

Predictive Capability Maturity Model Workshop



PRESENTED BY

Aubrey Eckert & Josh Mullins

Sandia National Laboratories

Verification, Validation, Uncertainty Quantification, & Credibility Processes Department

Erik Bailey & Lee Peterson

Jet Propulsion Laboratory

September 11, 2019 – JPL Pickering Auditorium



SAND2019-10327PE



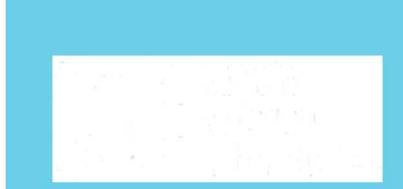
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Course Outline

Time	Topic	Presenter
9:00 am - 9:10 am	Introduction	Lee Peterson & Erik Bailey
9:10 am - 10:45 am	<p>Overview of V&V/UQ Concepts</p> <ul style="list-style-type: none">▪ Introduction and Motivation▪ V&V/UQ terminology▪ Introduction to short example problem▪ Class exercise▪ The V&V Process▪ Summary	Josh Mullins
10:45 am - 11:00 am	Break	---
11:00 am - 12:00 pm	<p>Introduction to PCMM</p> <ul style="list-style-type: none">▪ What is PCMM▪ Deployment of PCMM▪ Results of PCMM	Aubrey Eckert
12:00 pm - 1:00 pm	Lunch	---
1:00 pm - 1:30 pm	Introduction of Example Problem	Erik Bailey
1:30 pm - 2:30 pm	Application of PCMM to Example Problem	Aubrey Eckert & Josh Mullins
2:30 pm - 3:00 pm	Discussion & Questions	All



Introduction to using the Predictive Capability Maturity Model (PCMM)



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Credibility Evidence for Computational Simulation Predictions

How do we demonstrate that **predictions** derived from computational simulations are **credible**?



Expert judgement, I
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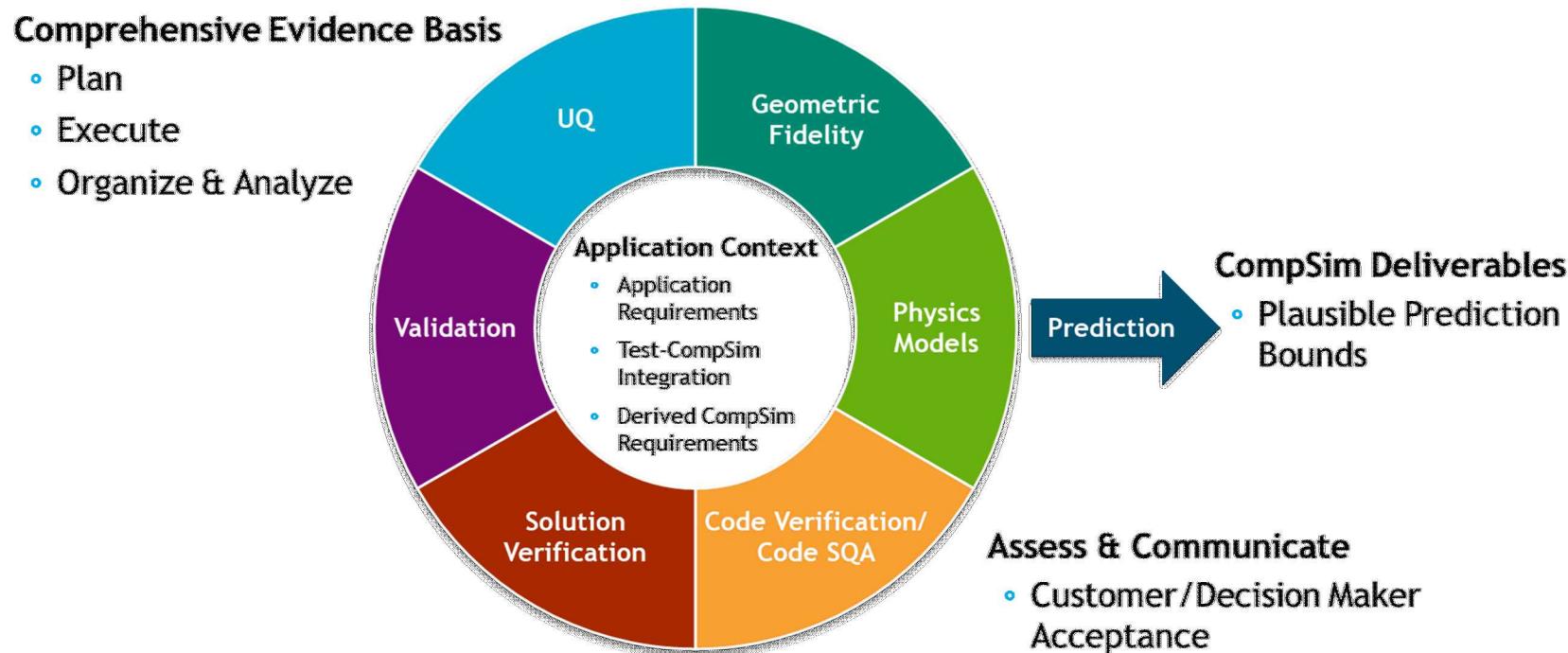
We used the same process we have always used, we have never been wrong before!

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Look, my presentation has a cool video!

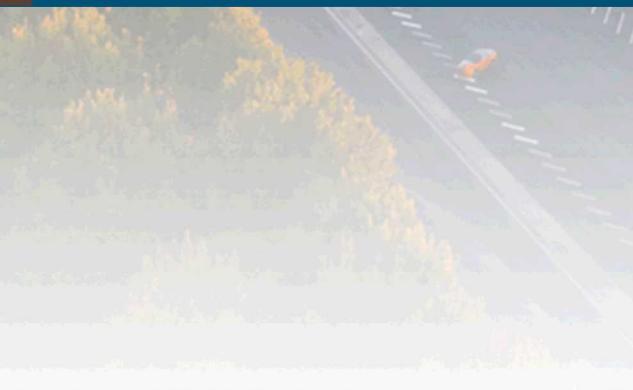
Credibility Evidence for Computational Simulation Predictions

- The computational simulation (CompSim) **credibility process** assembles and documents **evidence** to ascertain and communicate the **believability** of **predictions** that are produced from computational simulations.
- The **Predictive Capability Maturity Model** (PCMM) provides a **comprehensive framework** for planning, gathering, and communicating credibility evidence.





Introduction to the PCMM



What is the PCMM?

The Predictive Capability Maturity Model (PCMM) is a multi-dimensional qualitative metric to facilitate discussion and communication of **credibility evidence**.

- Primary purposes:
 - Provide evidence to help determine **readiness** of modeling capabilities and simulation products for use in various applications and decisions
 - **Identify gaps** in the current credibility evidence for an application and **prioritize** additional activities
 - **Measure progress** of an integrated simulation effort **over the lifetime** of an analysis
- PCMM components:
 - **Elements** – the dimensions of the credibility evidence
 - **Level of Rigor** – the state of the evidence and level of rigor around each element
 - **Element criteria** – major features of the credibility evidence to consider for each element

Origins of the PCMM

- The PCMM was developed at Sandia National Laboratories
 - The need to develop a framework to **assess** CompSim analyses arose as **CompSim** became more **heavily relied upon** to design and assess the safety of engineered systems.
 - Original report is publicly available:
 - <https://www.osti.gov/biblio/976951-predictive-capability-maturity-model-computational-modeling-simulation>
 - Sandia has deployed the PCMM across a wide variety of applications and physics disciplines
- The original PCMM has been **expanded** and **iterated upon** since its development
 - Iterations have increased the level of granularity for the PCMM elements
 - Method of deploying PCMM has changed through time and with lessons-learned

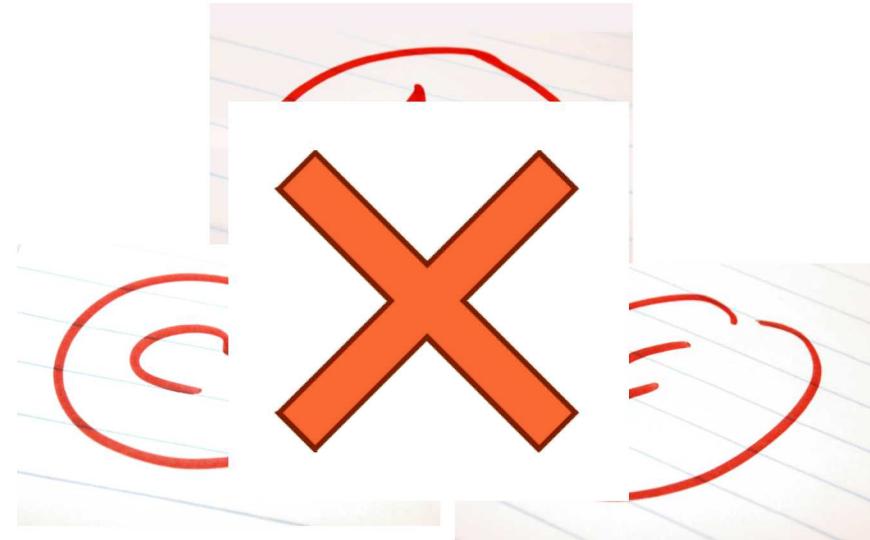
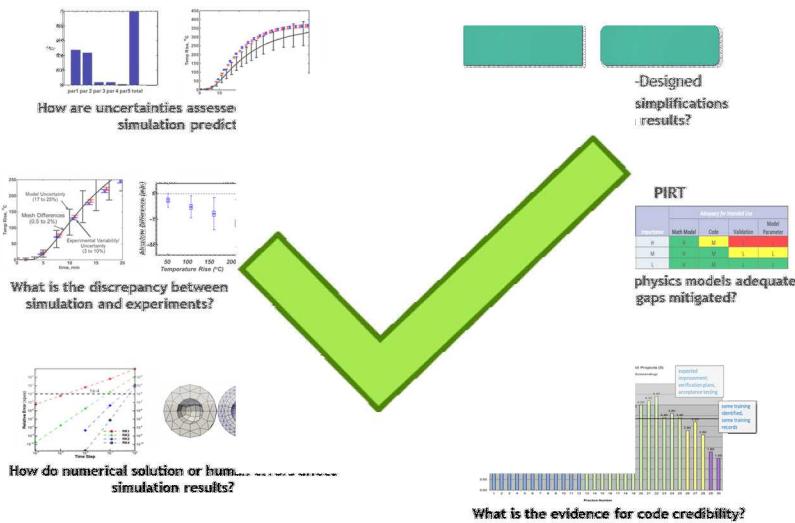
What the PCMM is and What the PCMM is Not

➤ The PCMM **IS**:

- A planning tool to **highlight** and **prioritize** detailed V&V/UQ activities at an early stage of an analysis
- A **communication tool** that *must* include a discussion of the **supporting evidence** to tell a credibility story
- A tool for **informing risk** related to the use of modeling and simulation

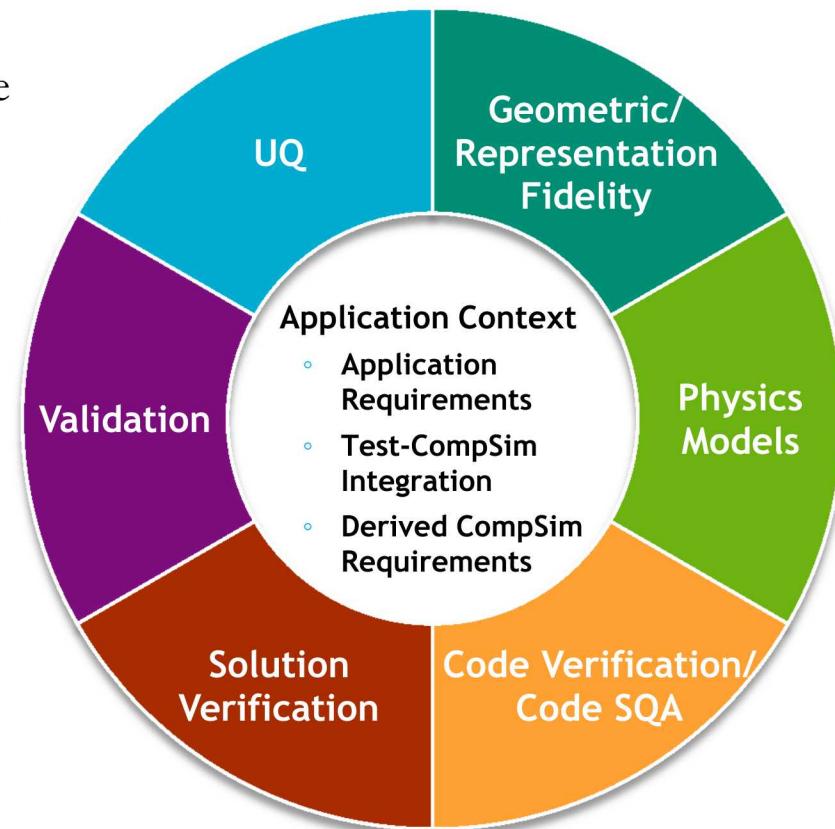
➤ The PCMM is **NOT**:

- An **absolute number** or a **score**
- A mechanism for **criticizing** or **poking holes** in analysis credibility



What are the Outcomes of the PCMM?

- The PCMM is used to:
 1. Guide the **collection** of a **comprehensive** set of **credibility evidence**
 2. Organize the evidence to **communicate** the credibility story to decision makers
- The credibility evidence must exist before it can be evaluated
 - What evidence will be generated?
 - Will it tell a coherent story?
 - Will it be adequate?
 - If evidence does not exist, the PCMM will identify this as a gap
- The PCMM elements represent the **dimensions** of the evidence
 - Representation and Geometric Fidelity
 - Physics and Material Model Fidelity
 - Code Verification
 - Solution Verification
 - Validation
 - Uncertainty Quantification



EAC1

Fix this one

Eckert, Aubrey C, 8/26/2019



PCMM Process Overview



Suggested Steps for Implementation of the PCMM

- The PCMM can be implemented at **any point** in a project.
- Implementation at the beginning of a project allows the PCMM to guide **planning** around V&V/UQ/Credibility activities.
- The PCMM can be **revisited** and **iterated upon** to demonstrate and document progress towards attaining the required level of credibility.
- General steps for implementing the PCMM include:
 1. Discuss the body of evidence that is currently available
 2. Identify key gaps in the evidence and prioritize additional detailed activities to perform (subject to project constraints)
 3. Generate additional evidence
 4. Manage the evidence
 - Document the existing evidence
 - Archive the existing evidence for traceability
 - Report evidence status periodically and update the PCMM as appropriate

PCMM Deployment

- The PCMM is deployed as a **guided discussion** taking place in a meeting or meeting series with team members
 - Meeting length depends on the **complexity** of the analysis and the team preference
 - An example of a meeting strategy is one hour per element (6 in total) of the PCMM
 - Team members **spanning all aspects** of the analysis should participate. This includes:
 - Analysts
 - Experimentalists
 - Project leads/project managers
 - Supporting experts (Statisticians, V&V/UQ practitioners)
 - A **facilitator** should be selected to lead the preparation for the meeting and guide the discussion during the meeting
 - Sandia often utilizes V&V/UQ experts to fill this role
 - Facilitators should have broad view of project goals and an understanding of the PCMM process and elements

Guidelines for this meeting

- Discuss each PCMM element in detail
 - Refer to **element descriptions** for detailed discussion points
 - Take notes on:
 - Status of related work
 - Existing evidence
 - Needed evidence
 - Level of rigor
 - Major priorities
- Suggested roles for the PCMM meetings:
 - **Facilitator** to lead discussion and take notes
 - Assign **primary stakeholder** for each PCMM element
 - Primary stakeholder for each element to **summarize findings** and communicate/track key **outstanding action items**

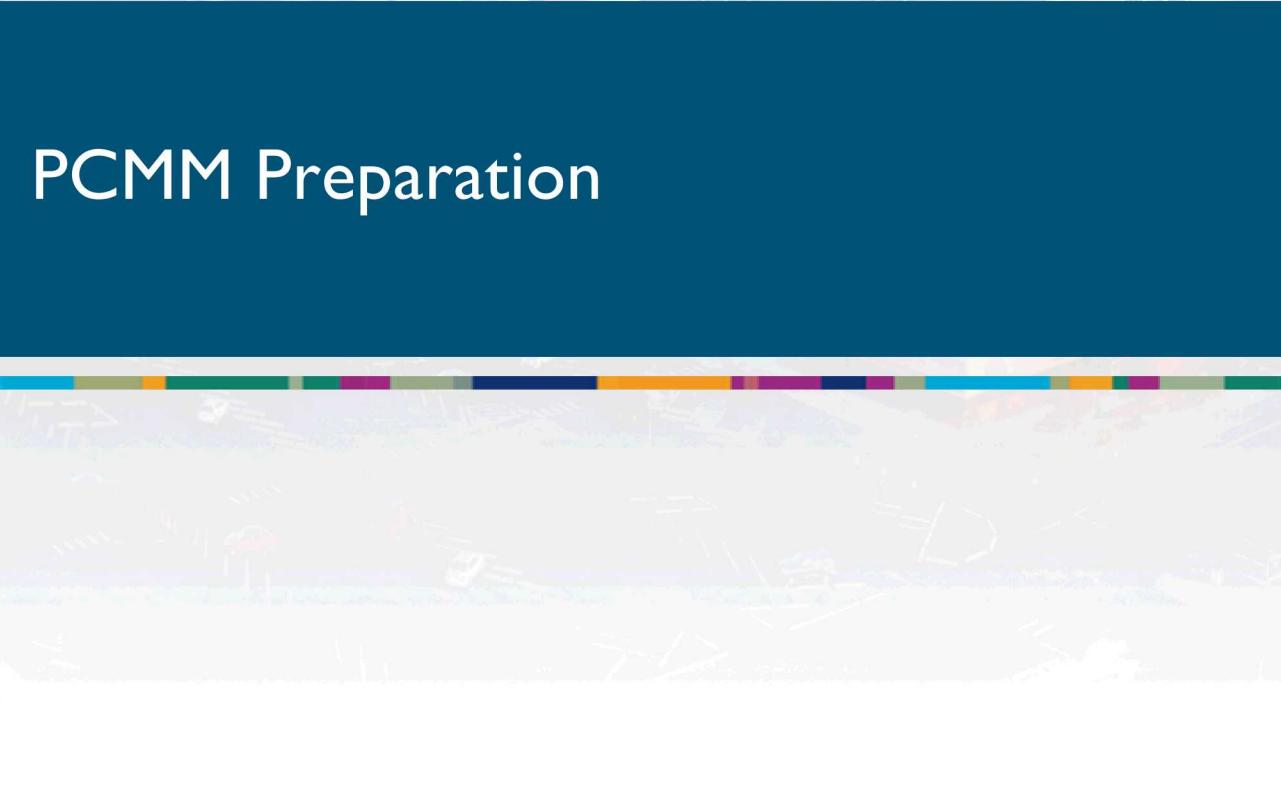
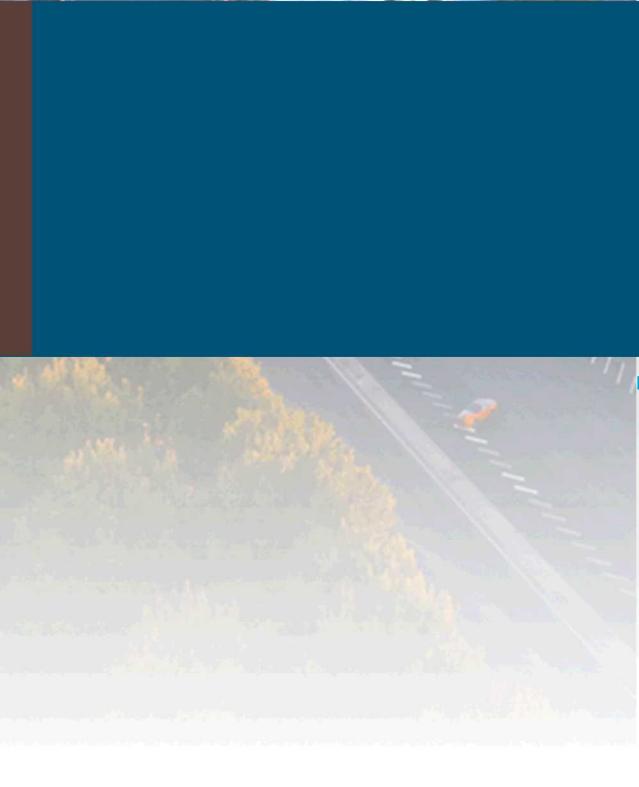
Process Outcomes and Conclusions

Following the PCMM meeting, the following actions should be taken:

- Summarize **key findings**
- Discuss **communication plan** for other project stakeholders
 - General high-level group consensus on status and readiness for decision making
 - Highlight any identified gaps
- Discuss **documentation** expectations
 - Has the existing evidence been documented?
 - Where does it need to go?
- Remaining **action items** (additional activities to perform and documentation):
 - Determine an owner
 - Define a path forward
- If PCMM is used in the planning stage of a project, use PCMM findings to develop a **V&V/UQ Plan**



PCMM Preparation



Prerequisite Steps

- A subset of the team including the PCMM facilitator and team lead should meet to review **prerequisite** materials and questions.
- Prerequisite materials include:
 - Defining CompSim **objectives**
 - Determining **status** of modeling and V&V/UQ efforts
 - Completing a PIRT (Phenomena Identification and Ranking Table)

Objectives of the CompSim Activities

- Defining the **overall objectives** of the CompSim activities is important to the success of the PCMM.
- Understanding the **application requirements** that need to be met helps to determine the required level of credibility evidence that must be gathered.
- The PCMM begins with answering the following questions:
 - What is the **context** of the modeling activities?
 - Who are the **primary stakeholders** for this effort?
 - How will the **simulation outcomes** be used by **decision makers**?
 - What are the analysis **scenarios of interest**?
 - What are the **quantities of interest** (QoIs) and **prediction objectives**?
 - What are the **deliverables** and **timelines** for these activities?

Status of Modeling and V&V/UQ Efforts

The following prerequisite steps and questions must be considered before the PCMM continues:

- Has a **PIRT** been conducted? If not, consider doing one first. If so, reference key high-level findings here.
- What is the **current stage** of the modeling effort for this application? (e.g., planning of activities, communication with stakeholders, etc.)
- What are the **goals** of this PCMM activity? (e.g., develop a V&V/UQ plan, develop a credibility story to communicate)

Prerequisite: Create a PIRT

- What is a PIRT (Phenomena Identification and Ranking Table)?
 - Define **key physical phenomena** that will be needed for an application of interest
 - **Rank importance** of each phenomena relative to a specific output **quantity of interest**
 - Assess adequacy and gaps in capabilities relative to the intended use

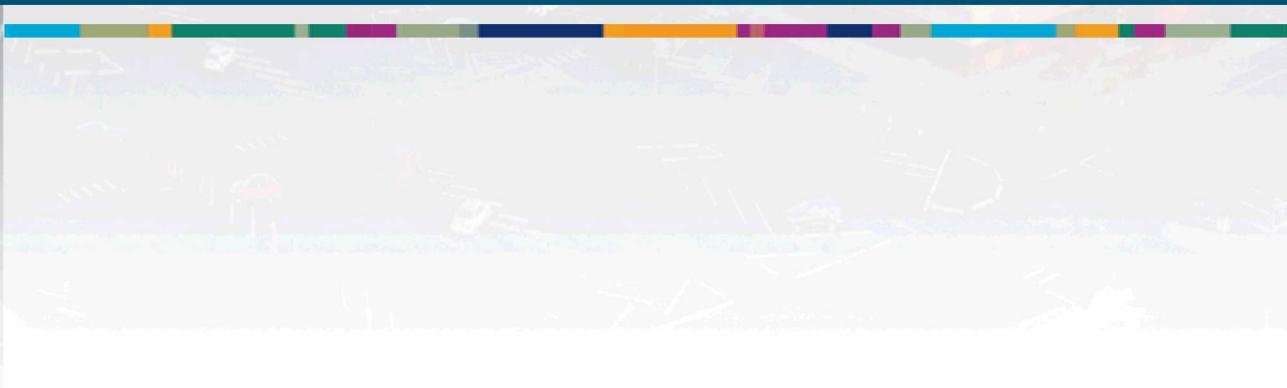
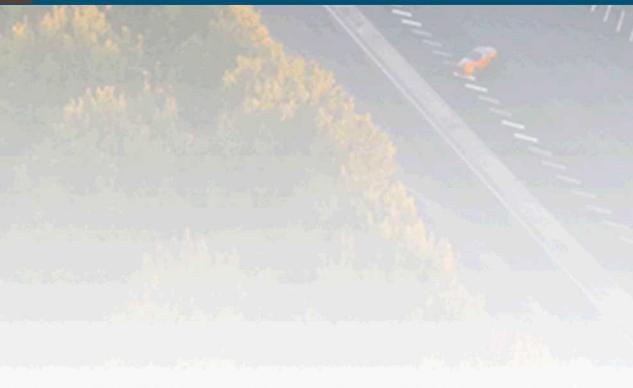
➤ PIRT adequacy elements

- Math model, Code, Validation, and Model parameters
- How does the PCMM differ from the PIRT?
 - The PIRT assesses how well the model captures the desired physics – **feeds directly into** physics and material model fidelity element of PCMM and also informs other elements
 - PIRT covers capability adequacy at high level, and then the PCMM focuses on **detailed V&V/UQ activities** and **evidence**

Phenomena	Importance	Adequacy for Intended Use			
		Math Model	Code	Validation	Model Parameter
Phenomena 1	H	H	M	L	L
Phenomena 2	M	H	M	L	L
Phenomena 3	L	H	M	L	L



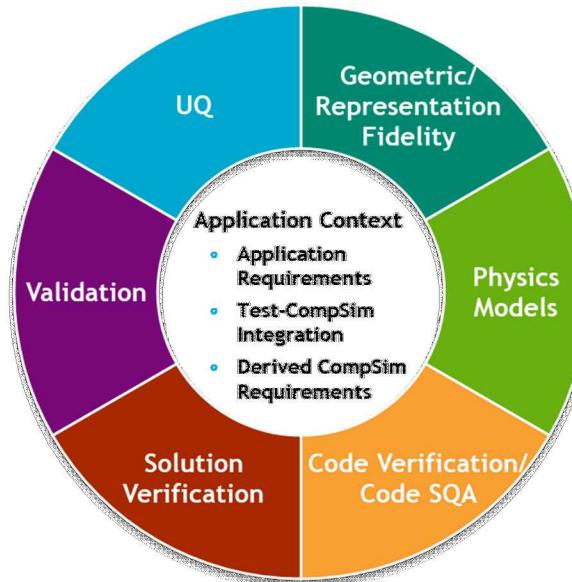
PCMM Elements Deep Dive



27 PCMM Elements Deep Dive

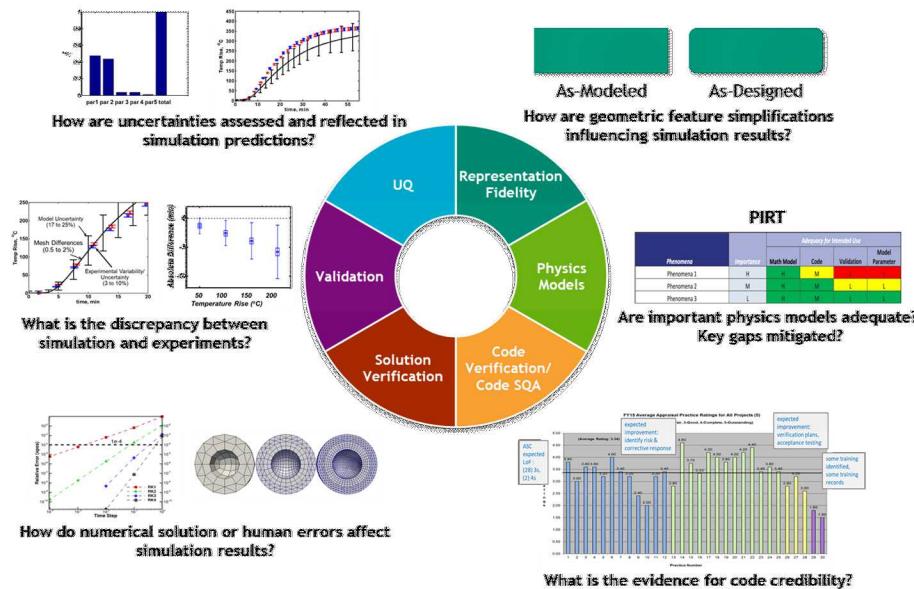
Following the completion of the prerequisite and initial PCMM activities, the PCMM meetings take place to dive into the PCMM elements.

- Each PCMM element is divided into **sub-elements**
- PCMM **sub-elements** have been broken into a **series of questions** that provide detailed information related to the collection of credibility evidence.
- As the project team answers each question, **existing credibility evidence** and **gaps** in this credibility evidence will be identified.
- Discussions should include a relationship back to the **application context** and **requirements**.



Slides for Deployment of PCMM Elements

- The following slides are used to deploy PCMM during the team PCMM meetings.
- Introductory slides provide broad information about each **element**.
- **Sub-elements** are introduced as questions that serve as **prompts** as the team discusses each element.



Representation and Geometric Fidelity (RGF)

➤ Goal:

- Identify the elements of the application geometry model that have been de-featured and understand the potential sensitivity to these approximations



As-Modeled

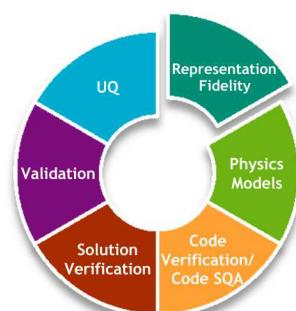


As-Designed

➤ Needed evidence:

- To what extent is the geometry important?
- Are approximations/simplifications being made and why?

How are geometric feature simplifications influencing simulation results?



Representation and Geometric Fidelity Sub-elements

1. Characterize Representation and Geometric Fidelity

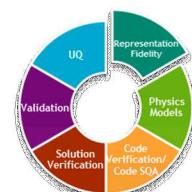
- Has the model been de-featured and to what extent are the “major” or “minor” features included (ex. Fillets, bolts, holes, cables, etc.)?

2. Geometric Sensitivity

- Has the computational error due to the given level of geometric resolution on the QoIs been studied or discussed (at least two simulations conducted for varying levels of de-featuring)?
- If so, for which major features was the sensitivity quantified (few, some, all)?

3. Technical review of representation and geometric fidelity

- Has the representation/geometry for the simulation been rigorously checked (by the analyst, by other analysts, by multiple other users, peer review panel (external or internal))?



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Physics and Material Model Fidelity (PMMF)

➤ Goal:

- Identify the important physics and material models and their readiness for the intended use and identify gaps

➤ Needed evidence:

- Model selection
 - What choices were made and why?
 - Is it sufficient for the given application?
- Physics-based vs. empirical models
 - Are we within the range of applicability for our assumptions?

PIRT

Phenomena	Importance	Adequacy for Intended Use			
		Math Model	Code	Validation	Model Parameter
Phenomena 1	H	H	M	L	L
Phenomena 2	M	H	M	L	L
Phenomena 3	L	H	M	L	L

Are important physics models adequate?
Key gaps mitigated?



Physics and Material Model Fidelity Sub-elements

1. Characterize completeness versus the PIRT
 - A PIRT should have already been completed for this analysis.
 - Are all relevant material/physics models in the capability correlated with the PIRT for the intended application?
2. Quantify model accuracy (i.e., separate effects model validation)
 - What is the rigor of the validation comparisons (i.e., are they quantitative or qualitative)?
 - Do the validation comparisons include experimental uncertainty/error in the test data and model outputs?
 - Is the pedigree information presented in any form (none, some but incomplete, complete)?
3. Assess interpolation vs. extrapolation of physics and material model
 - To what extent does the application domain intersect the validation domain for this physics and material model (does not intersect, partially intersects, entirely contained)?
4. Technical review of physics and material models
 - Have the physics and material models, PIRT coverage and model accuracy been subjected to peer review (by the team, internal, external), and where are these results documented?



Physics and Material Model Fidelity Sub-elements

1. Characterize completeness versus the PIRT

- A PIRT should have already been completed for this analysis.
- Are all relevant material/physics models in the capability correlated with the PIRT for the intended application?

2. Quantify model accuracy (i.e., separate effects model validation)

- What is the intended use of the model (e.g., predictive, prescriptive, or qualitative)?
- Do the validation results support the intended use of the model? (e.g., does the model output support the intended use)?
- Is the pedigree information present for the validation results? (e.g., is the pedigree information complete)?

Phenomena	Importance	Adequacy for Intended Use			
		Math Model	Code	Validation	Model Parameter
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- Is the pedigree information presented in any form (none, some but incomplete, complete)?

3. Assess interpolation vs. extrapolation of physics and material model

- To what degree does the model extrapolate beyond the range of the test data?

this physics and material model coverage is acceptable?

Phenomena	Importance	Adequacy for Intended Use			Model Parameter
		Math Model	Code	Validation	
Phenomena 1	H	H	M	L	L
Phenomena 2	M	H	M	L	L
Phenomena 3	L	H	M	L	L

4. Technical review of physics and material models

- Have the physics and material models, PIRT coverage and model accuracy been subjected to peer review?

High: **Relevant test data** is available for the phenomenon, and **quantitative comparisons** have been made between the test data and the model outputs.

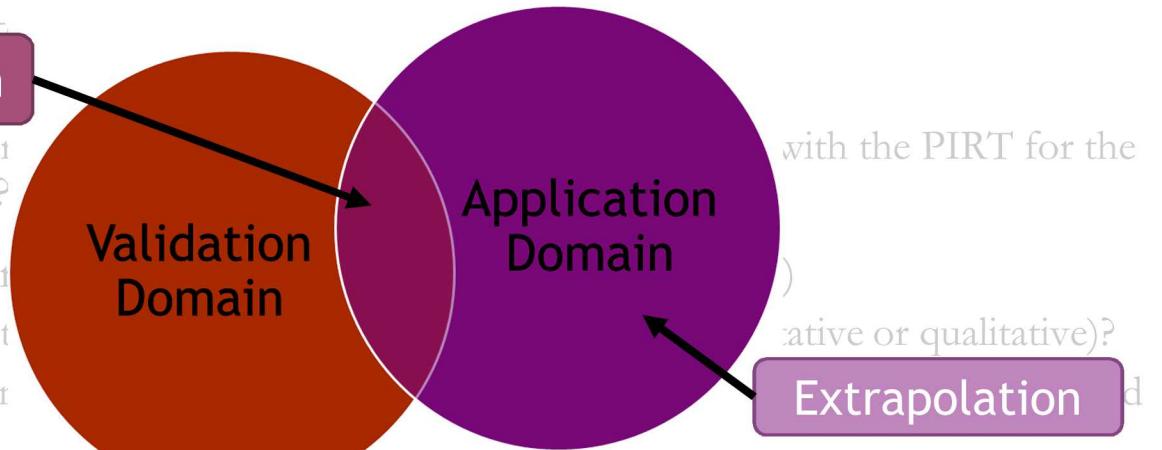
Medium: **Some relevant test data** is available for the phenomenon, but it has only been **qualitatively compared** with the model outputs or no comparison has been performed.

Low: **No relevant test data** is available for the phenomenon.



Physics and Material Model Fidelity Sub-elements

1. Characterize completeness of the validation domain
 - Are all relevant materials and conditions included in the intended application?
2. Quantify model accuracy
 - What is the rigor of the validation?
 - Do the validation conditions represent the intended application?
 - Is the pedigree information presented in any form (none, some but incomplete, complete)?
3. Assess interpolation vs. extrapolation of physics and material model
 - To what extent does the application domain intersect the validation domain for this physics and material model (does not intersect, partially intersects, entirely contained)?
4. Technical review of physics and material models
 - Have the physics and material models, PIRT coverage and model accuracy been subjected to peer review (by the team, internal, external), and where are these results documented?



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)

ative or qualitative)?

Extrapolation



Code Verification (CVER)

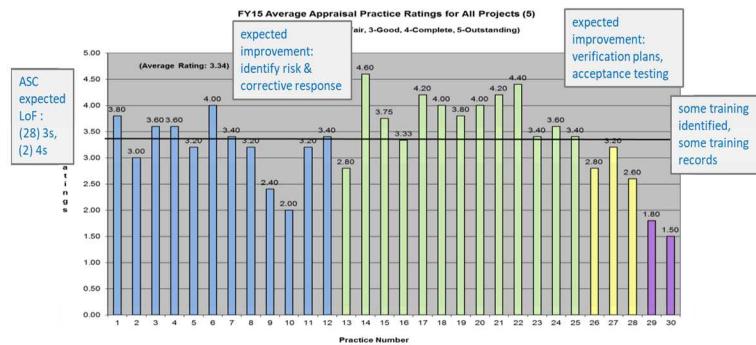
➤ Goal:

- Identify the important code capabilities for the intended use and understand their current readiness and verification pedigree

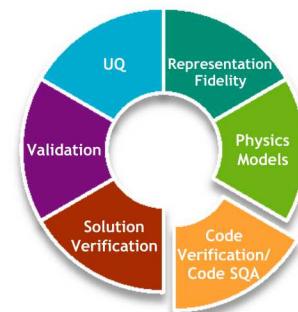
➤ Needed evidence:

- Software development process
 - What is the process for developing the code base?
 - What are the SQA standards?
- How is the code base maintained?
- Verification testing
 - Are there tests for important features?
 - Verification tests or regression tests?
 - Do the available tests cover what the code is being used for?

Summary of Verification Test Coverage



What is the evidence for code credibility?



Code Verification Sub-elements

1. Apply software quality engineering (SQE) processes (requires input from a capability developer)
 - Is the code capability managed to identified SQE practices?
 - Is the SQE process managed and optimized?
2. Provide test coverage information
 - Are the capabilities subject to regression testing and VERTS (verification test suite) testing?
 - Are all of the physics/engineering features required for the intended application covered by the reported VERTS?
3. Identification of code or algorithm attributes, deficiencies and errors
 - Are the code/algorithm attributes, deficiencies and errors from VERTS presented?
 - Are these mapped to the intended application?
4. Verify compliance to Software Quality Engineering (SQE) processes
 - To what extent has the SQE process been reviewed and/or certified (none, self-assessment, external, certification)?
5. Technical review of code verification activities
 - Have these activities been subjected to peer review (by the team, internal, external), and where are these results documented?



Code Verification Sub-elements

1. Apply software quality engineering (SQE) processes (requires input from a capability developer)
 - Is the code capability managed to identified SQE practices?
 - Is the SQE process managed and optimized?

2. Provide test coverage information

- Are the code coverage reports available?
- Are all of the code coverage reports up-to-date?

3. Identification

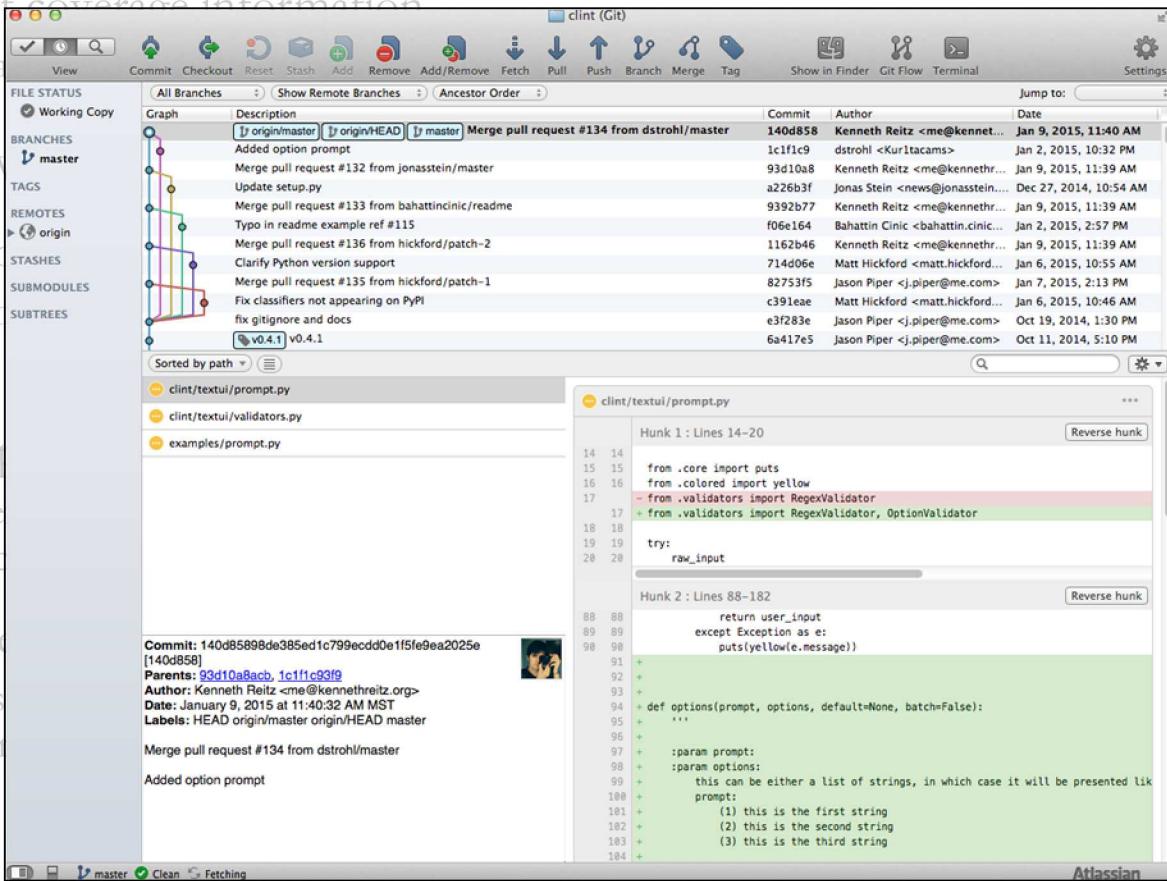
- Are the code identifiers unique?
- Are these identifiers well-documented?

4. Verify compliance

- To what external standards and regulations does the code conform?

5. Technical review

- Have these technical reviews been completed?
- Are these reviews up-to-date?



The screenshot shows the Atlassian Git client interface. The main window displays a commit history for the 'master' branch. The commits are listed in chronological order, with the most recent at the top. Each commit includes the author, date, and a brief description of the changes made. A detailed code diff is shown for a specific commit, highlighting changes in the file 'client/textui/prompt.py'. The diff shows two hunks of code with changes marked in red and green. The commit history and code diff are as follows:

Commit History:

Commit	Author	Date
140d858	Kenneth Reitz <me@kennethreitz.org>	Jan 9, 2015, 11:40 AM
1c1f1c9	dstrohl <KurtAcams>	Jan 2, 2015, 10:32 PM
93d10a8	Kenneth Reitz <me@kennethreitz.org>	Jan 9, 2015, 11:39 AM
a226b3f	Jonas Stein <news@jonasstein.de>	Dec 27, 2014, 10:54 AM
9392b77	Kenneth Reitz <me@kennethreitz.org>	Jan 9, 2015, 11:39 AM
f06e164	Bahattin Cinic <bahattin.cinic@gmail.com>	Jan 2, 2015, 2:57 PM
1162b46	Kenneth Reitz <me@kennethreitz.org>	Jan 9, 2015, 11:39 AM
714d06e	Matt Hickford <matt.hickford@me.com>	Jan 6, 2015, 10:55 AM
82753f5	Jason Piper <j.piper@me.com>	Jan 7, 2015, 2:13 PM
c391eae	Matt Hickford <matt.hickford@me.com>	Jan 6, 2015, 10:46 AM
e3f283e	Jason Piper <j.piper@me.com>	Oct 19, 2014, 1:30 PM
6a417e5	Jason Piper <j.piper@me.com>	Oct 11, 2014, 5:10 PM

Code Diff (client/textui/prompt.py):

```

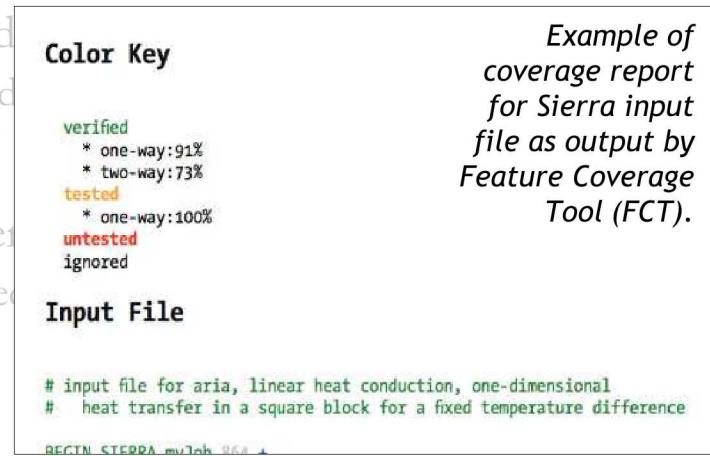
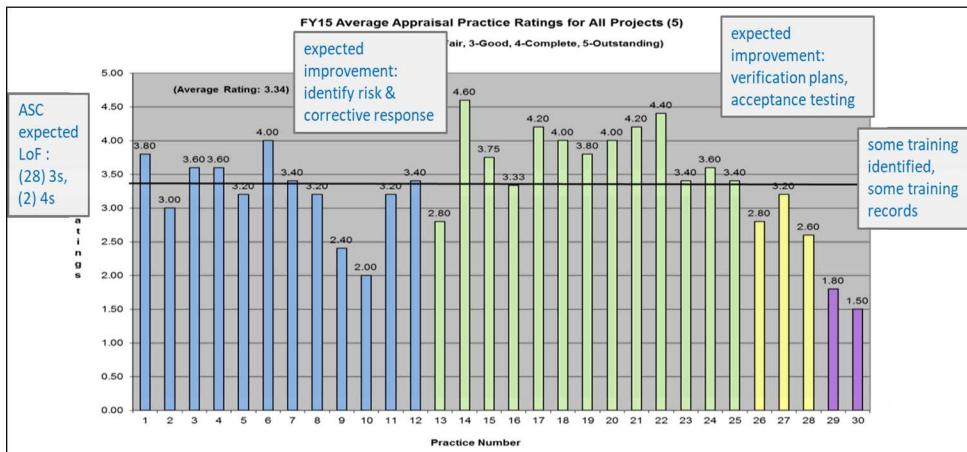
14 14
15 15
16 16
17 17 from .core import puts
18 18 from .colored import yellow
19 19 - from .validators import RegexValidator
20 20 + from .validators import RegexValidator, OptionValidator
21 21
22 22 try:
23 23     raw_input
24 24
25 25
26 26
27 27
28 28
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91 91
92 92
93 93
94 94
95 95
96 96
97 97
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104 104

```



Code Verification Sub-elements

1. Apply software quality engineering (SQE) processes (requires input from a capability developer)
 - Is the code capability managed to identified SQE practices?
 - Is the SQE process managed and optimized?
2. Provide test coverage information
 - Are the capabilities subject to regression testing and VERTS (verification test suite) testing?
 - Are all of the physics/engineering features required for the intended application covered by the reported VERTS?



- Have these activities been subjected to peer review (by the team, internal, external), and where are these results documented?



Code Verification Sub-elements

1. Apply software quality engineering (SQE) processes (requires input from a capability developer)
 - Is the code capability managed to identified SQE practices?
 - Is the SQE process managed and optimized?
2. Provide test coverage information
 - Are the capabilities subject to regression testing and VERTS (verification test suite) testing?
 - Are all of the physics/engineering features required for the intended application covered by the reported VERTS?
3. Identification of code or algorithm attributes, deficiencies and errors
 - Are the code/algorithm attributes, deficiencies and errors from VERTS presented?
 - Are these mapped to the intended application?
4. Verify compliance to Software Quality Engineering (SQE) processes
 - To what extent has the SQE process been reviewed and/or certified (none, self-assessment, external, certification)?
5. Technical review of code verification activities
 - Have these activities been subjected to peer review (by the team, internal, external), and where are these results documented?



Code Verification Sub-elements

1. Apply software quality engineering processes (by developer)
 - Is the code capability mapped to a capability?
 - Is the SQE process mapped to a process?

Change-Id:		120c97908d0e03b45051d4a1da9484eea0ee429bc
Owner:	Stephen Ray Kennon	
Project:	code	
Branch:	master	
Topic:	new-geom-kernel-greg-patch	
Uploaded:	Mar 9, 2015 10:48 AM	
Updated:	Mar 9, 2015 10:48 AM	
Submit Type:	Fast Forward Only	
Status:	Review in Progress	

Reviewer	Code-Review	Verified
Kevin D Coppers	<input checked="" type="checkbox"/>	
Brian Barnes		

• Need Verified
• Need Code-Review

Name or Email or Group Add Reviewer

Dependencies

Subject	Owner	Project	Branch	Updated
Merge branch 'master' into srk-br-022615-gregory-find-closest	Stephen Ray Kennon	code	master (new-geom-kernel-greg-patch)	Mar 9

Needed By
(None)

Reference Version: 20c97908d0e03b45051d4a1da9484eea0ee429bc (gitweb)

Author: Stephen Kennon <srkennon@sandia.gov> Mar 9, 2015 10:47 AM
 Committer: Stephen Kennon <srkennon@sandia.gov> Mar 9, 2015 10:47 AM
 Parent(s): d81d6d7542f20857b0c94f9687ee1dc7f8ec28e Merge branch 'master' into srk-br-022615-gregory-find-closest
 Download

Review

File Path	Comments	Size	Diff	Reviewed
Commit Message			Side-by-Side	Unified
M percept/adapt/Refiner.cpp		+19, -3	Side-by-Side	Unified
M percept/adapt/main/AdaptMain.cpp		+1, -2	Side-by-Side	Unified
M percept/percept/PerceptMesh.cpp		+54, -6	Side-by-Side	Unified
M percept/percept/PerceptMesh.hpp		+5, -1	Side-by-Side	Unified

Commit Message

Percept: add Gregory Patch geometry kernel.

* enable surface projection and smoothing code to access geometry fit to meshes using Gregory patches.

Code Review for Git

2. Provide test coverage
 - Are the capabilities mapped to a test suite?
 - Are all of the physical phenomena and application covered by the reported VERTS?
3. Identification of code review
 - Are the code/algorithms mapped to a code review?
 - Are these mapped to a code review?
4. Verify compliance to Software Quality Engineering (SQE) processes
 - To what extent has the SQE process been reviewed and/or certified (none, self-assessment, external, certification)?
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Solution Verification (SVER)

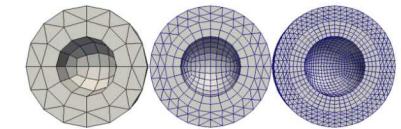
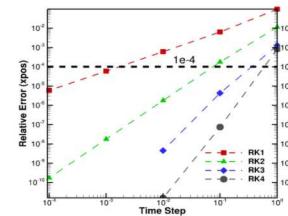
➤ Goal:

- Identify spatial, temporal, and/or stochastic resolution limitations in the application simulation

➤ Needed evidence:

- What type of solvers are being used in the code?
 - Do they converge?
 - What are the limitations?
- Are approximations/simplifications needed?
 - How much error is incurred?
 - Has the numerical error been quantified?

Mesh Refinement Study



How do numerical solution or human errors affect simulation results?



Solution Verification Sub-elements

1. Quantify numerical solution errors

- Has the magnitude of numerical errors incurred from spatial, temporal, and stochastic resolution been accounted for qualitatively or quantitatively?
- Has the sensitivity or robustness of all of the relevant QoIs to this error been studied?

2. Quantify uncertainty in computational (or numerical) error

- Is the quantified numerical error deterministic or stochastic?
- Are there appropriate error bars for the stochastic error for all the relevant QoIs?

3. Verify simulation input decks

- Has the accuracy of the input decks for the simulation been rigorously checked (by the analyst, by other analysts, by multiple other users)?

4. Verify simulation post-processor input decks

- Are a common set of post-processing tools used for the analysis, and are they held to a common set of SQE standards?
- Has the accuracy of the inputs to the post-processing tools been checked (by the analyst, by other analysts, by multiple other users)?

5. Technical review of solution verification

- Have these activities been subjected to peer review (by the team, internal, external), and are these results documented?



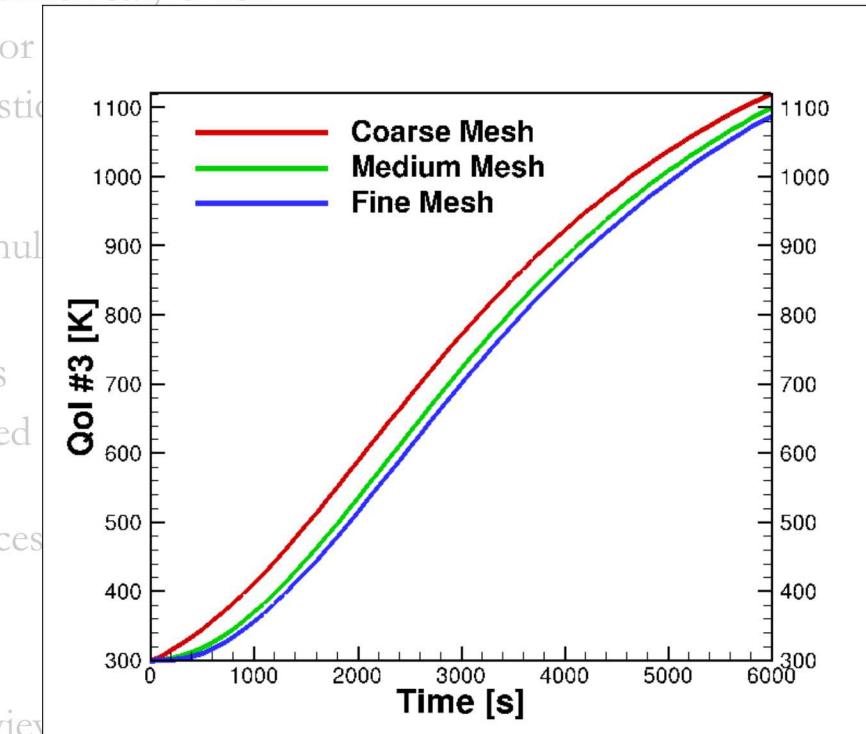
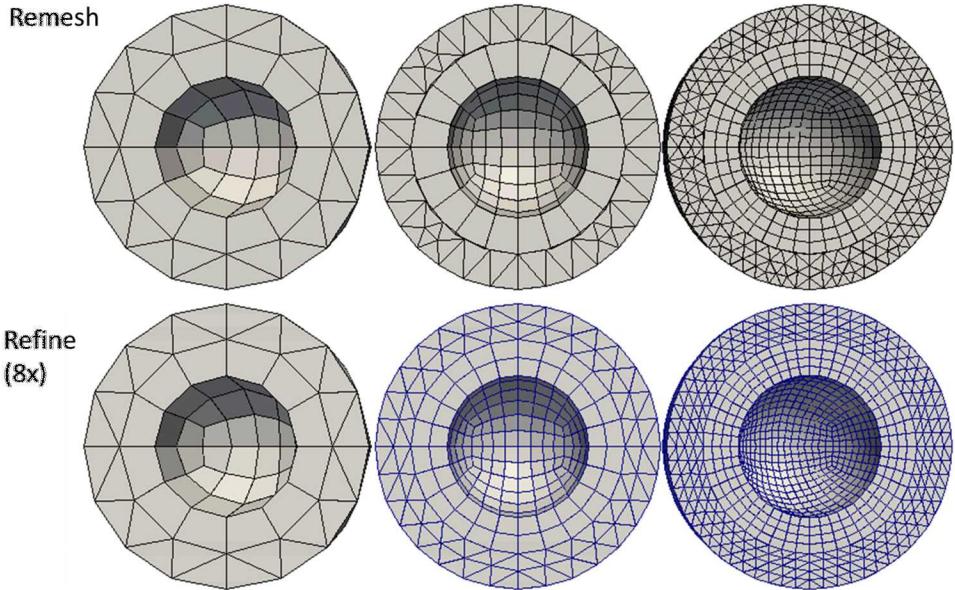
Solution Verification Sub-elements

1. Quantify numerical solution errors

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2. Quantify uncertainty in computational (or numerical) error

- Is the quantified numerical error deterministic or



3. Technical review of solution verification

- Have these activities been subjected to peer review
are these results documented?



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Validation (VAL)

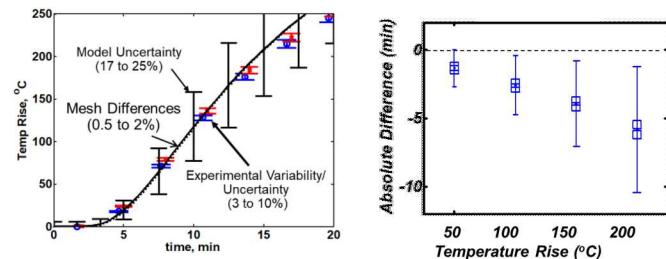
➤ Goal:

- Identify existing validation comparisons and understand hierarchy coverage and the degree of extrapolation from the validation conditions to the application conditions

➤ Needed evidence:

- Do we have test data available for this application?
- How similar are the tested conditions to the ones we want to predict?
- Have we assessed our model with the data?
 - How did it perform?
 - Were the results quantitative or qualitative?
 - Did we consider uncertainty in the comparison?

Model Validation Assessment



What is the discrepancy between simulation and experiments?



Validation Sub-elements

1. Define a validation hierarchy

- Has a validation hierarchy been defined (i.e., mapping from material to component to subsystem to full system levels)?

2. Apply a validation hierarchy

- What is the methodology for how available experimental data connects the levels of the hierarchy?
- Have the steps in this methodology been performed (i.e., have quantitative comparisons been made at different levels of the hierarchy)?

3. Quantify physical accuracy

- What is the rigor of the validation comparisons (i.e., are they quantitative or qualitative)?
- Do the validation comparisons include uncertainty/error in the test data and model outputs?

4. Validation domain vs. application domain

- Is the application of the model an extrapolation from the conditions where test data is available for validation, and to what extent (materials, environments, hardware, etc.)?
- What evidence exists that provides confidence in the ability to extrapolate?

5. Technical review of validation

- Have these activities been subjected to peer review (by the team, internal, external), and are these results documented?



Validation Sub-elements

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3. Quantify physical accuracy

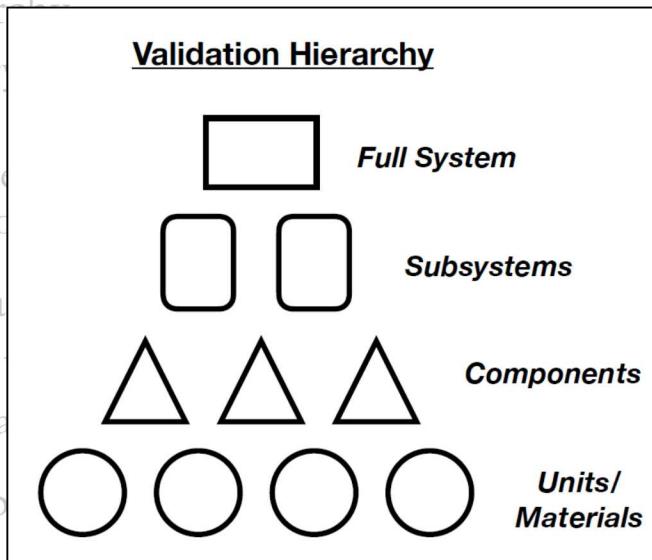
- What is the rigor of the validation comparisons?
- Do the validation comparisons connect the levels of the validation hierarchy?

4. Validation domain vs. application domain

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3. Quantify physical accuracy

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- Do the validation comparisons

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- data and model outputs?

4. Validation domain vs.

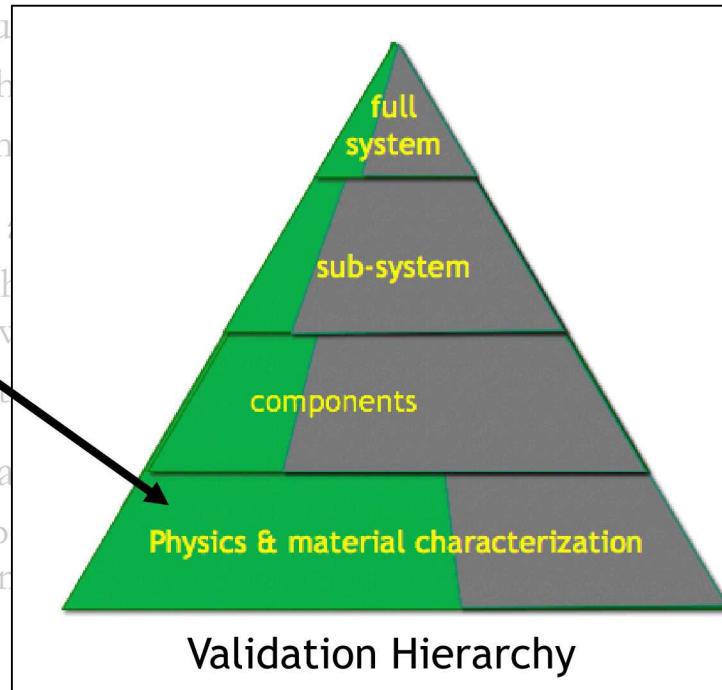
- Is the application of the validation methodology valid?
- What is the domain of validation?

is where test data is available
(internal, external, etc.)?
- interpolate?

5. Technical review of validation

- Have these activities been completed?
- Are these results documen

internal, external), as well as



Validation Sub-elements

1. Define a validation hierarchy

- Has a validation hierarchy been defined (i.e., mapping from material to component to subsystem to full system levels)?

2. Apply a validation hierarchy

- What is the methodology for how available experimental data connects the levels of the hierarchy?
- Have the steps in this methodology been performed (i.e., have quantitative comparisons been made at different levels of the hierarchy)?

3. Quantify physical accuracy

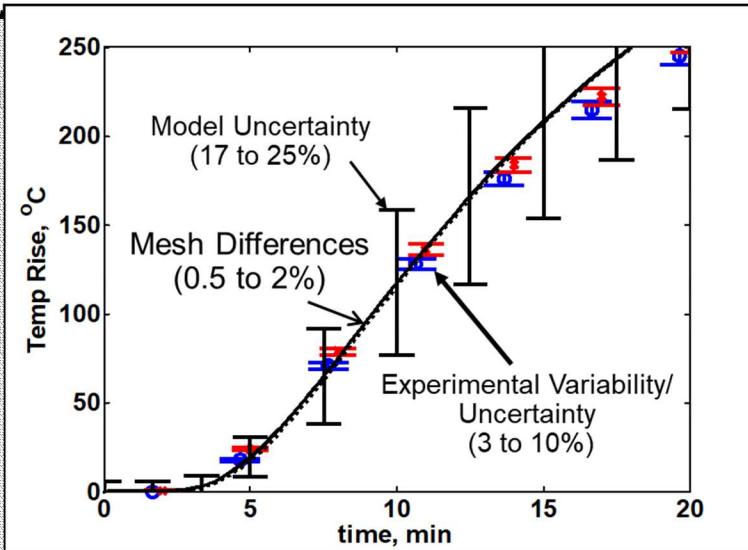
- What is the rigor of the validation comparisons (i.e., are they quantitative or qualitative)?
- Do the validation comparisons include uncertainty/error in the test data and model outputs?

4. Validation domain vs.

- Is the application of _____ for validation, and to _____
- What evidence exists _____

5. Technical review of v

- Have these activities been completed? _____
- Are these results documented? _____



• where test data is available
• etc.)?
• interpolate?

internal, external), as



Validation Sub-elements

1. Define a validation hierarchy

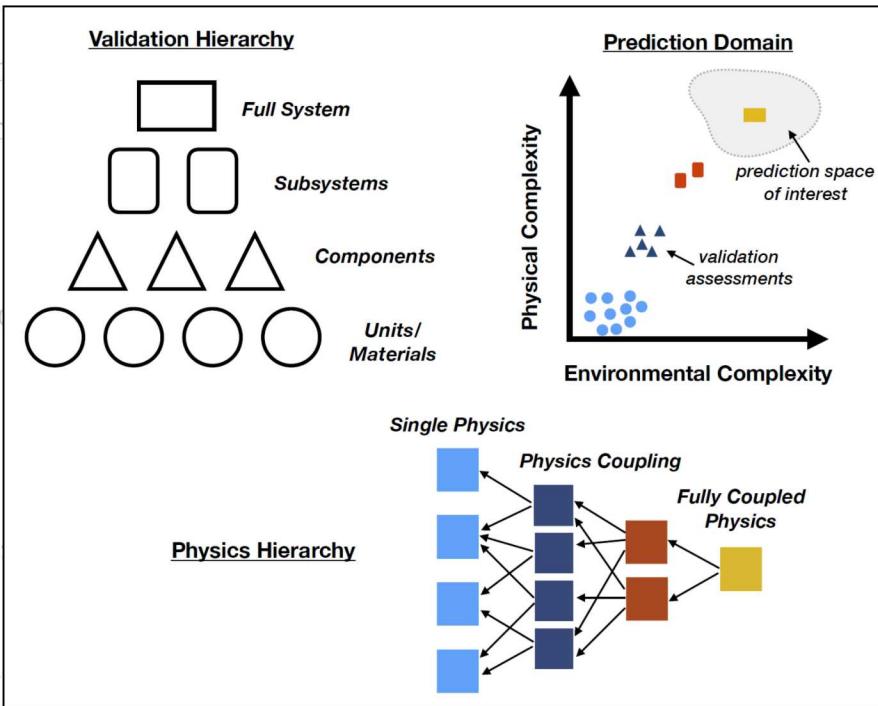
- Has a validation hierarchy from component to full system

2. Apply a validation hierarchy

- What is the method for defining the validation hierarchy?
- Have the steps in the validation hierarchy been made at different levels of the hierarchy?

3. Quantify physical complexity

- What is the rigor of the validation hierarchy?
- Do the validation hierarchy and model outputs? provide quantitative or qualitative comparisons?



4. Validation domain vs. application domain

- Is the application of the model an extrapolation from the conditions where test data is available for validation, and to what extent (materials, environments, hardware, etc.)?
- What evidence exists that provides confidence in the ability to extrapolate?

5. Technical review of validation

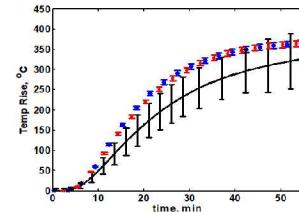
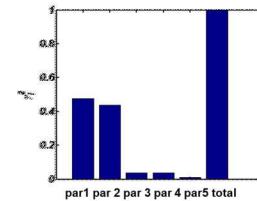
- Have these activities been subjected to peer review (by the team, internal, external), and are these results documented?



Uncertainty Quantification (UQ)

➤ Goal:

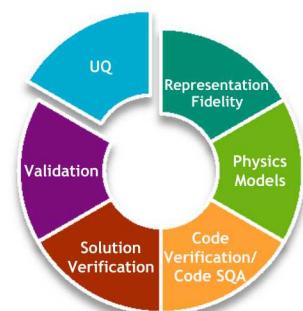
- Understand the identification and characterization of input uncertainties, the quantification of output uncertainties, and the extrapolation of the validation uncertainties to the application



How are uncertainties assessed and reflected in simulation predictions?

➤ Needed evidence:

- Have we considered known uncertainty sources?
 - How well are they understood?
 - Can they be characterized well?
- Have we studied the effect of these uncertainty sources on the output?



Uncertainty Quantification Sub-elements

1. Aleatory and epistemic uncertainties identified and characterized
 - Aleatory = natural variability; epistemic = lack of knowledge
 - Has an inventory of uncertainty sources been taken, and have they been classified according to these forms?
 - What is the source of information (e.g., legacy, literature, direct measurement, calibration, etc.) that is used for uncertainty characterization (e.g., classification as aleatory vs. epistemic, uncertainty representation, distributional assumptions, etc.)?
2. Perform sensitivity analysis
 - How have the most important uncertainty sources for the relevant QoIs been identified (e.g., SME judgment, local sensitivity analysis, global sensitivity analysis, etc.)?
3. Quantify impact of uncertainties on QoIs
 - Have identified sources of uncertainty (see 1 above) been propagated to the important output QoIs?
 - What is the procedure for propagation and what additional errors are introduced?
4. UQ aggregation and roll-up
 - How have sources of uncertainty been combined and transferred across different levels of the system (i.e., validation hierarchy) and to the application domain?
5. Technical review of uncertainty quantification
 - Have these activities been subjected to peer review (by the team, internal, external), and where are these results documented?

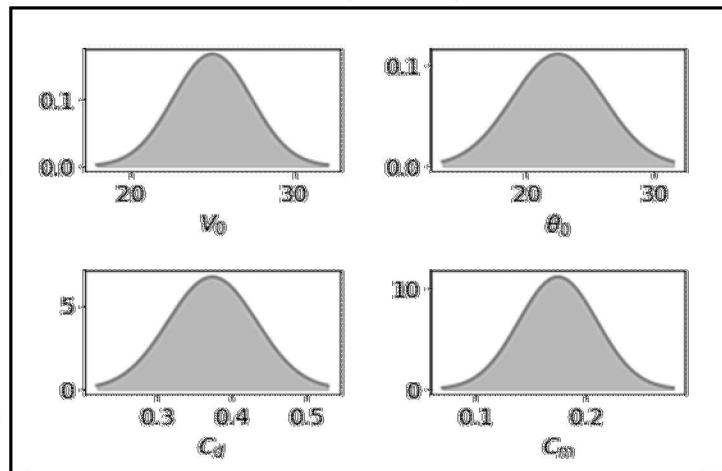


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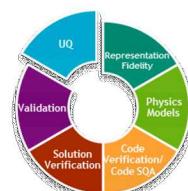
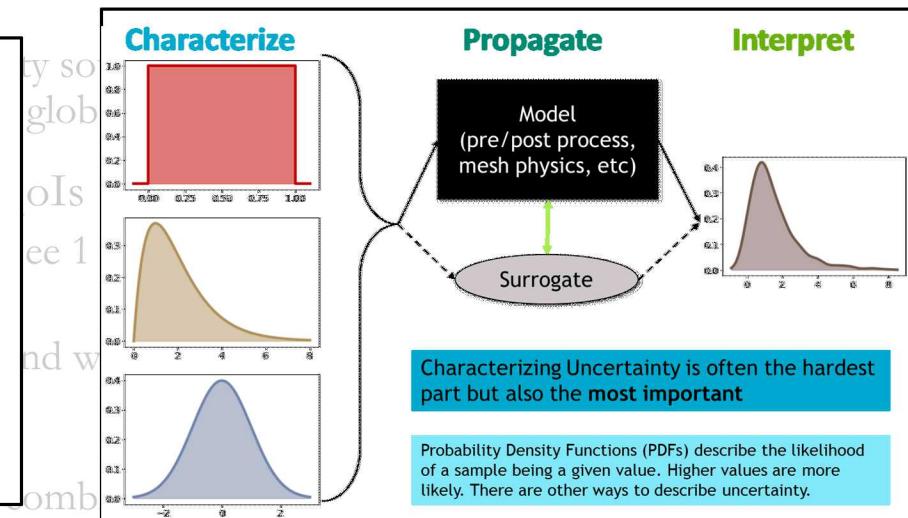
3.

4.

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5. Technical review of uncertainty quantification

- Have these activities been subjected to peer review (by the team, internal, external), and where are these results documented?



Uncertainty Quantification Sub-elements

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3. Quantify imp...

- Have identified QoIs?

- What is the

4. UQ aggrega...

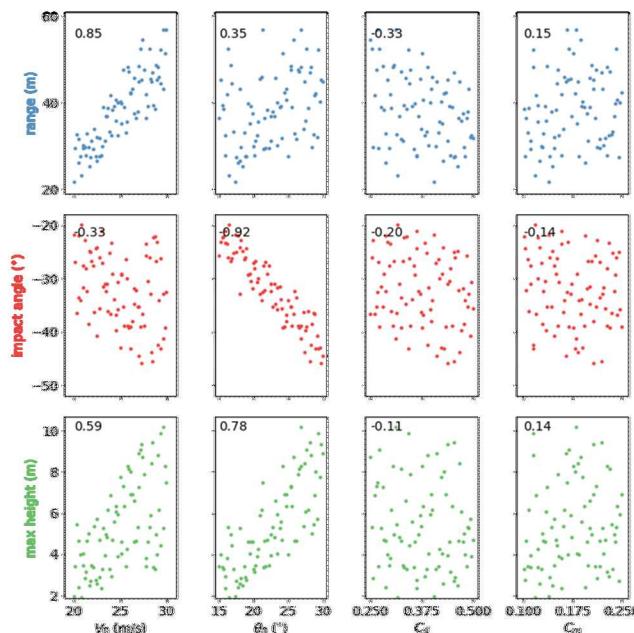
- How have s... system (i.e.,

5. Technical re...

- Have these ... and where a

*Sensitivity analysis
using correlation
coefficients for
projectile problem.*

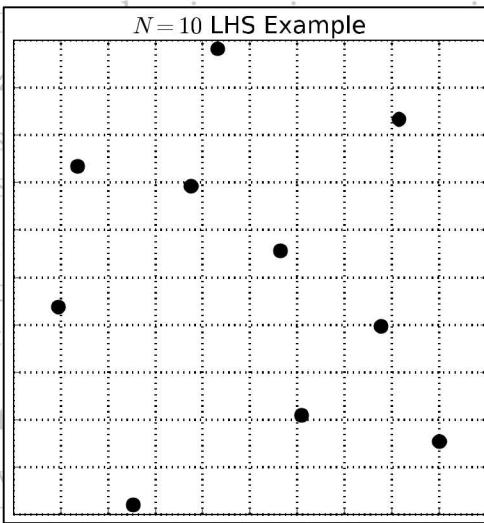
	Range (m)	Impact angle (°)	max height (m)
v_0 (m/s)	+0.85	-0.33	+0.59
θ_0	+0.35	-0.92	+0.78
c_d	-0.33	-0.20	-0.11
c_m	+0.15	0.14	+0.14



Uncertainty Quantification Sub-elements

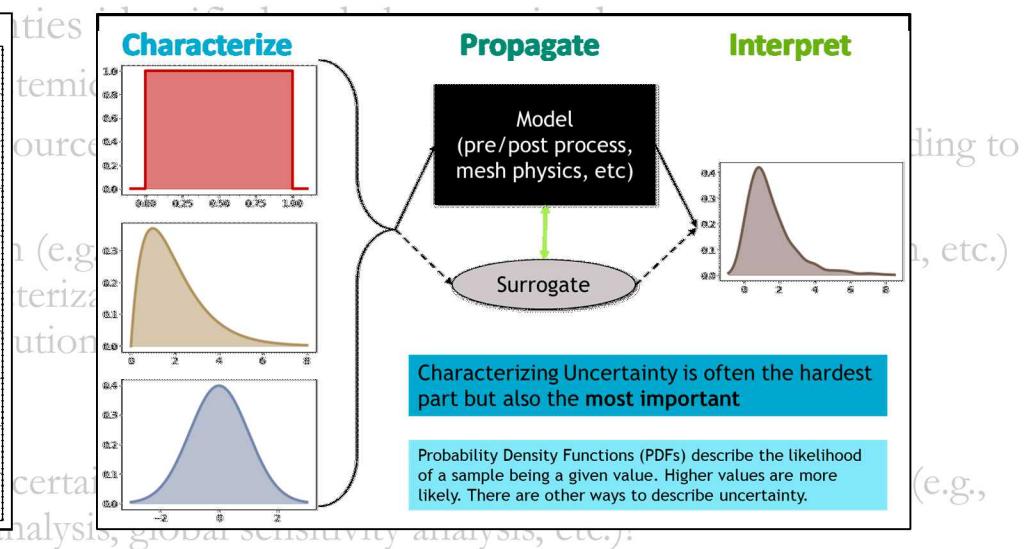
1. Aleatory

- Aleatory uncertainty
- Has a random component that cannot be removed
- What is the distribution of uncertainty?



2. Performance

- How to characterize uncertainty?
- SME judgment, local sensitivity analysis, global sensitivity analysis, etc.



3. Quantify impact of uncertainties on QoIs

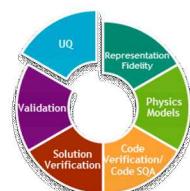
- Have identified sources of uncertainty (see 1 above) been propagated to the important output QoIs?
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- How have sources of uncertainty been combined and transferred across different levels of the system (i.e., validation hierarchy) and to the application domain?

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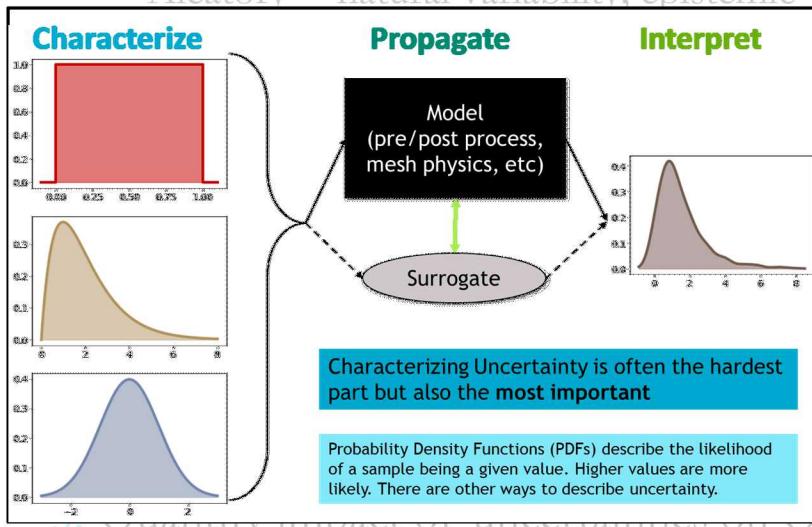
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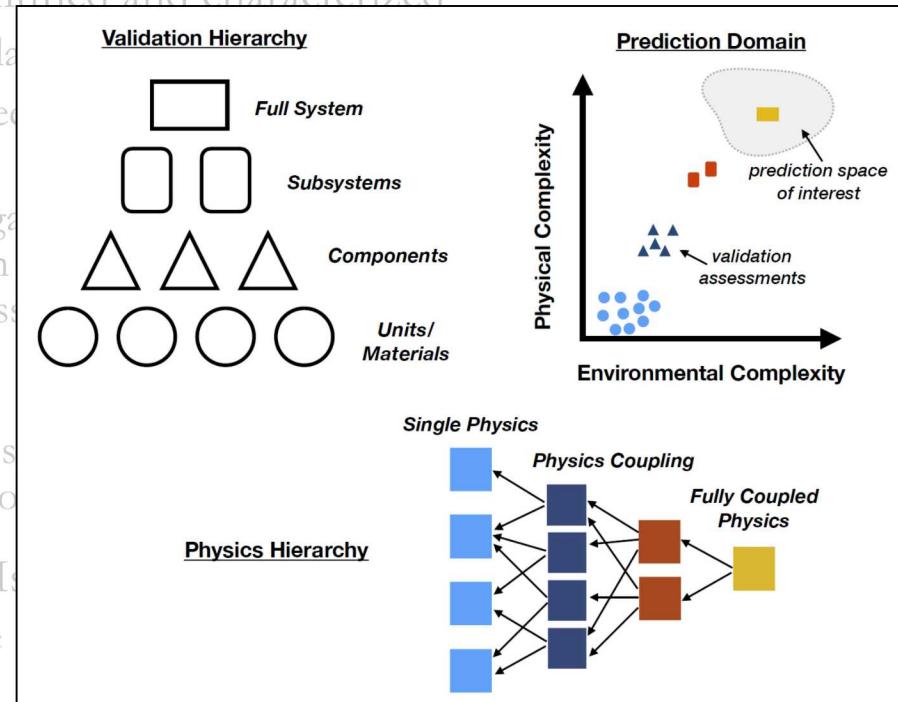
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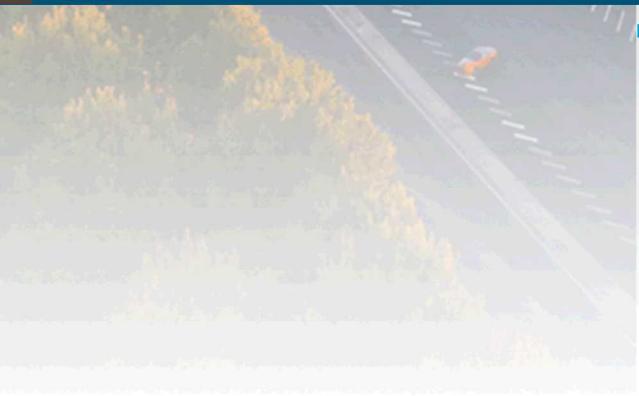
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PCMM Outcomes and Conclusions



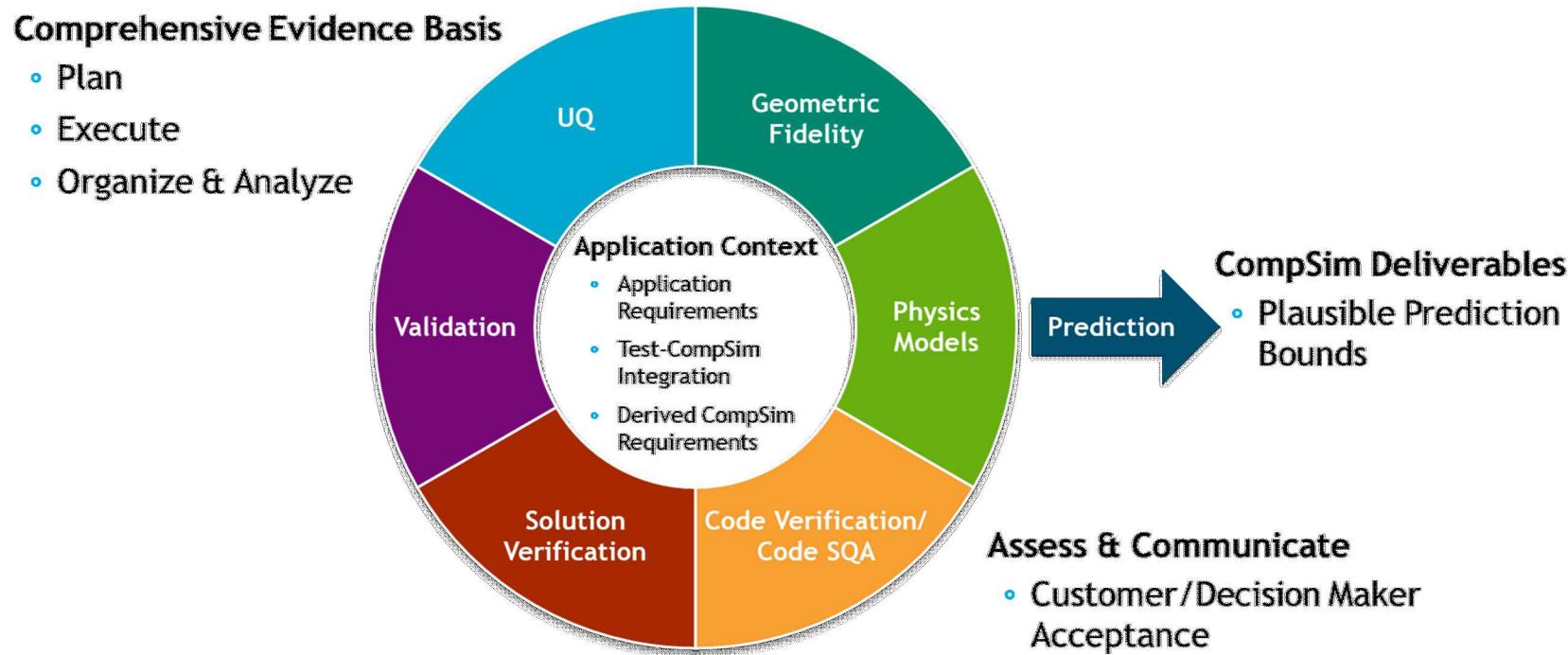
Process Outcomes and Conclusions

Following the PCMM meeting, the following actions should be taken:

- Summarize **key findings**
- Discuss **communication plan** for other project stakeholders
 - General high-level group consensus on status and readiness for decision making
 - Highlight any identified gaps
- Discuss **documentation** expectations
 - Has the existing evidence been documented?
 - Where does it need to go?
- Remaining **action items** (additional activities to perform and documentation):
 - Determine an owner
 - Define a path forward
- If PCMM is used in the planning stage of a project, use PCMM findings to develop a **V&V/UQ Plan**

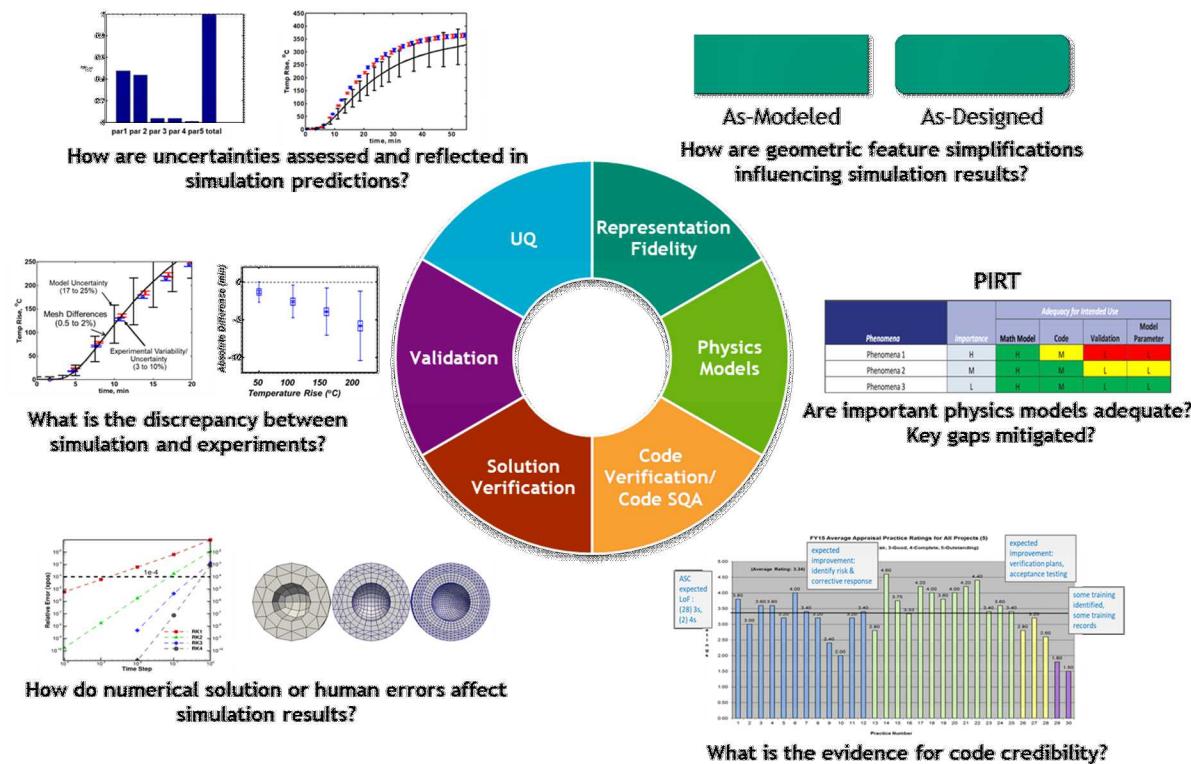
Credibility of Computational Simulation Predictions

- The computational simulation (CompSim) **credibility process** assembles and documents **evidence** to ascertain and communicate the **believability** of **predictions** that are produced from computational simulations.
- The **Predictive Capability Maturity Model** (PCMM) provides a **comprehensive framework** for planning, gathering, and communicating credibility evidence.



Credibility of Computational Simulation Predictions

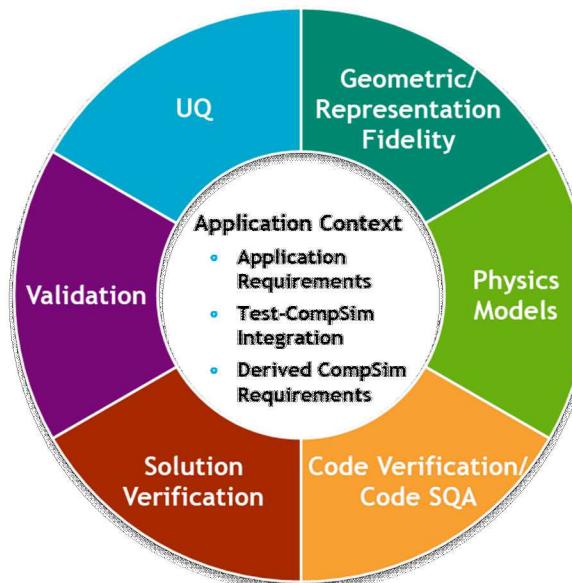
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64 Now you can deploy PCMM!

You should now have the information and materials you need to deploy PCMM for your project:

- Introductory V&V/UQ material provides a **basis for understanding** related technical activities
- PCMM introduction provides a **background** and **motivation** for using this framework
- PCMM slides including prerequisite material and element deep dive provide **discussion materials for facilitators** to use in PCMM meetings



Course Outline

Time	Topic	Presenter
9:00 am - 9:10 am	Introduction	Lee Peterson & Erik Bailey
9:10 am - 10:45 am	Overview of V&V/UQ Concepts <ul style="list-style-type: none"> ▪ Introduction and Motivation ▪ V&V/UQ terminology ▪ Introduction to short example problem ▪ Class exercise ▪ The V&V Process ▪ Summary 	Josh Mullins
10:45 am - 11:00 am	Break	---
11:00 am - 12:00 pm	Introduction to PCMM <ul style="list-style-type: none"> ▪ What is PCMM ▪ Deployment of PCMM ▪ Results of PCMM 	Aubrey Eckert
12:00 pm - 1:00 pm	Lunch	---
1:00 pm - 1:30 pm	Introduction of Example Problem	Erik Bailey
1:30 pm - 2:30 pm	Application of PCMM to Example Problem	Aubrey Eckert & Josh Mullins
2:30 pm - 3:00 pm	Discussion & Questions	All