SAND2014-3984P

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Sandia National Laboratories

ESP 700: Class Summary, Evidence and Credibility

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Validation, Verification,
Uncertainty Quantification and
Credibility Processes Dept.

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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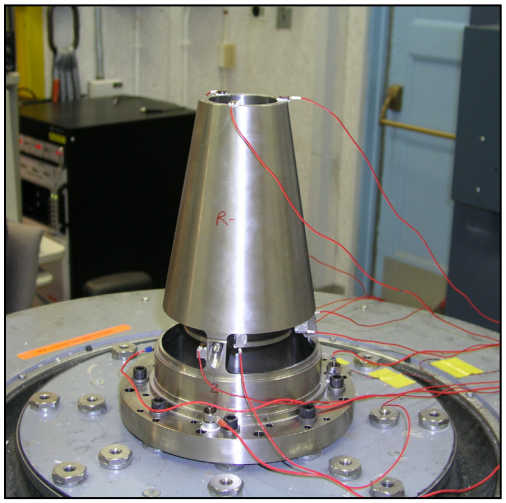
Overall Course Outline

- Summary of class
  - The example (revisited)
  - What have we learned?
  - What do we do next?
- How does V&V/UQ help establish credibility in computational simulations
  - Predictive Capability Maturity Model (PCMM)
  - Credibility Evidence Package (CEP)
- Q&A
- Before we start

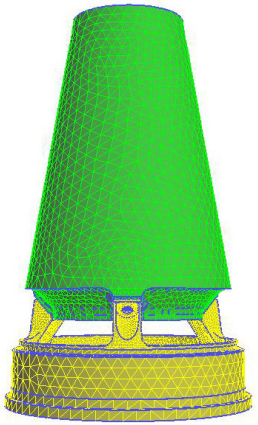
The Example

The Example (Credibility)

Response of physical system, *j* $\overset{?}{\approx}$ Response of model system, *j*



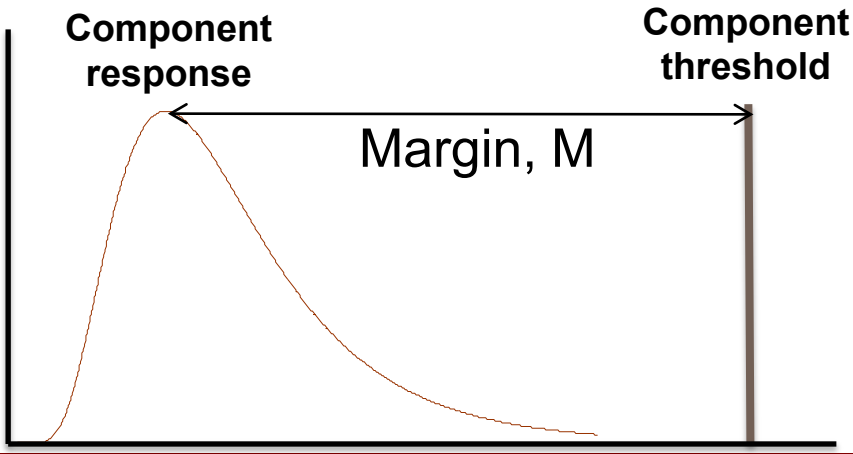
$\overset{?}{\approx}$



Key questions:

- Are model predictions "good enough" to be used in lieu of the real thing?
- How do establish credibility in these predictions?

Intended use of CompSim: Qualification Support



What Gives CompSim Results Credibility?

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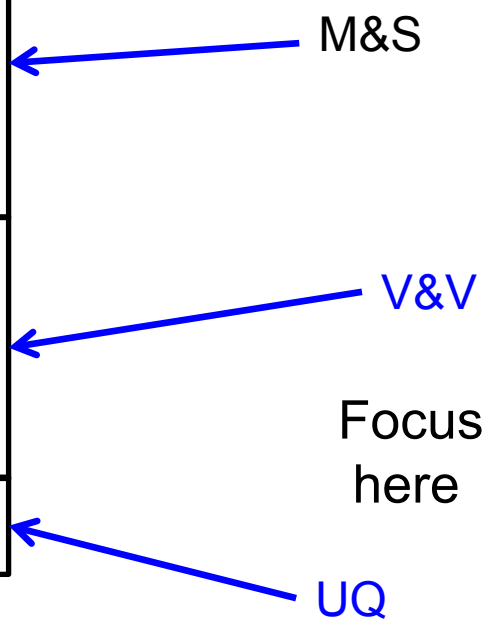
- PCMM is an assessment of credibility

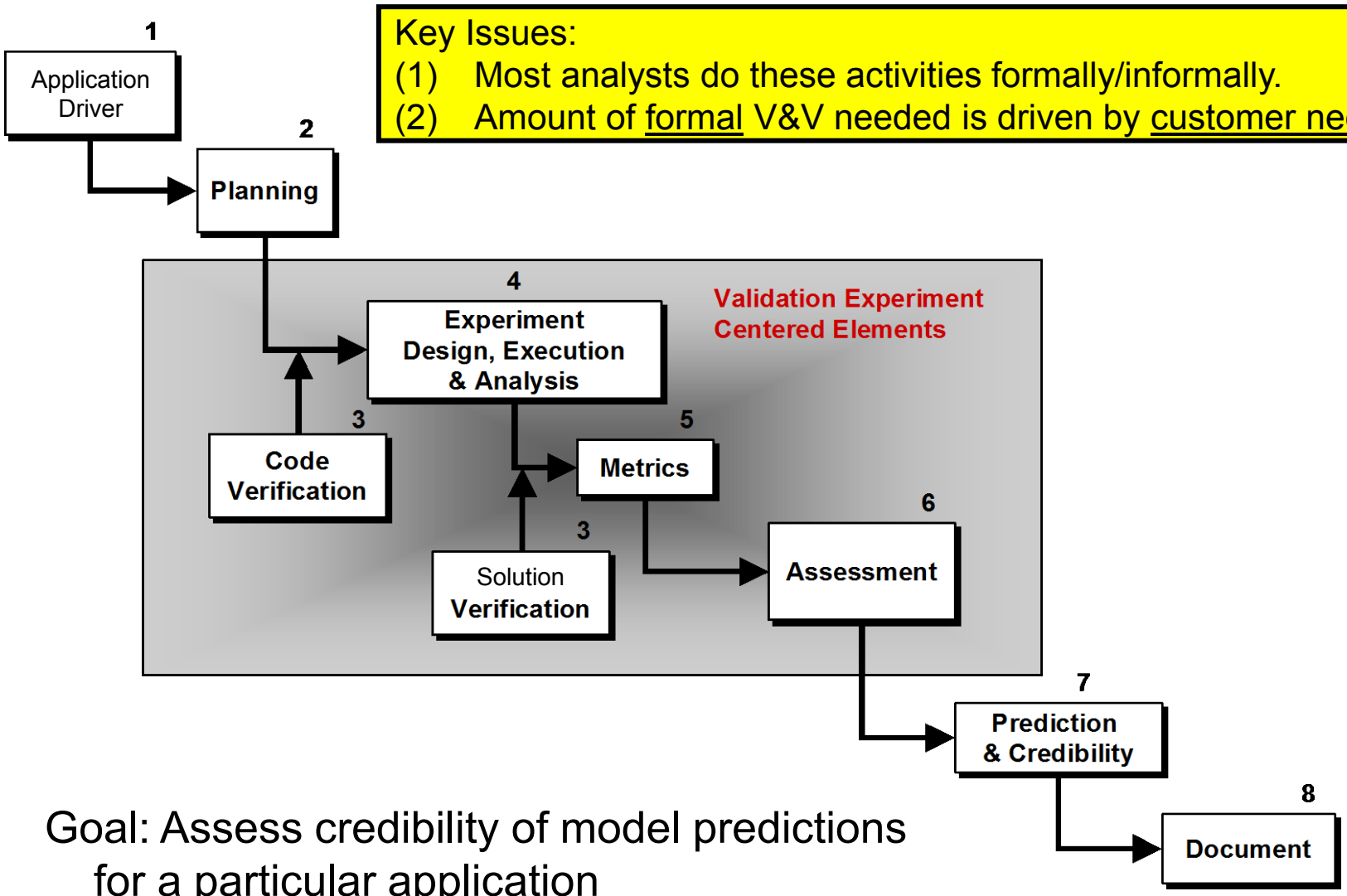
Seven components

1. RGF: Representation and geometric fidelity
2. PMMF: Physics and material model fidelity
3. CVER: Code verification
4. SVER: Solution verification
5. VAL: Validation
6. UQ: Uncertainty quantification
7. Documentation and archiving



The V&V Process

Overview of the Sandia V&V Process



Goal: Assess credibility of model predictions for a particular application

Code and Solution Verification

Code and Solution Verification

Code Verification is the activity of ensuring that the code correctly implements the numerical model.

- Errors in computer models are called code defects or bugs
- The code developers/testers have primary responsibility for identifying and eliminating code bugs

➢ Tool: Feature Coverage Tool (FCT)

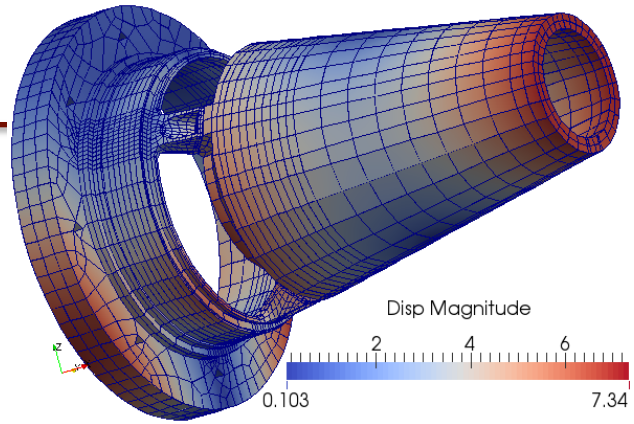
Solution Verification is the quantification and reduction of numerical error.

- Done in the context of the overall uncertainty budget.
- Error may or may not need to be reduced.

➢ Tool: Percept

An FCT Analysis

Example: the structural dynamics cone problem.




```
SOLUTION
//    eigen nmodes=20
// uncomment all the lines below this to the END and comment the
line above to run a nonlinear blast analysis
    NLtransient
    time_step 2.0e-5
    nsteps 8192
    nskip 1
    rho 0.9
    solver = gdsw
END

[...]

GDSW
   max_iter=1000
   solver_tol 1e-10
   krylov_method=1  //0
   overlap = 2
   orthog = 1000
//   orthog_option = 2
END
```

The main input file.

Specifies the problem domain, a grid, boundary conditions, material properties, algebraic solver, etc.

FCT 1-way coverage

```
verified
  * one-way:93%
  * two-way:66%
tested
  * one-way:100%
untested
ignored
```

One Way
Percent of features (non-commented lines) in your input file that are covered by at least one verification test.

Two Way
Percent of pairs of every two features in the input file that were present in one or more verification tests.

Input File

```
SOLUTION 1087 +
//    eigen nmodes=20
// uncomment all the lines below this to the END and comment the line above to run a nonlinear blast
    NLtransient 31 +
    time_step 31 +  2.0e-5
    nsteps 31 +  8192
    nskip 10 -
Salinas_rtest/verification/visco/visco_poissons_ratio_nl.test|visco_poissons_ratio_nl.np1_feti-dp
Salinas_rtest/verification/visco/visco_poissons_ratio_nl.test|visco_poissons_ratio_nl.np1_sparsepak
Salinas_rtest/verification/visco/visco_poissons_ratio_nl.test|visco_poissons_ratio_nl.np1_gdsw
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Salinas_rtest/verification/visco/visco_stress_relaxation_nl.test
Salinas_rtest/verification/visco/visco_poissons_ratio_nl.test|vi
Salinas_rtest/verification/visco/visco_stress_relaxation_nl.test
 1
    rho 27 +  0.9
    solver = gdsw 292 +
END
```
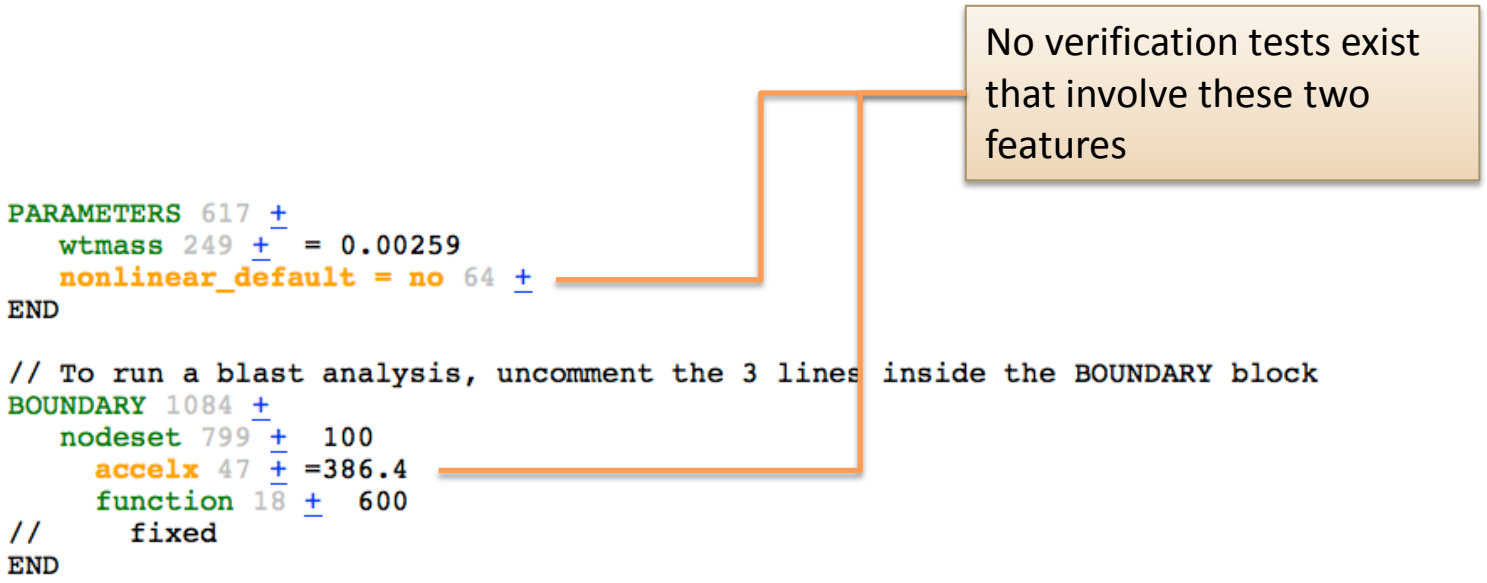

Clicking on the expansion +/- symbol opens a list of the verification tests.

Items in the list will soon link to documentation and a directly of all the test inputs and outputs.

FCT 1-way coverage

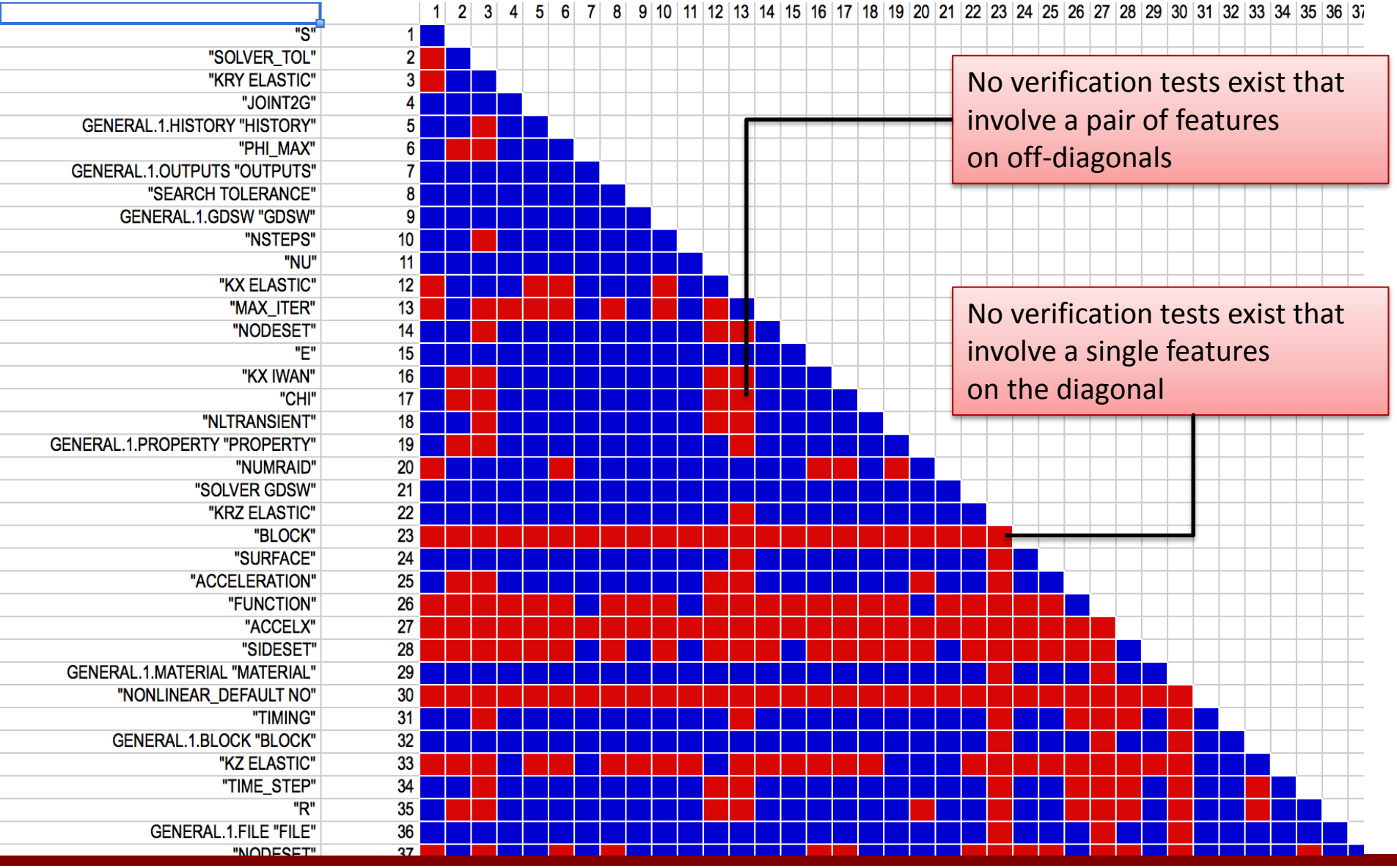


Amber color signifies a limited form of testing: a *regression test* (ensures the feature works the same as it did yesterday).

Red color signifies no test of any kind was found that included that feature.

- Results are an opportunity to discuss these features with developers and whether additional or higher quality testing would be useful.
- 1-way coverage snapshot can be pasted into reports and documentation of your analysis.

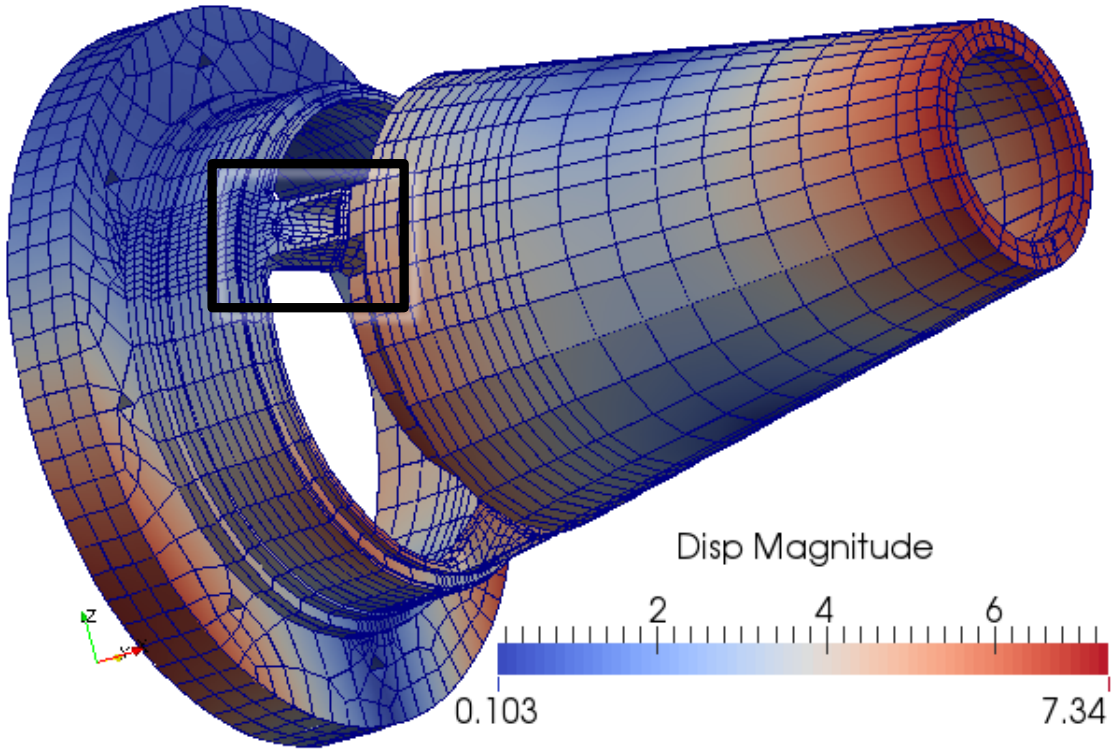
FCT 2-way coverage (Excel table)



Solution Verification for Modal Analysis

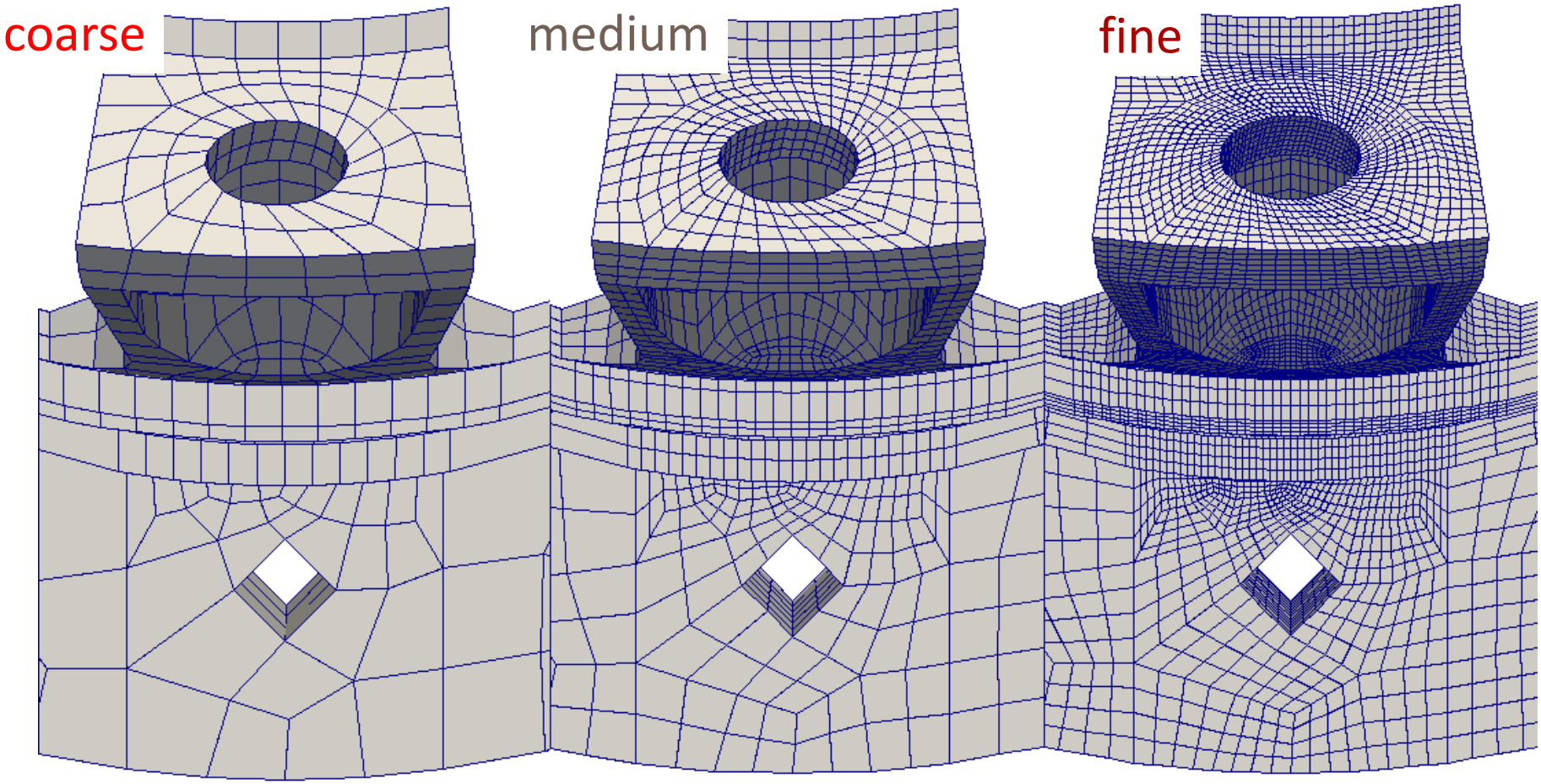
- This problem has a complex mesh, but few numerical controls (only solver tolerance, contact search tolerance)
- QoIs are the eigenvalues

Next slide we will zoom to the region indicated



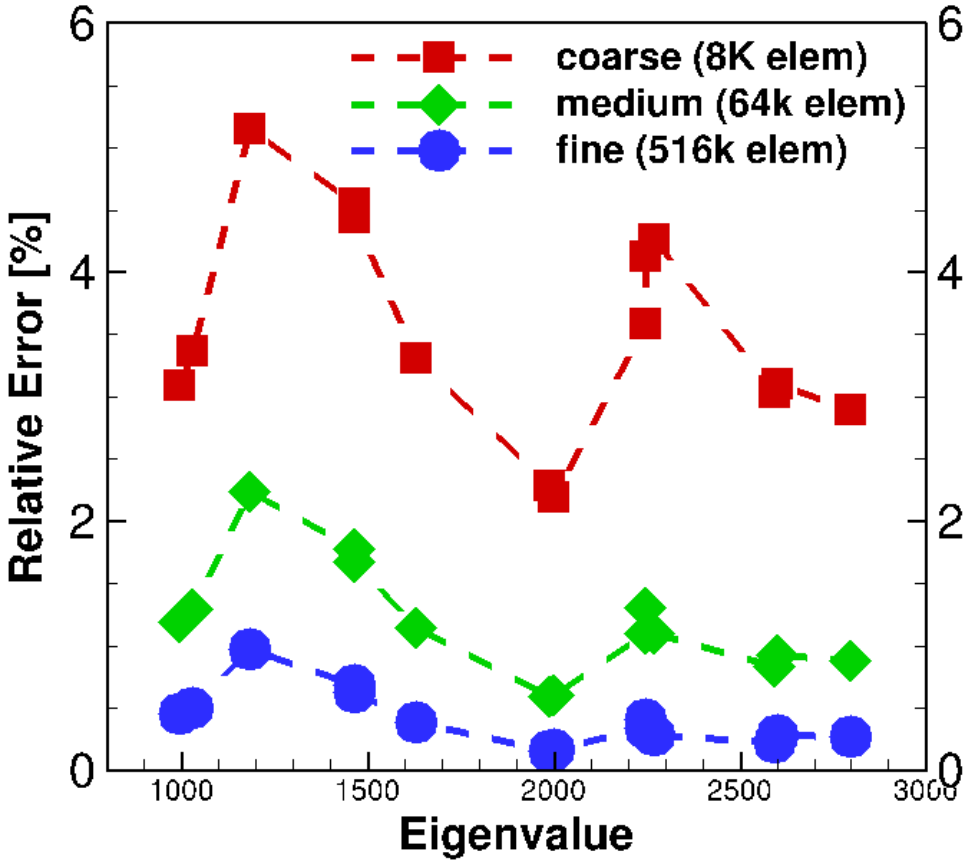
Generation of Refined Meshes

- We used Sierra/Percept to generate refined meshes



Numerical Error Estimates

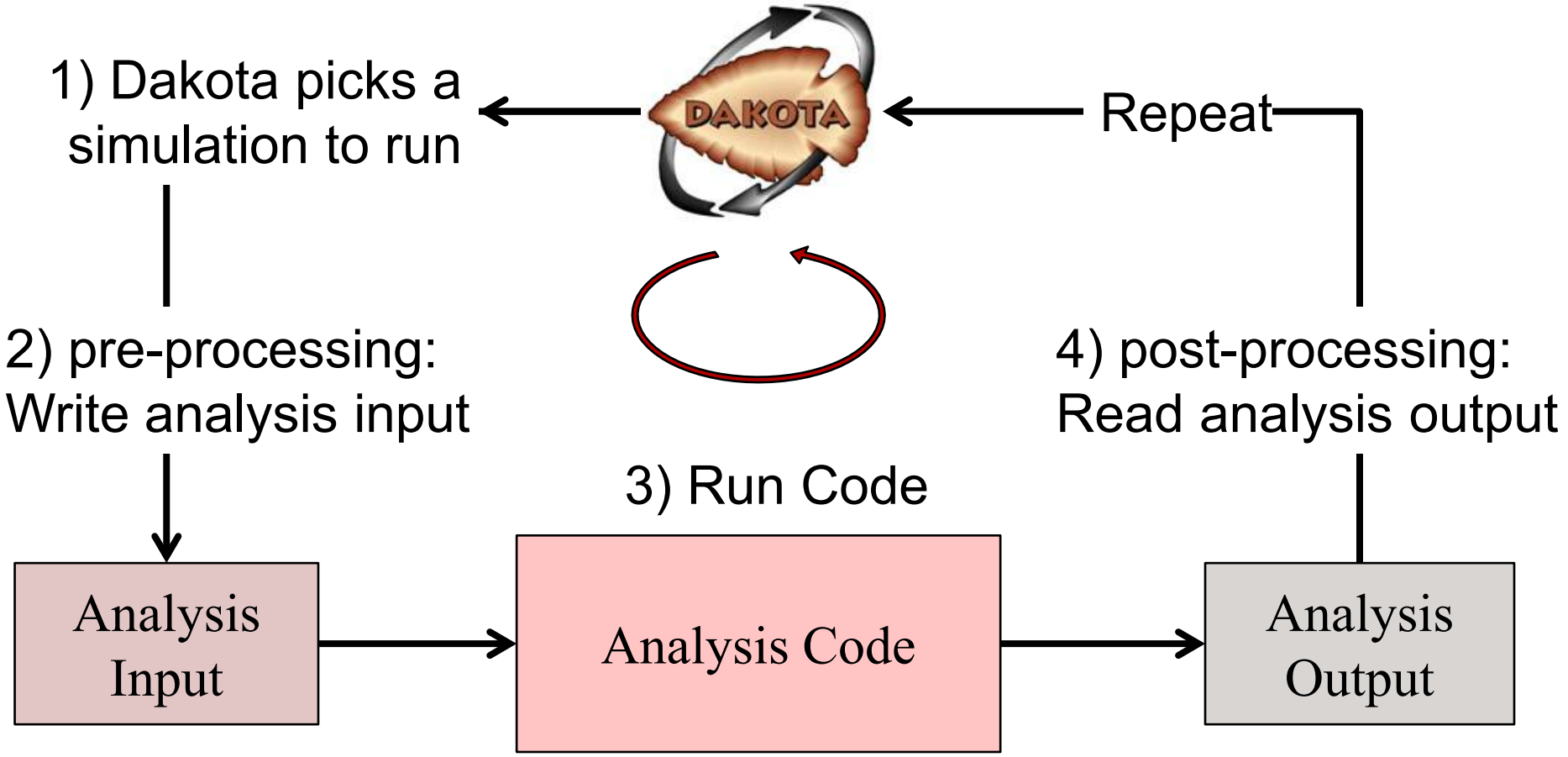
- Errors from extrapolation (first 14 nonzero frequencies)



- In this case, we see convergence for all frequencies
- This allows us to assess the accuracy of each mesh
- Suitable accuracy depends on the application and other uncertainties (parametric, validation data, etc.)

Sensitivity Analysis and Uncertainty Quantification

The Tool: DAKOTA



Sensitivity Analysis

- How do changes to inputs affect the response?
  - How "sensitive" is the response to each input?
  - Direction and magnitude

Simple Correlation Matrix MaxAccel

# samples	10	20	40
chi	-0.33	-0.43	-0.46
R	-0.14	0.25	0.17
S	0.62	0.52	0.49
phi_max	0.39	0.45	0.39

Partial Correlation Matrix MaxAccel

# samples	10	20	40
chi	-0.68	-0.56	-0.59
R	-0.59	0.18	0.15
S	0.78	0.64	0.61
phi_max	0.62	0.57	0.52

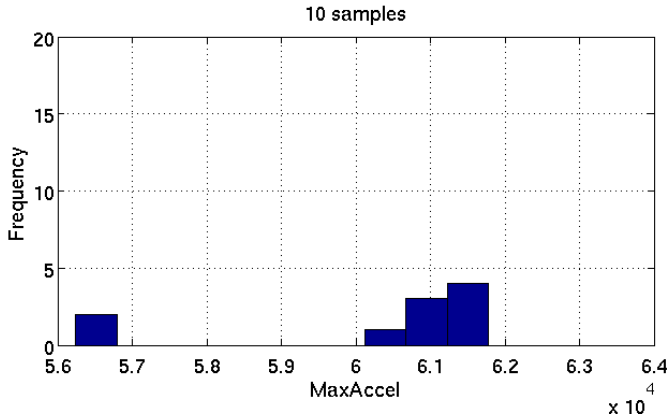
Uncertainty Quantification

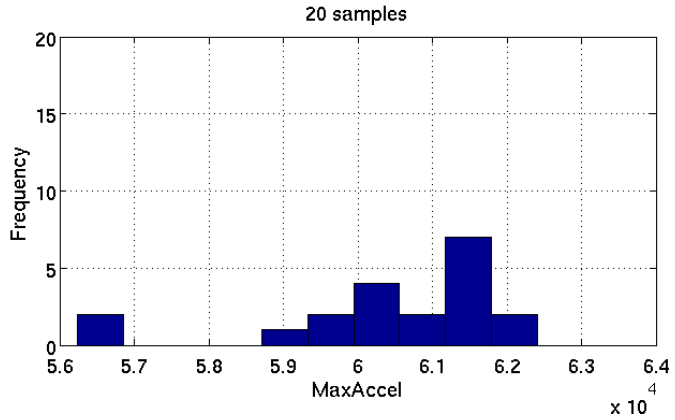
- What is uncertainty? Lack of information
- Uncertainty quantification = information quantification
  - Have a model, know the significant inputs, etc…
  - How much information do you have about QoI's?
  - What are the significant sources of uncertainty?

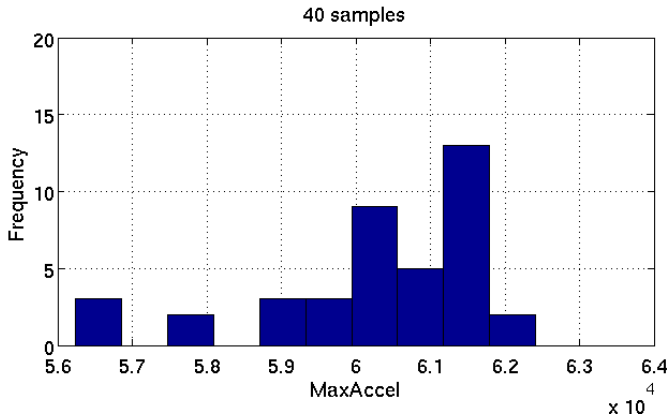
1. Characterize the uncertainty in significant inputs
2. Propagate
3. Interpret

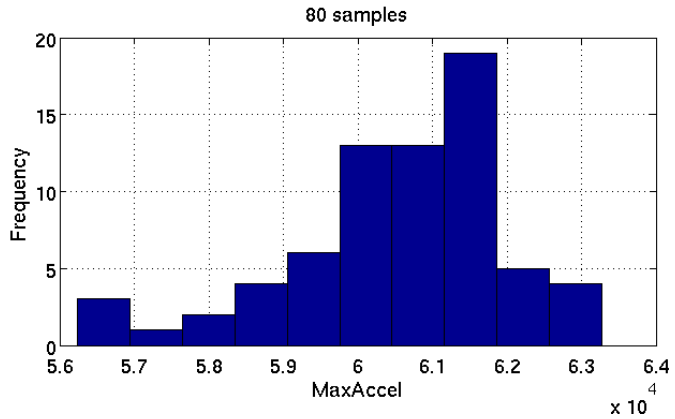
Example: 3leg

- 20 sets of best estimates for 4 parameters
  - Assume Gaussian distributions w/ correlations
- Propagate w/ incremental LHS: 10, 20, 40, 80 samples









Samples	Mean	Std Dev
10	60297	2131.5
20	60488	1700.4
40	60365	1558.6
80	60589	1496.3

Higher moments need more samples to converge

Model Validation

Model Validation

Definition:

The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

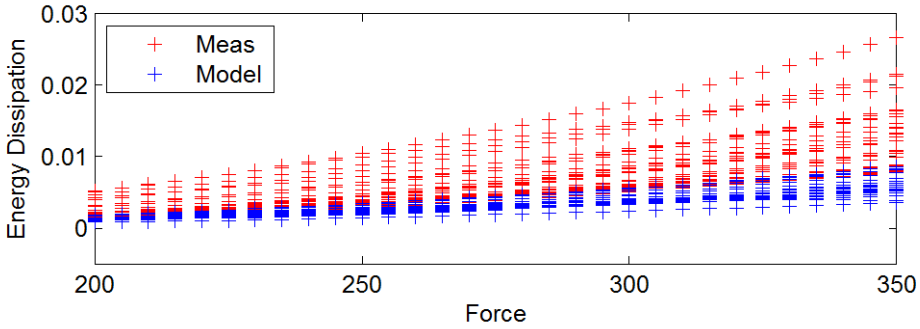
Model validation assesses a model for a specific application using experimental observation.

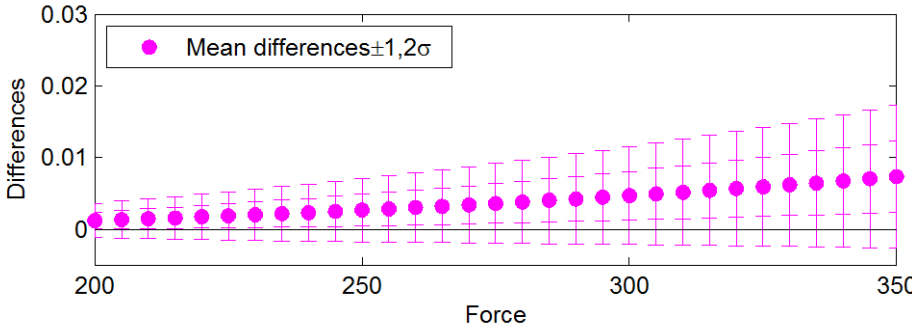
Here the focus is on the assessment of a model for use near the specific conditions of the validation experiments (e.g. not extrapolating validation results)

Model validation quantifies the agreement between modeled prediction and truth relative to the estimated uncertainty of the validation exercise.

Model Validation

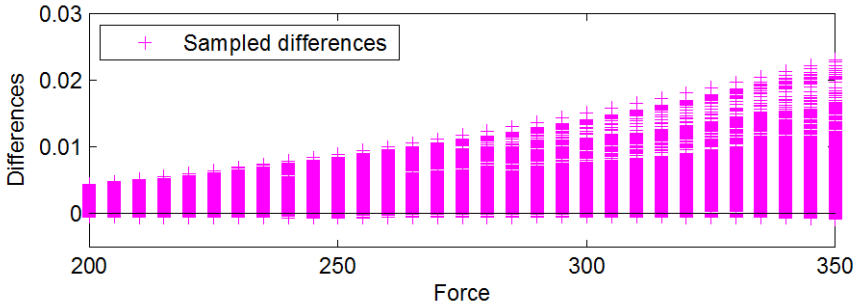
Based on Means and Standard Deviations

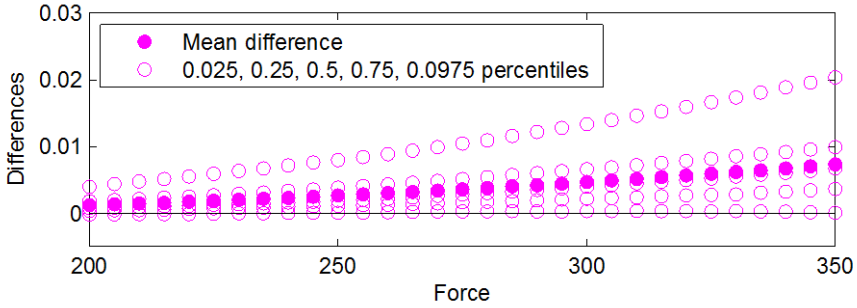




A 'perfect' model would tend toward a zero difference in means with more data.

Based on Samples of Differences





Is this model useful?

- Depends on how useful is defined
- Under predicts energy dissipation and under predicts unit-to-unit variability

Predictive Capability Maturity Model
PCMM

Credibility Assessment

- The Predictive Capability Maturity Model (PCMM) is a communication tool for informing stakeholders of the level of maturity of an application-specific simulation capability
  - It is a multidimensional, qualitative metric
    - Determine readiness for stockpile issues
    - Identify gaps in credibility of application
    - Measure progress of integrated simulation effort
  - 6 Dimensions of the model:
    - Geometric fidelity
    - Physics fidelity
    - Code Verification (inc. SQE)
    - Solution Verification
    - Model Validation
    - Uncertainty Quantification

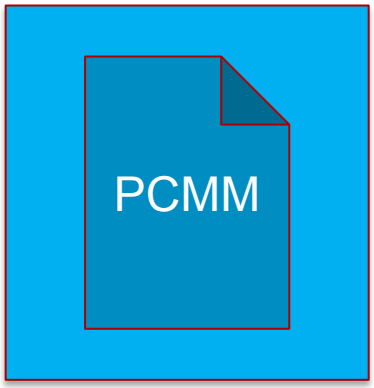
PCMM allows to qualitatively measure our CompSim "due diligence"

PCMM is intended to be a communication and a planning tool

It is not intended to be a report card

PCMM Assessment

- Let's do a assessment on our example problem



Resource Balance

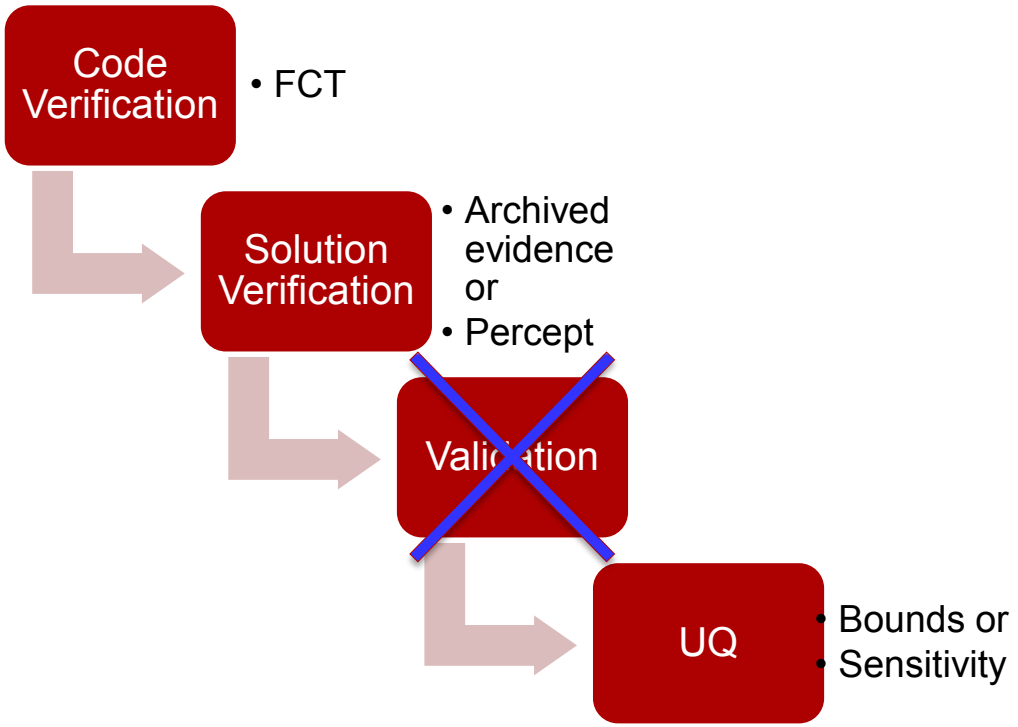
- V&V/UQ takes effort (Effort = Time & funding)

- To reach an appropriate level of V&V/UQ activities relative to CompSim end-use, keep in mind:
  - It's a function of the intended use of CompSim and what is available (i.e. is there test data for validation???)
  - It should be an informed decision. Knowing what the intended use should guide decision on what V&V/UQ activities should be done
  - Identify risks incurred in not performing some/all V&V/UQ activities

- Let's look at a couple of scenarios …

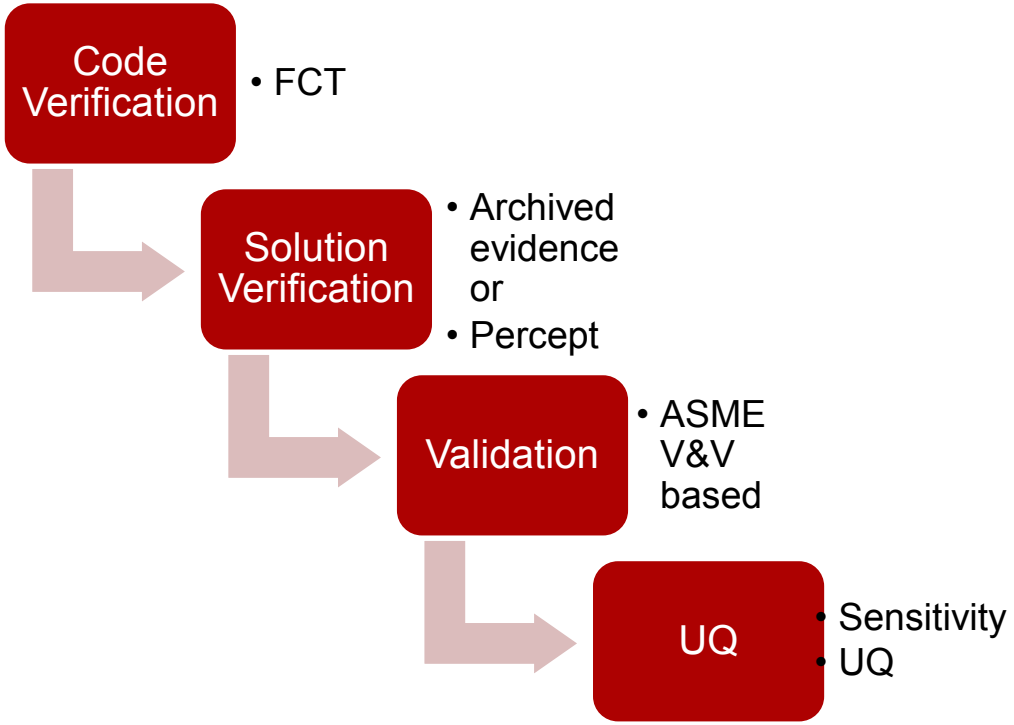
Scenario 1 - Design Support

- CompSim need:
  - Design Support
- What's available:
  - A CAD drawing
  - Historical data/Expert opinion
- Benefits:
  - Sensitivity to design parameters
  - Pre-test information
- Risks:
  - CompSim results are "blind" predictions (i.e. no validation)



Scenario 2 - Environments Definition

- CompSim need:
  - Environments definition support
- What's available:
  - A CAD drawing
  - Historical data/Expert opinion
  - Validation test (but not at application space, i.e. F-35)
- Benefits:
  - Uncertainty can be quantified
- Risks:
  - CompSim results are "blind" predictions in application space



Summary

- The basic terminology relating to V&V/UQ was presented
- One of the main reasons for having a V&V/UQ process is to increase the confidence in CompSim results
  - PCMM is a way to communicate this confidence
- When in doubt about UQ/Validation/PCMM, please contact me
  - Angel Urbina, aurbina@sandia.gov; 844-4988

Dept. 1544 support of your Credibility Evidence Package (CEP)

- PCMM Framework
  - PCMM Tool → **communication** device
    - Planning tool
    - Assessment tool
    - Evidence catalog/organizer
- V&V Tools
  - Suggested V&V/UQ Workflow with pruning
  - V&V Plan Standard Template
  - V&V Resource Allocation Tool
  - FCT
  - Percept
- V&V Office Hours/Consulting
- V&V/UQ Portal Website
  - Guidelines/How Tos
  - Template Scripts
  - References
  - Technical Points of Contact
  - Knowledge Archive
  - Use Cases