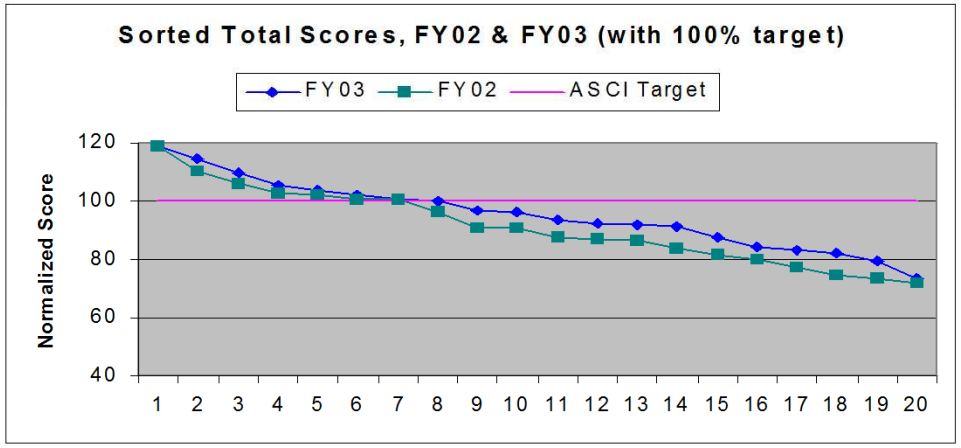
Improvement



FY03 AVG = 95.36

Calore = 96

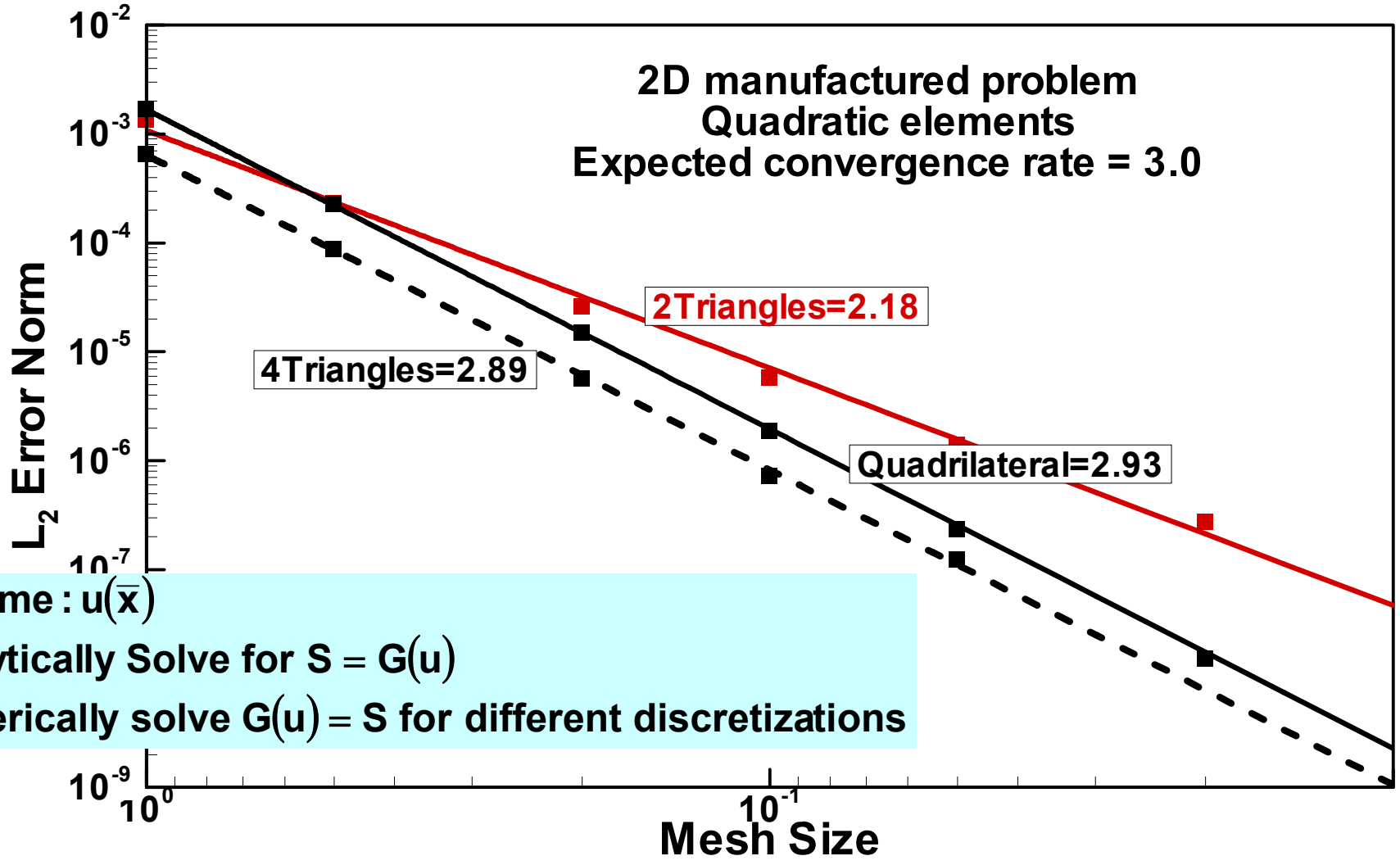
FY02 AVG = 91.06



Assessments

Verification with Manufactured Solution

CEPTRE: Radiation Transport



Assume : $u(\bar{x})$

Analytically Solve for $S = G(u)$

Numerically solve $G(u) = S$ for different discretizations

Measuring Progress in Code Verification Coverage and Interactions

	Features & Capabilities	Unit Tests	Verification Test Suite: VERT 1	VERT 2	VERT 3	Ideal
Code A	FC1		VT1			
	FC2	UT1	VT1			
	FC3	UT2	VT1			
	FC4	UT3	VT1			
	FC5			VT2		
Code B	FC6	UT4		VT2		
	FC7	UT5			VT3	
	FC8	UT6			VT3	
	FC9	UT7			VT3	
	FC10	UT8			VT3	
	Code or Appl Perspective	Line or Cap Coverage	Capability+Interaction Coverage			
		80%	3.22%			

$$f = \frac{\sum_{i=1}^{Nverts} \left(\sum_{r=1}^{nv} C_r \right)_i}{\sum_{r=1}^{NFC} C_r}$$

Solution Verification

Hyperlinks

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Inference

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Code Verification: Convergence to correct answer, *wrong application*

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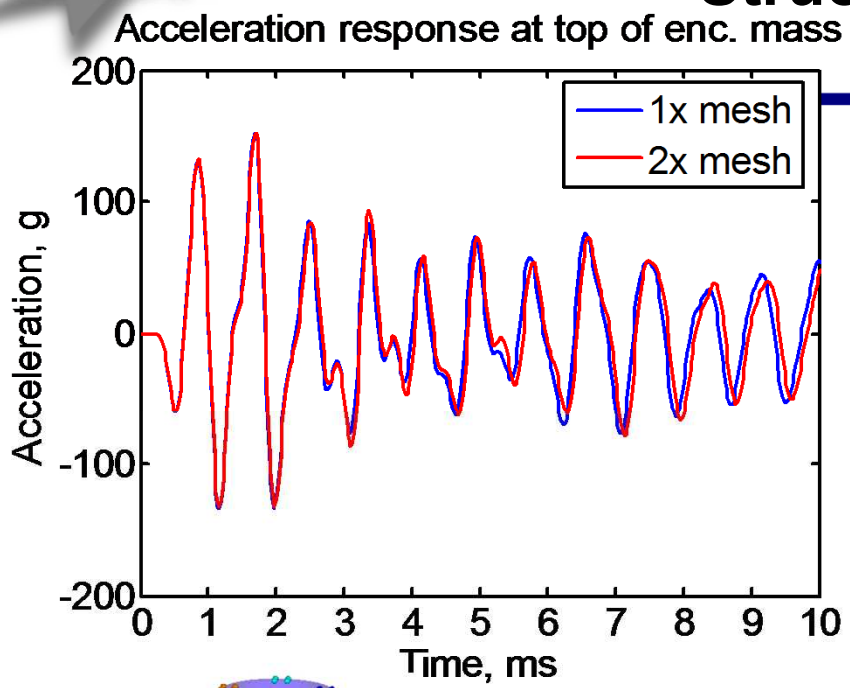
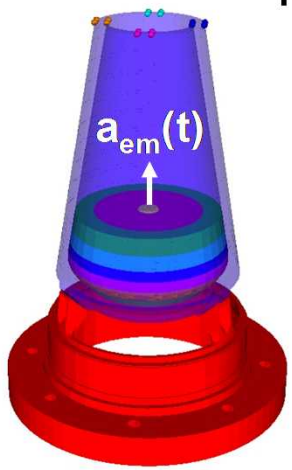
SQE(A)

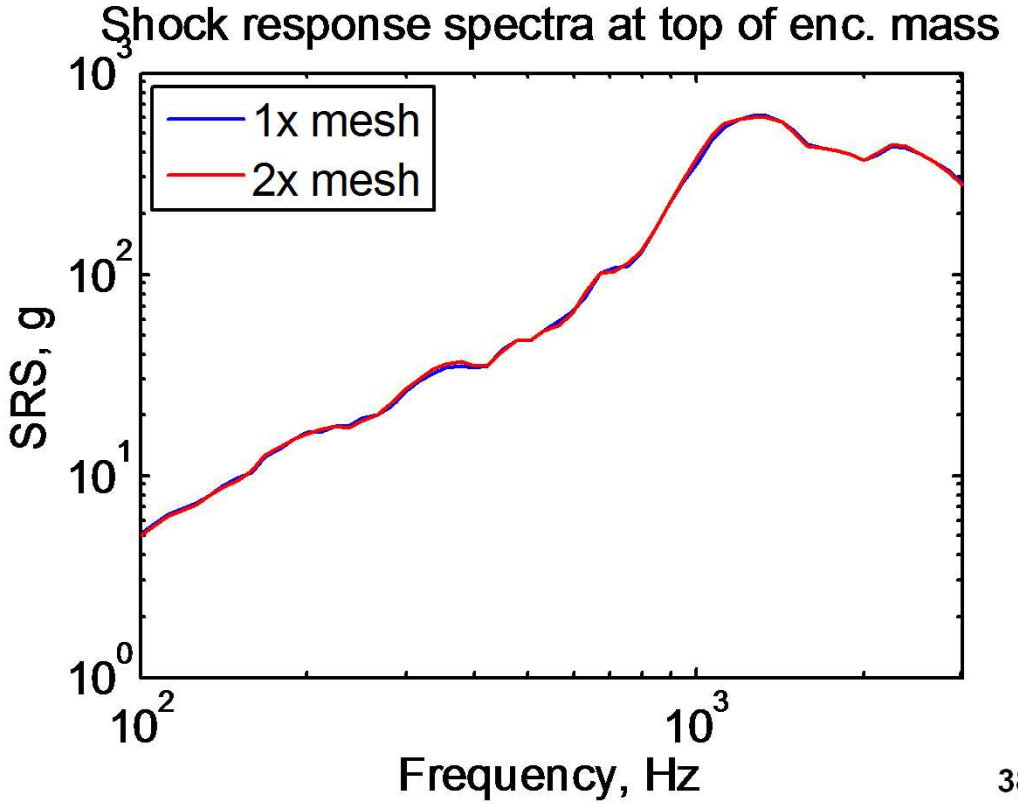
Sensitivity to Mesh Parameters

Structural Dynamics



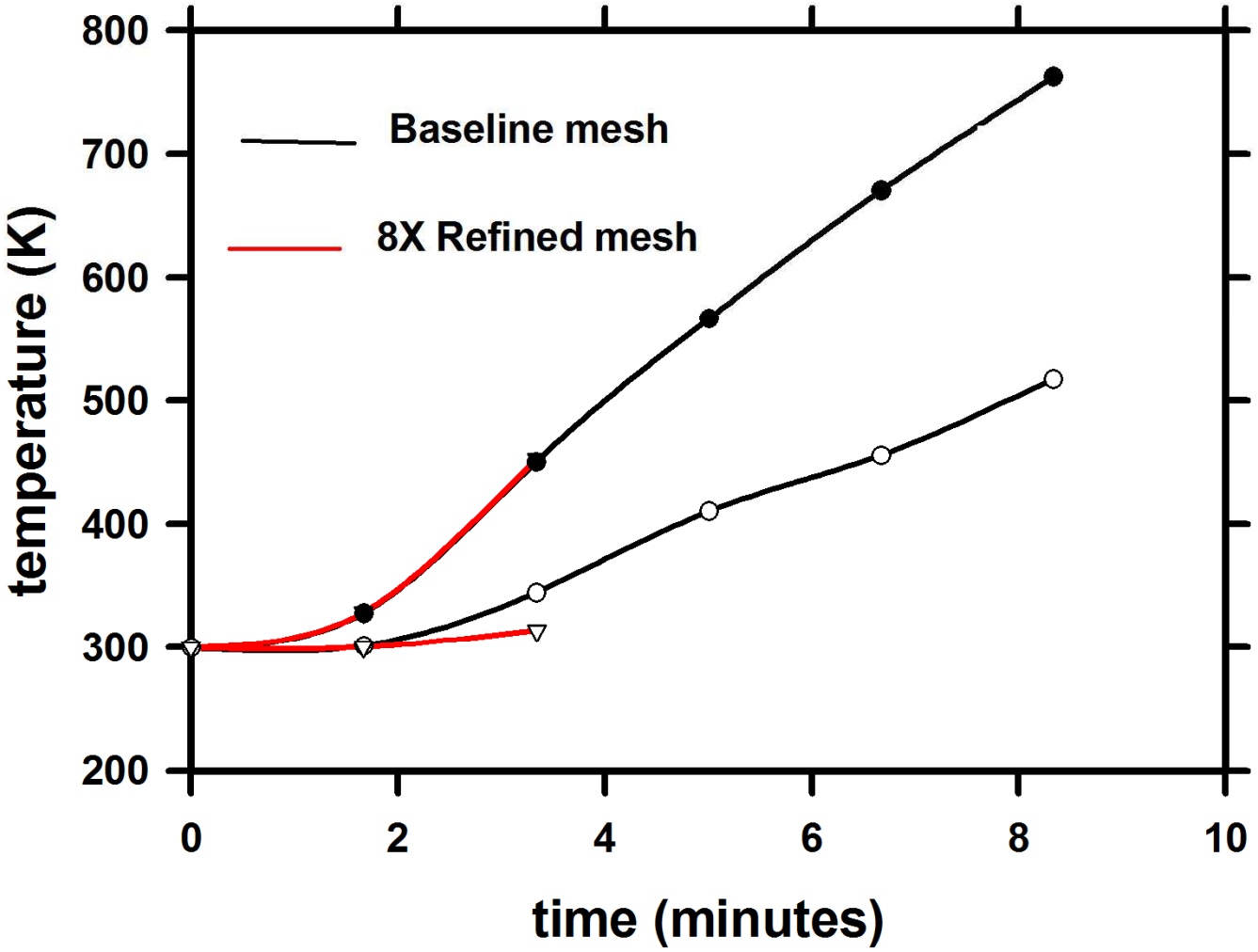
Max. relative error between SRS: +/- 5%



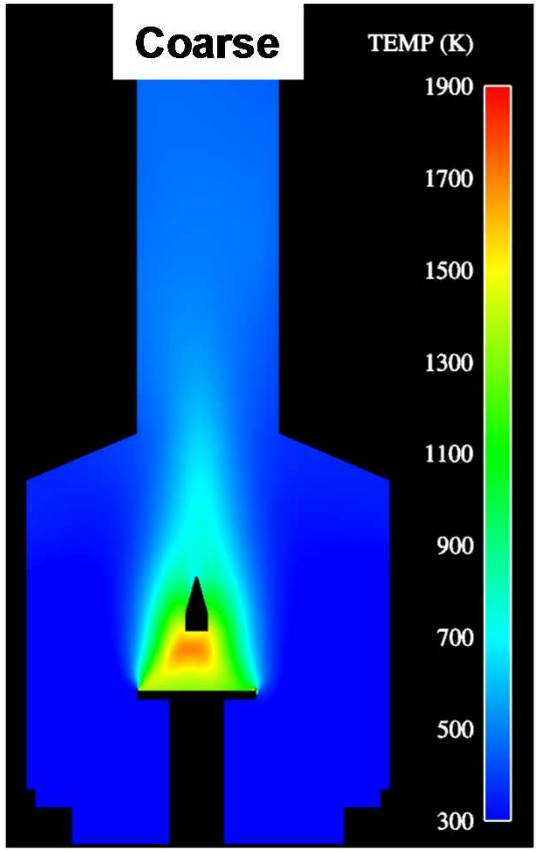


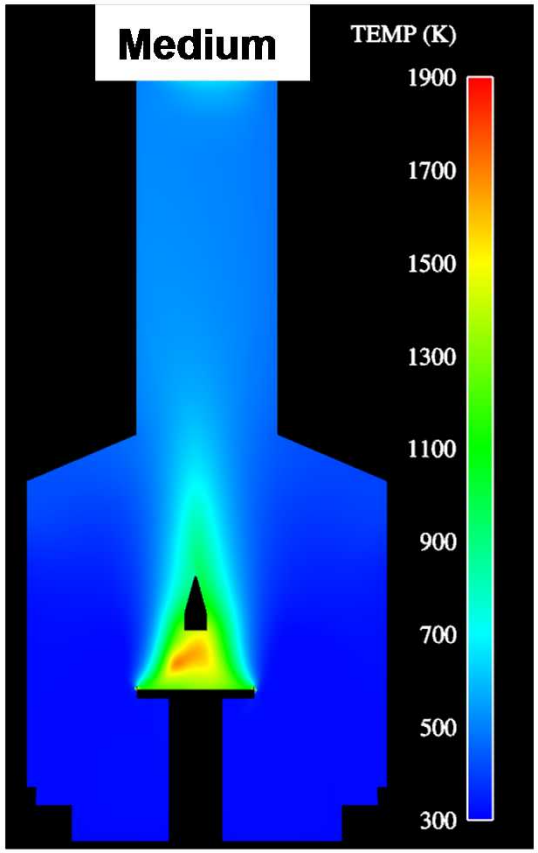
Solution Verification on High Fidelity Models is Hard

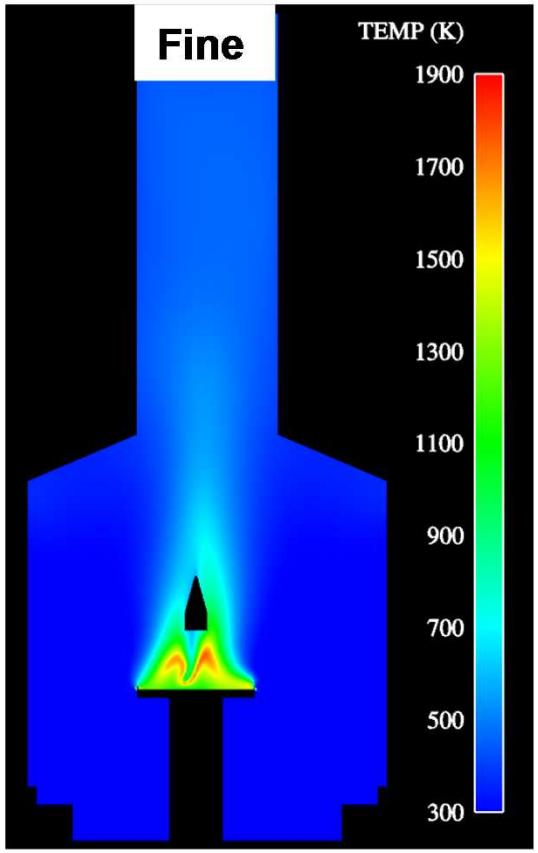
Solution Verification: Is the Discretization Adequate?

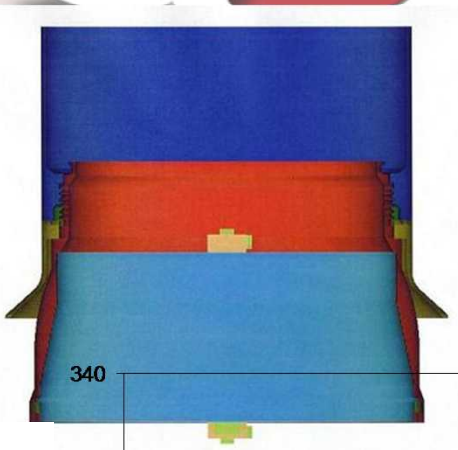


Calorimeter Fire
BVG Solutions



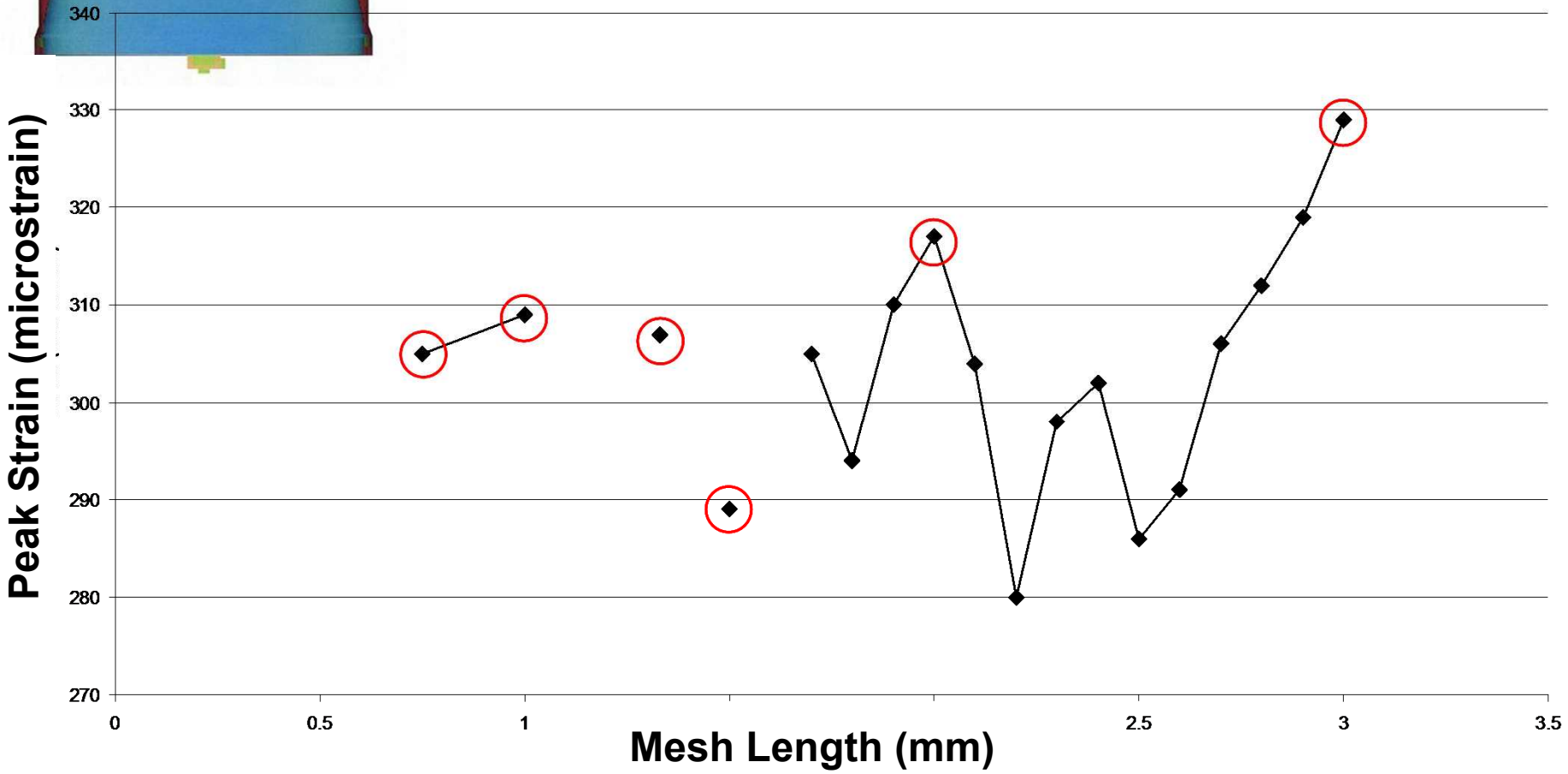






Calculation Verification for a Threaded Assembly

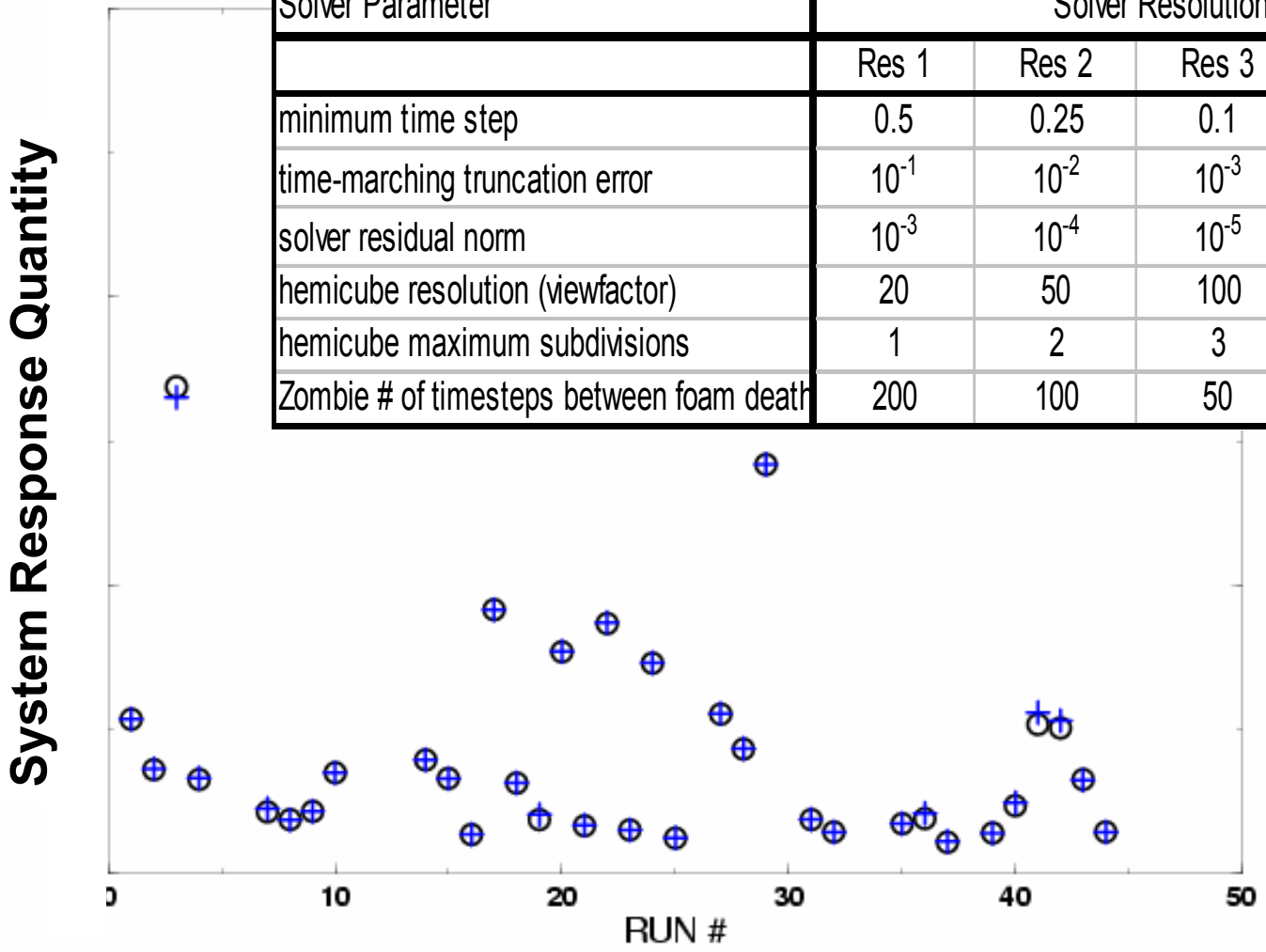
Ryan Maupin, ESA-WR, LANL: IMAC-XXIV 1/31/06



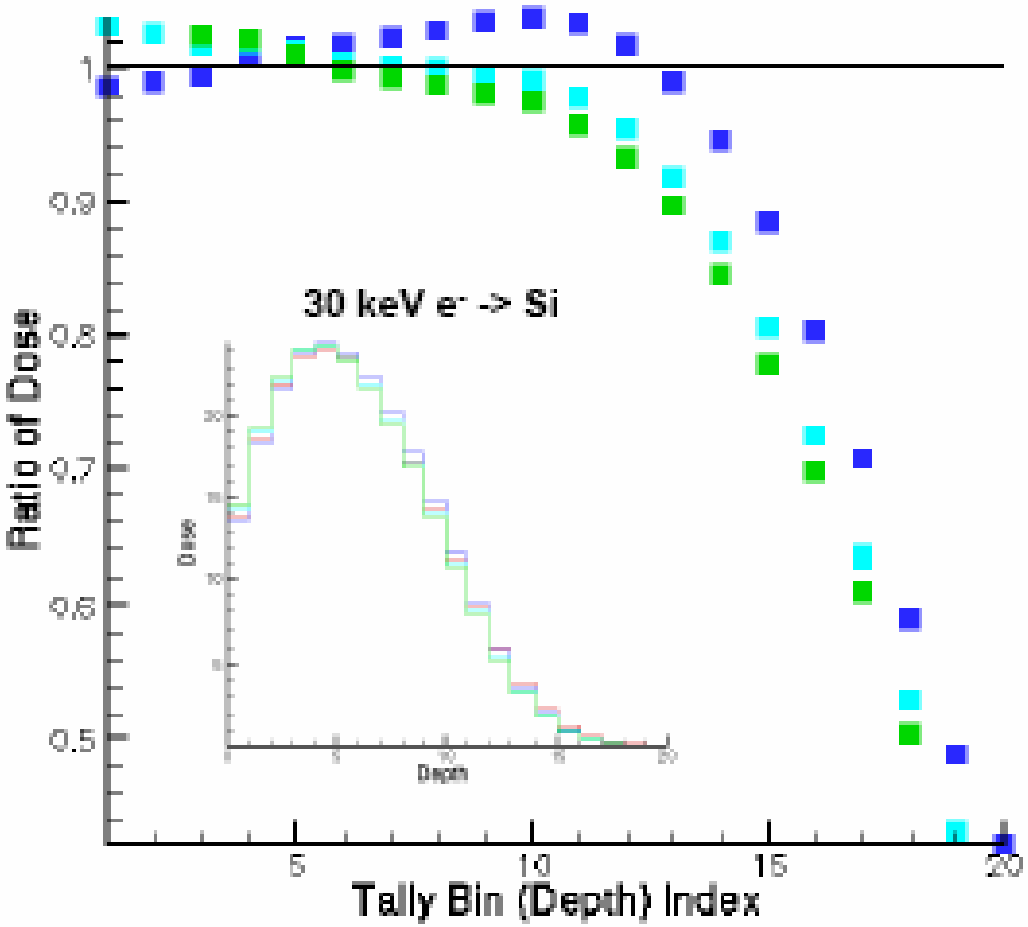
Solver Resolution Over UQ Parameter Space

Solution Verification: Are the solver settings adequate?

Solver Parameter	Solver Resolution Settings				
	Res 1	Res 2	Res 3	Res 4	Res 5
minimum time step	0.5	0.25	0.1	0.05	0.01
time-marching truncation error	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
solver residual norm	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
hemicube resolution (viewfactor)	20	50	100	200	300
hemicube maximum subdivisions	1	2	3	4	5
Zombie # of timesteps between foam death	200	100	50	20	1

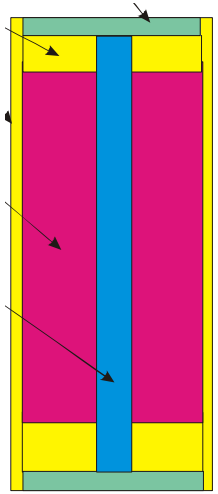


Dose Sensitivity to Electron Boundary Crossing Algorithm

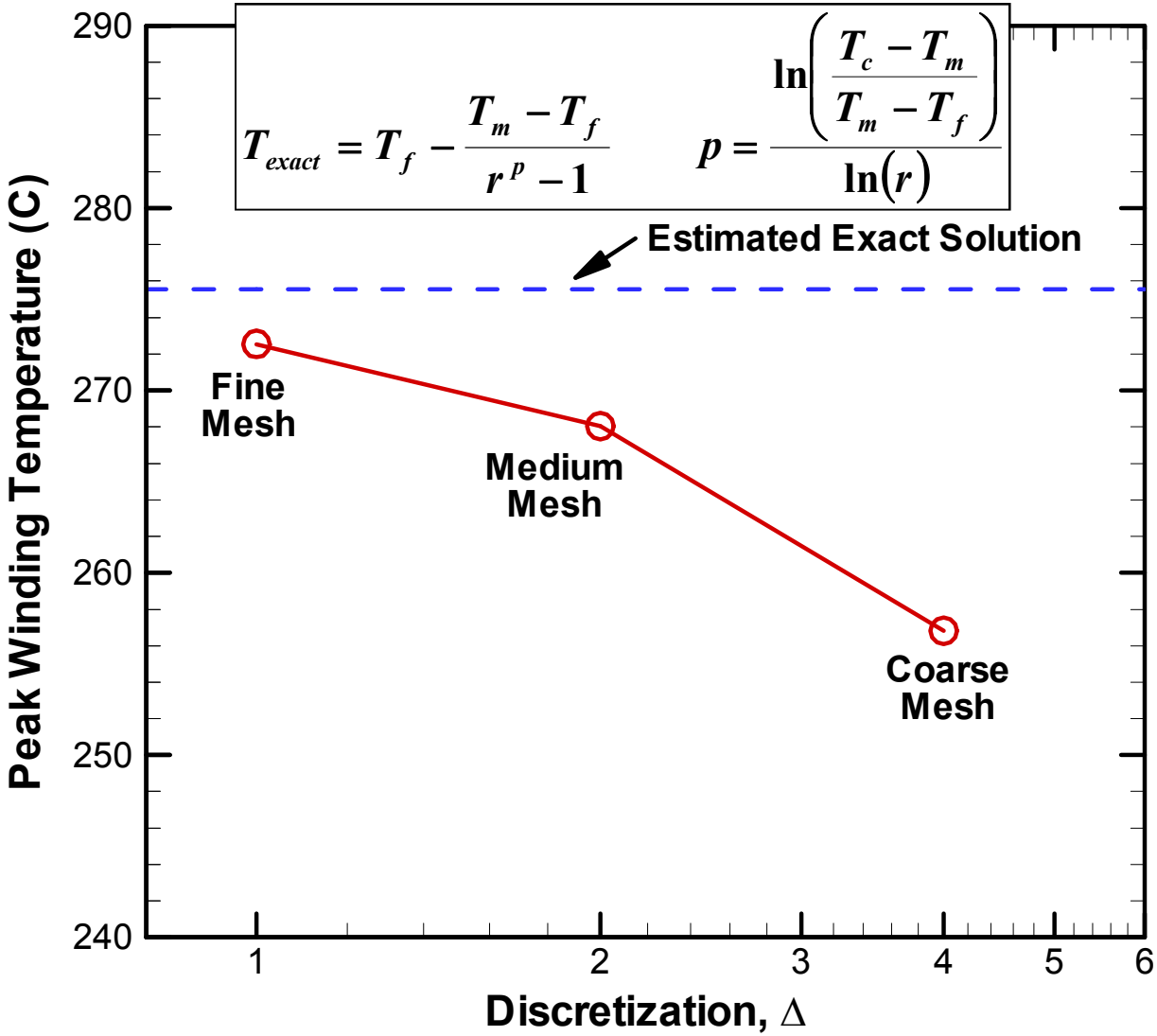


- Evaluation of ITS electron boundary-crossing error: (All with respect to no internal boundaries, default substep size.
- Blue: internal boundaries, default subtep size
- Cyan: Internal boundaries half-default substep size
- Green: Internal boundaries quarter-default substep size

Numerical Errors
Pollute Validation Assessments



$$T_{exact} = T_f - \frac{T_m - T_f}{r^p - 1} \qquad p = \frac{\ln\left(\frac{T_c - T_m}{T_m - T_f}\right)}{\ln(r)}$$



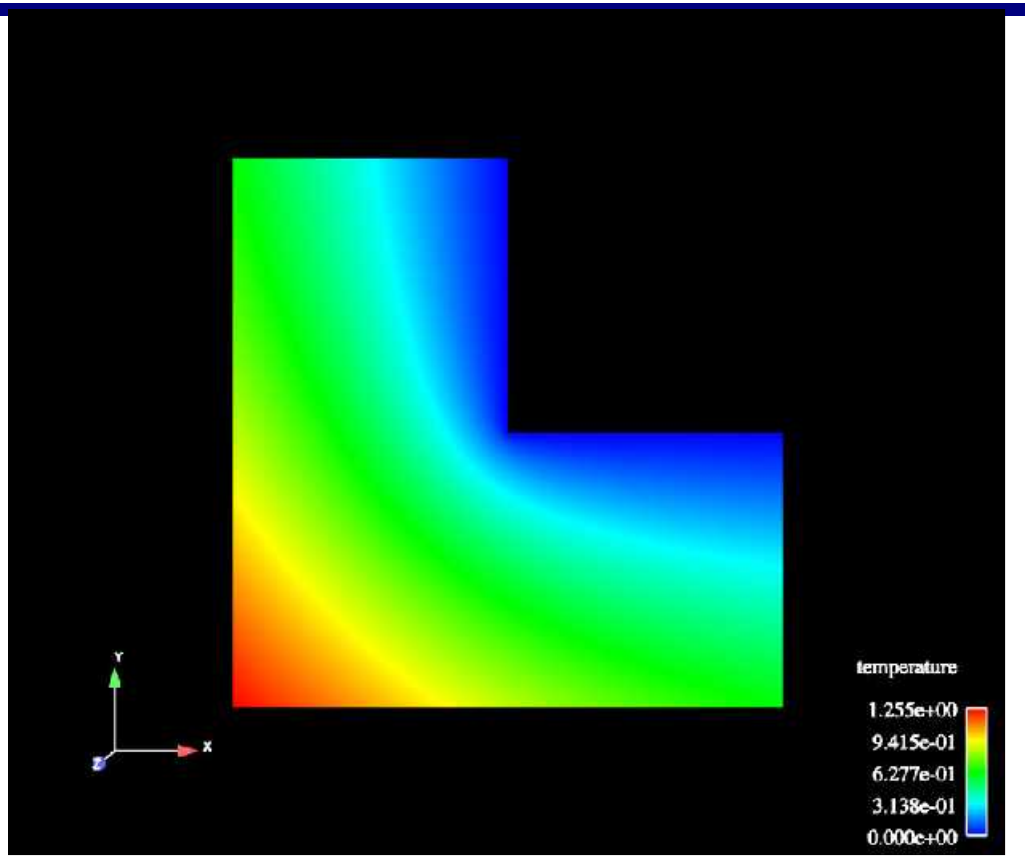
Verification of Error Estimator and Adaptive Algorithm

- 2D Exact Solution:

$$u = r^{2/3} \sin\left(\frac{2}{3}\theta\right)$$

- Linear elements
- ZZ error estimator

- Feedback adaptive algorithm:



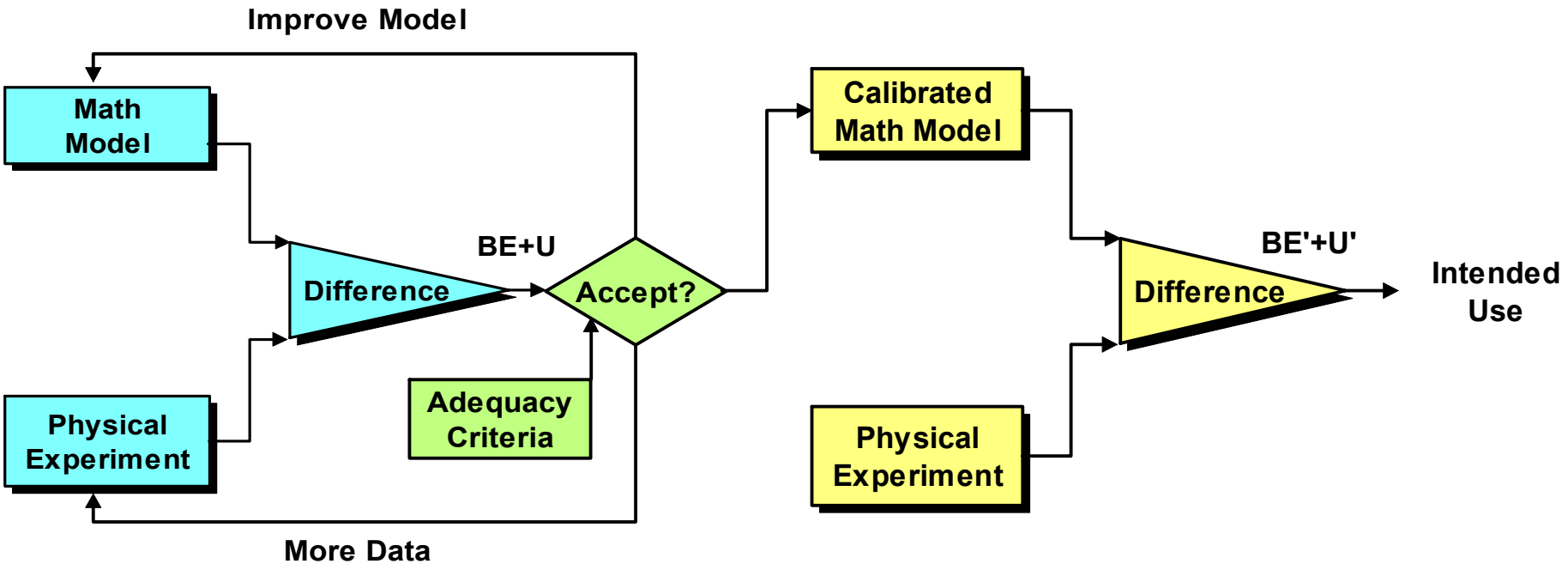
$$\text{if } \left(||e^*||_{H_1(\omega_j)} > 0.995 \max_{1 \le i \le N_\omega} ||e^*||_{H_1(\omega_i)} \right) \text{ then refine } \omega_j$$

Validation

Hyperlinks

Validation is Assessment

Calibration is not Validation

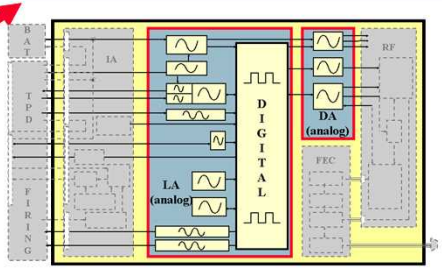


Science-Based Validation Experiments

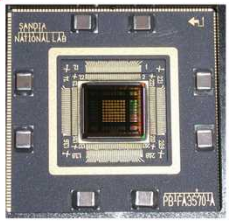
Validation: Are You Solving the Right Equations?

Hierarchal Validation: Right answer for the right reason

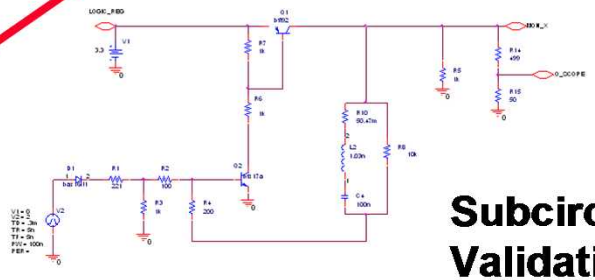
Increasing complexity, Decreasing number of tests



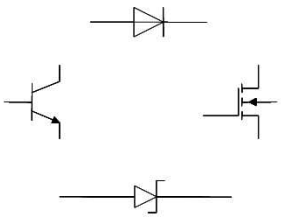
System-Level Circuit Validation



Single ASIC Validation



Subcircuit Validation



Single Device Characterization and Validation

- **Application relevant parameter space**
- **Formal DOE and replicate tests**
- **Attention to diagnostic bias and precision**

Science-Based Validation Experiments

Validation: Are You Solving the Right Equations?

Hierarchal Validation: Right answer for the right reason

Full System Test

Increasing complexity, Decreasing number of tests

Mockup with jointed structure and foam embedded object

Jointed structure validation

Single joint validation

Joint parameter characterization

- **Application relevant parameter space**
- **Formal DOE and replicate tests**
- **Attention to diagnostic bias and precision**

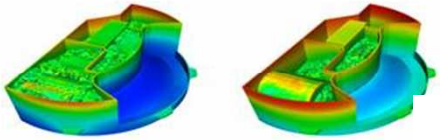
Science-Based Validation Experiments

Validation: Are You Solving the Right Equations?

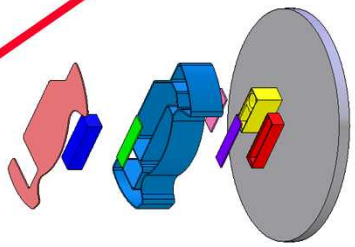
Hierarchal Validation: Right answer for the right reason

Increasing complexity, Decreasing number of tests

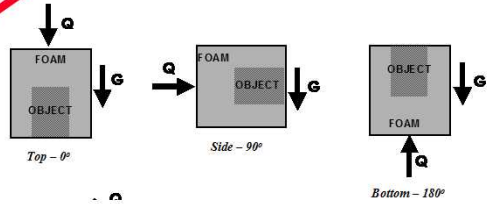
Full System Test



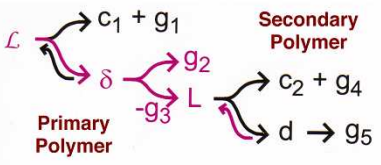
Validation Real Sub-systems



Validation with mockups



Foam recession

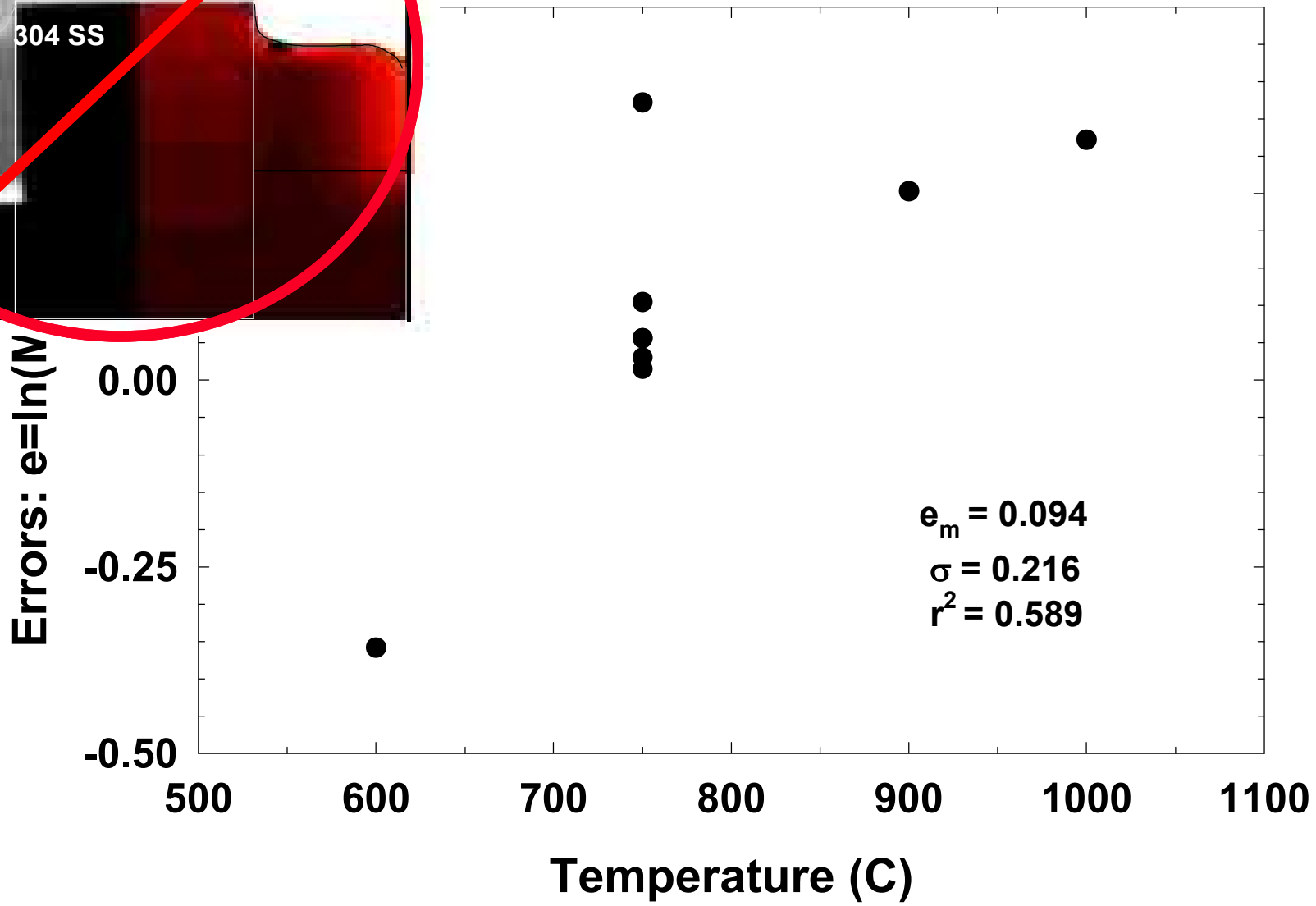


Chemistry characterization/validation

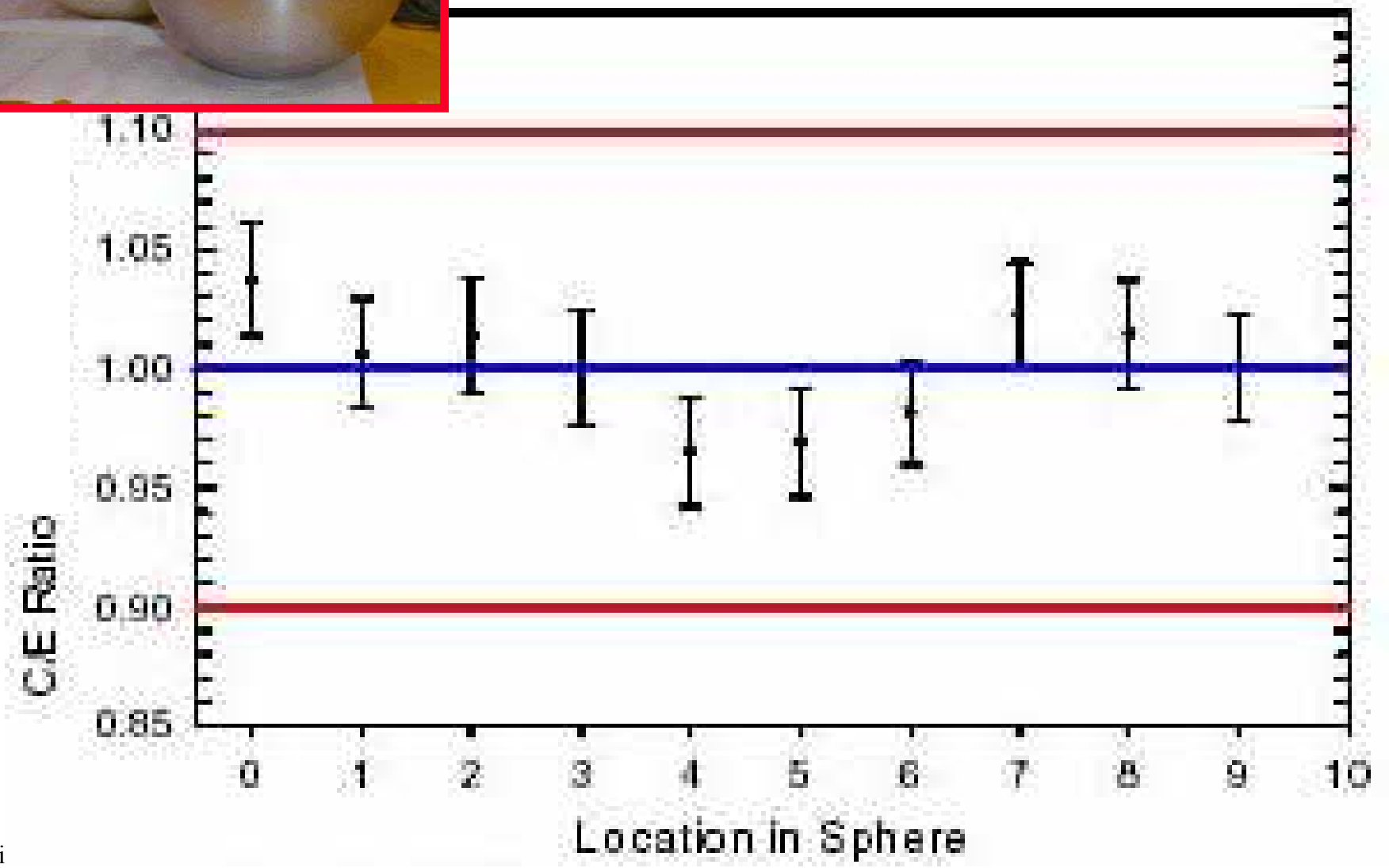
- **Application relevant parameter space**
- **Formal DOE and replicate tests**
- **Attention to diagnostic bias and precision**

Validation is Statistical

Vugraph Norms Are Not Adequate



Neutron Attenuation in Test Objects

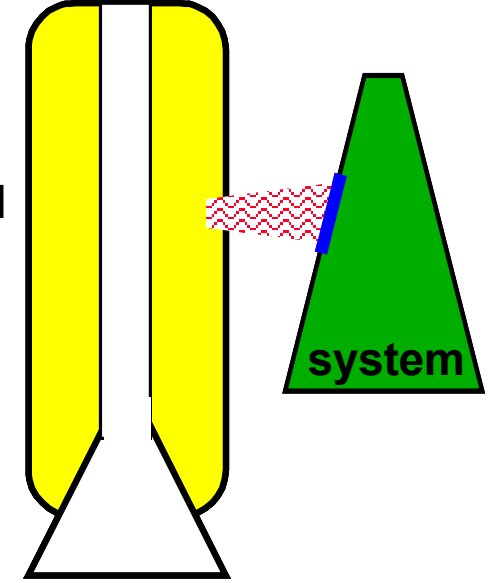


QMU and Sensitivities

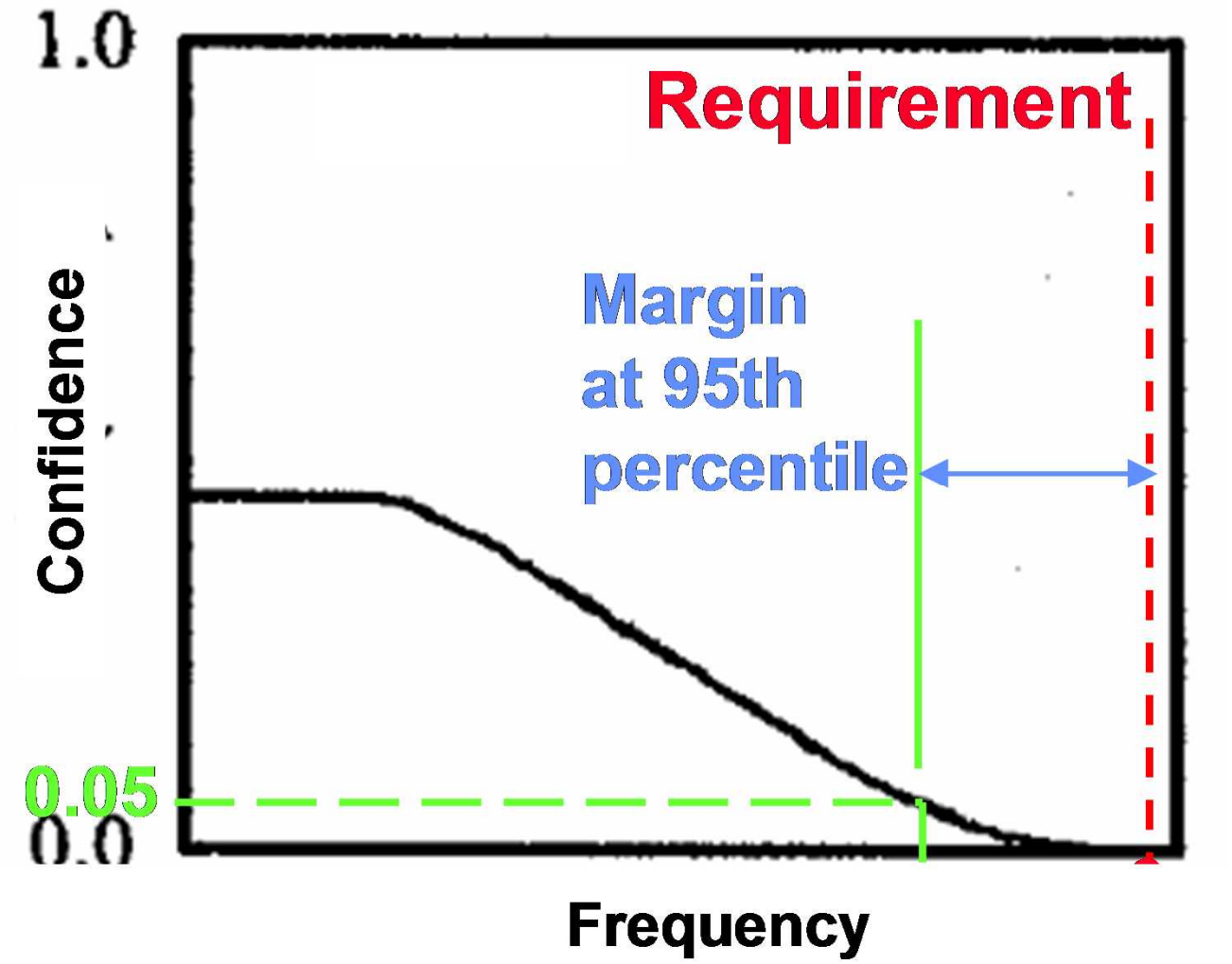
Hyperlinks

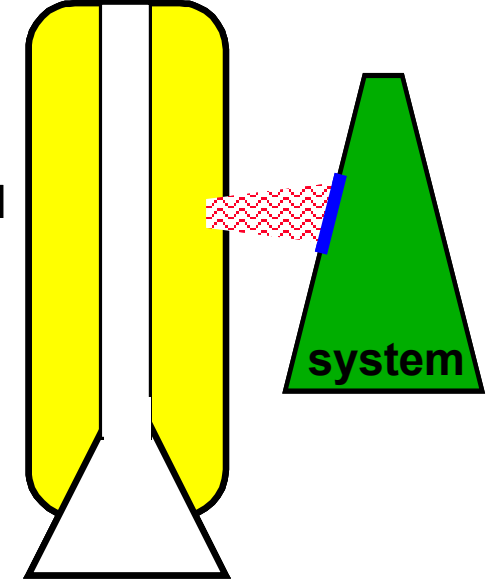
Aleatory and Epistemic Uncertainties

- **Aleatory uncertainty**: Inherent randomness in behavior of system under study **(frequency interpretation)**
  - Alternatives: Variability, stochastic uncertainty, irreducible uncertainty, type A uncertainty
  - Examples: component failures or material properties derived from statistically significant testing under conditions relevant to intended application
- **Epistemic uncertainty**: Lack of knowledge about appropriate value to use for a quantity that is assumed to have a fixed value in the context of a specific analysis **(confidence or belief interpretation)**
  - Alternatives: state of knowledge uncertainty, subjective uncertainty, reducible uncertainty, type B uncertainty
  - Examples: representative scenarios, unknown parameters in frequency distributions, parameters or models with defensible bounds but no sense of frequency



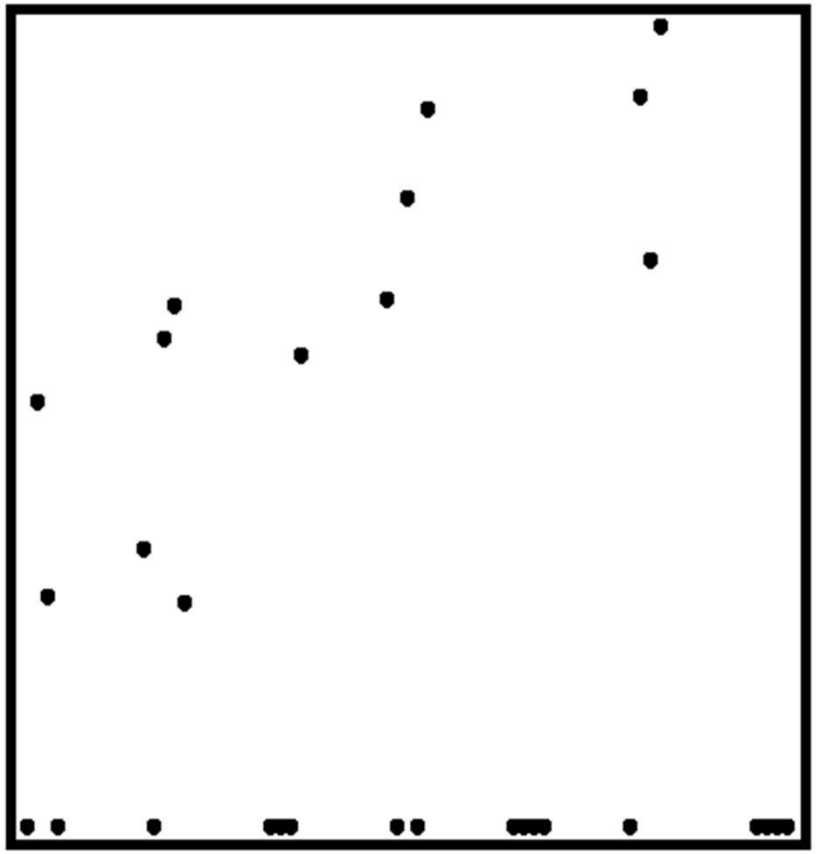
Quantified Margins and Uncertainties

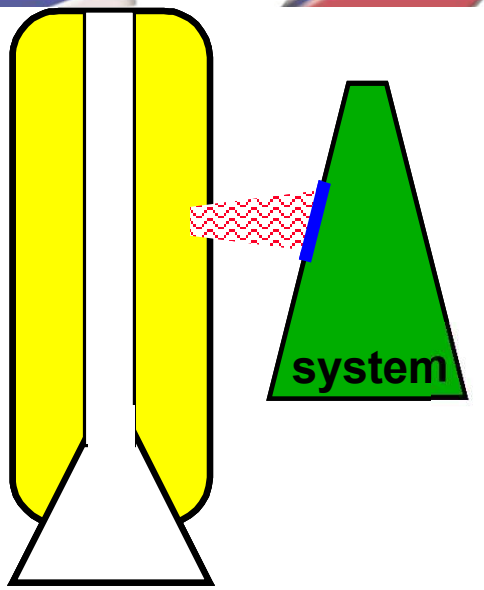




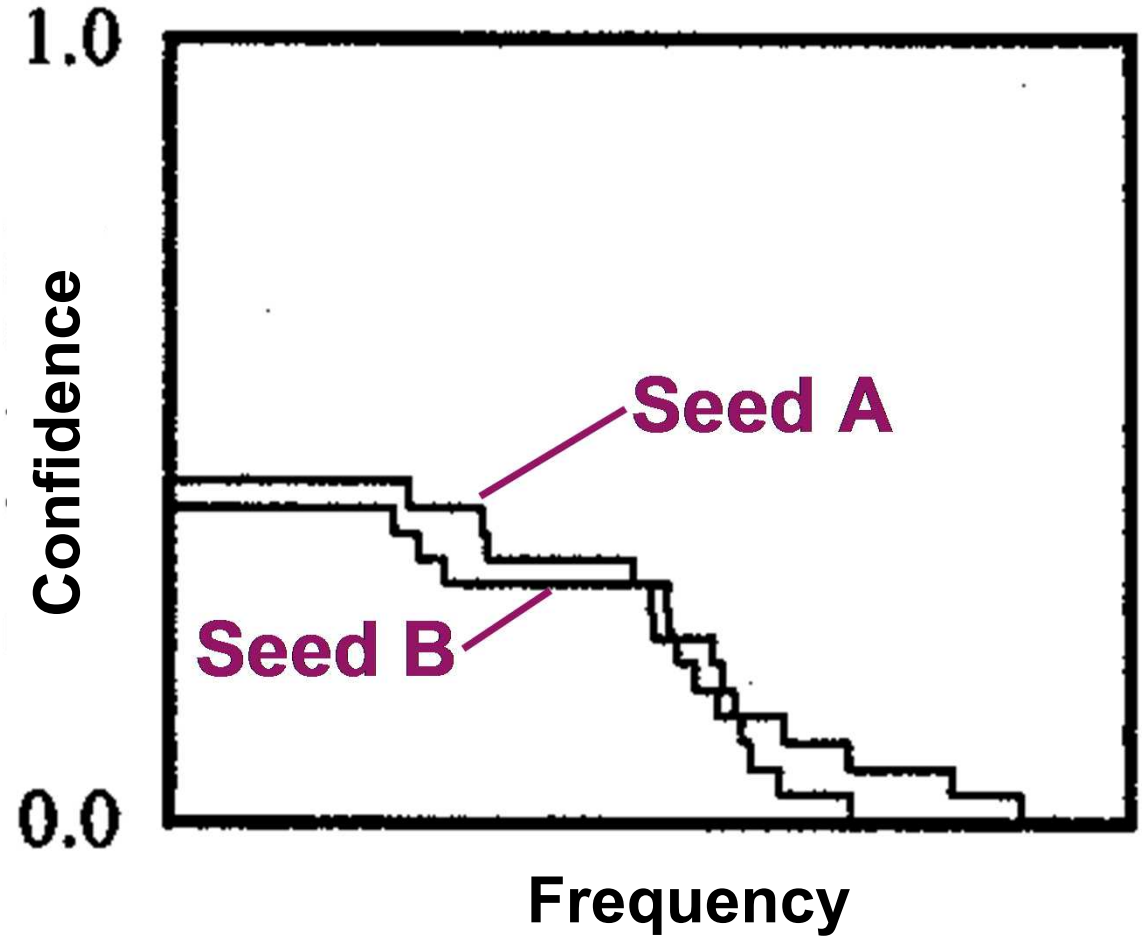
Sensitivity Analysis

SCorr = 0.809





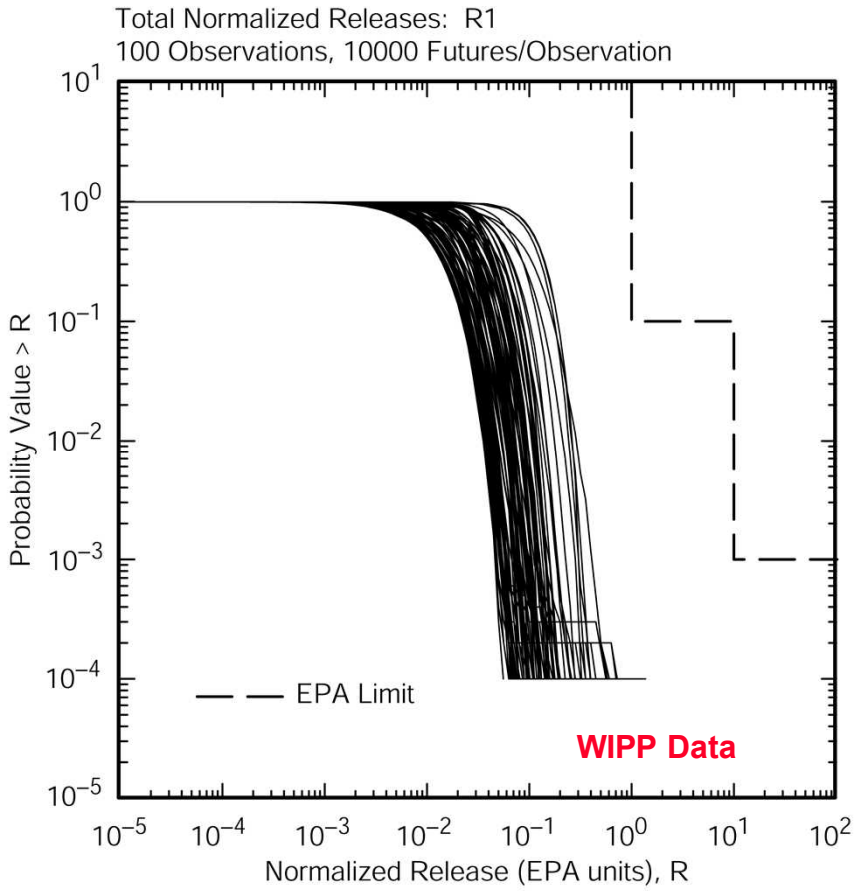
UQ Solution Verification

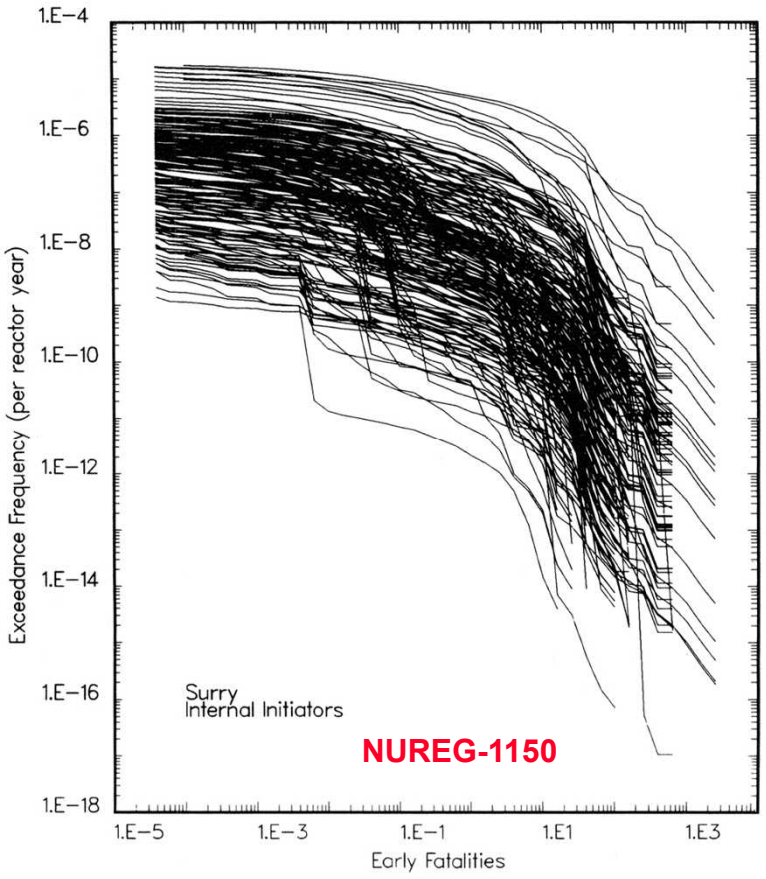


Seed Effects from limited sampling

WIPP and NUREG-1150 Precedents

High Consequence Regulatory Issues in the National Interest Addressed Primary Through Modeling and Simulation

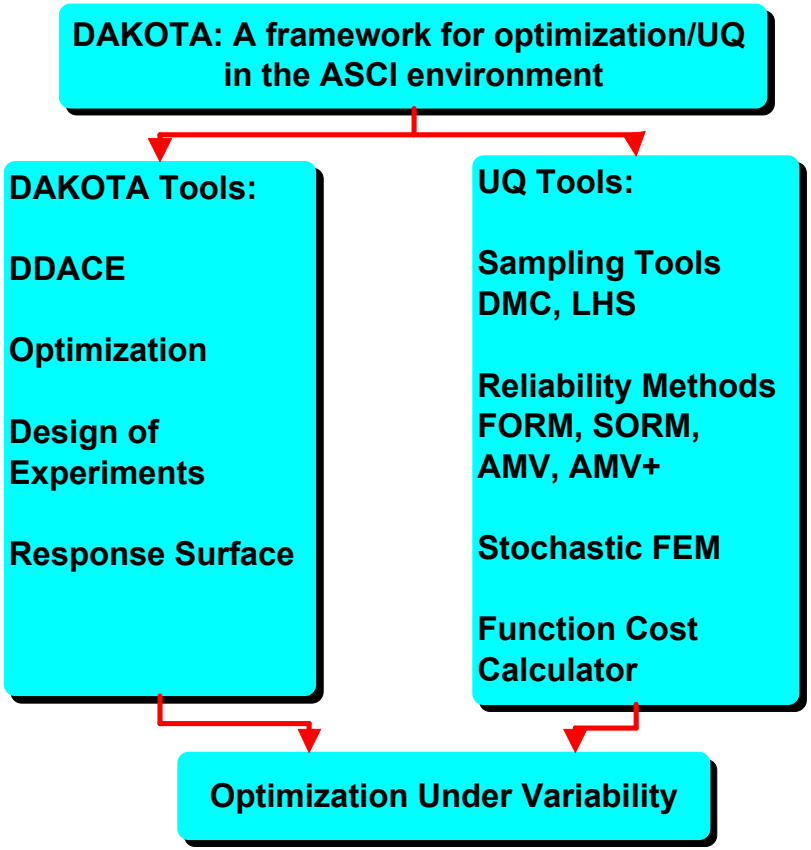




Lessons Learned: (1) Seek BE + Uncertainty

(2) It takes more than one shot to get it right

Infrastructure for ASC-Scale UQ Analyses



1. ***Algorithmic coarse-grained parallelism:*** **independent concurrent fn. evaluations**
2. ***Algorithmic fine-grained parallelism:*** **parallel computation of internal linear algebra**
3. ***Function evaluation coarse-grained parallelism:*** **concurrent execution of separable simulations within a fn. eval. (e.g., multiple loading cases)**
4. ***Function evaluation fine-grained parallelism:*** **parallelization of the solution steps within a single analysis code (e.g., SALINAS, MPSalsa)**