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Predictive Capability Maturity Model (PCMM)

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VERIFICATION VALIDATION

Template slides for Specific Analysis Project

NOTE: coordinate the contents of these slides with analysis lead prior to conducting a PCMM meeting

Objectives of the CompSim Activities

What is the context of the modeling activities? (capability development or milestone vs. stockpile support)

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 QoIs and prediction objectives?

What are the deliverables and timelines for these activities?

Status of Modeling and V&V Efforts

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 plan, develop a credibility story to communicate)

Introduction to PCMM

Pre-requisite: 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
- 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

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:
  - Determine readiness of modeling capabilities and simulation products for use in various applications and decisions (e.g., design, ES derivation, qualification)
  - 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
  - Maturity levels – a relative measure of the state of the evidence and level of effort around each element
  - Element criteria – major features of the evidence to consider for each element

PCMM: What it is and what it is not

PCMM is:

- A planning tool to highlight and prioritize detailed V&V 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 in the use of modeling and simulation

PCMM is NOT:

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

What does PCMM do?

Use PCMM to:

(1) Help collect a comprehensive set of evidence

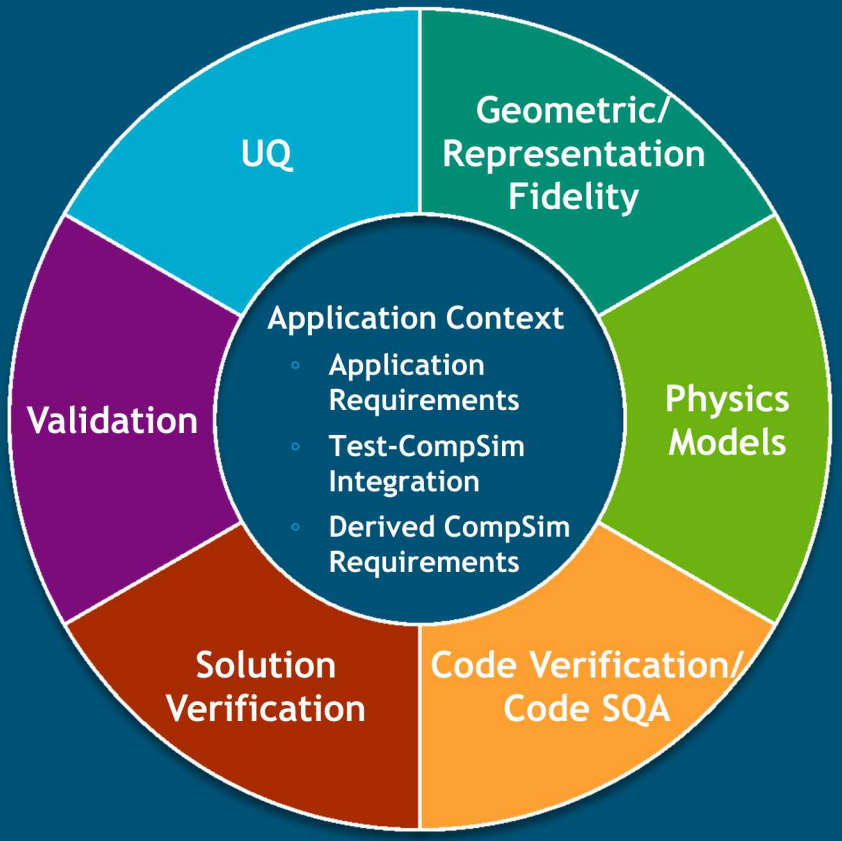
(2) Organize the evidence to tell the story

The *evidence* must exist before it can be evaluated

- What evidence will be generated?
- Will it tell a coherent story?
- Will it be adequate?

PCMM elements – dimensions of the evidence

- Representation and Geometric Fidelity
- Physics and Material Model Fidelity
- Code Verification
- Solution Verification
- Validation
- Uncertainty Quantification



This evidence feeds into a credibility story - 1544 has developed a template for communicating this story

PCMM Process

Suggested Implementation of the PCMM

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 it
   - Archive it
   - Report evidence status periodically – update PCMM as appropriate

Guidelines for this meeting

Discuss each element in detail (refer to element descriptions)

- Take notes on status, existing evidence, needed evidence, current maturity, and major priorities

Roles for the meeting

- 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

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 risks

Discuss documentation expectations
- Has the existing evidence been documented?
- Where does it need to go?

Remaining action items (additional activities to perform and documentation):
- Owner
- Path forward

PCMM Element Discussion (Use the sub-element slides as prompts for facilitation)

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

Needed evidence:

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

As-Modeled As-Designed

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, 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))?

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?

Code Verification (CVER)

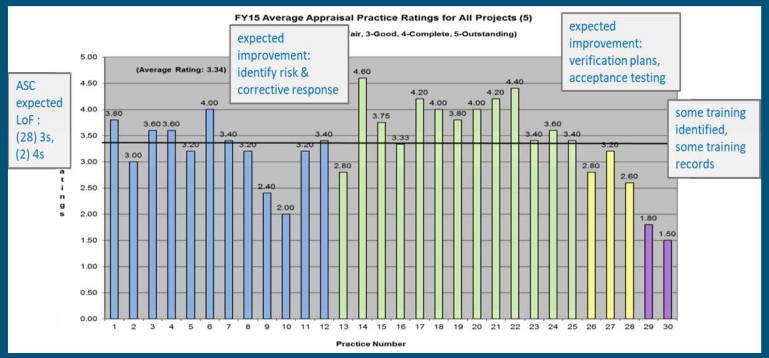
Goal:

- 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? ("Managed" = ASC IC management (for example). Defined in SNL ASC SQE Guidance)
   - Is the SQE process managed and optimized? (as defined in SNL ASC SQE Guidance)
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-assessement, 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?

Note: The evidence for the SQE sub-element may be already documented in a memo by the software code team. Please refer to such documents (if they exist).

Solution Verification (SVER)

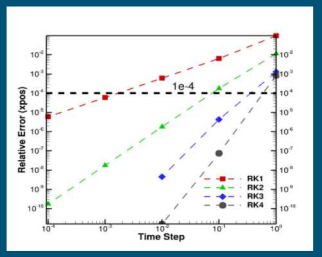
Goal:

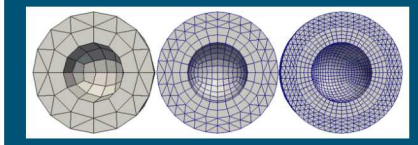
- Identify spatial, temporal, and/or stochastic resolution limitations in the application simulation

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 where are these results documented?

Validation (VAL)

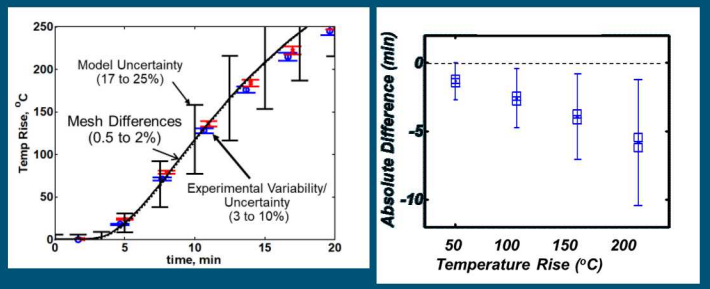
Goal:

- 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?

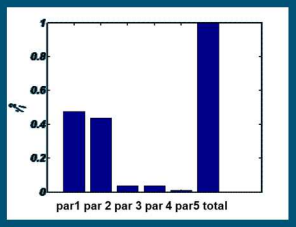
Validation Sub-elements

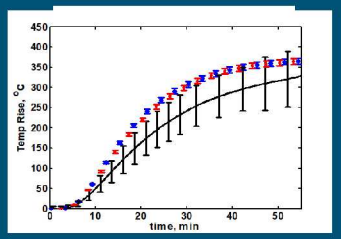
1. Define a validation hierarchy
   - Has a validation hierarchy been defined (i.e., mapping from material to component to subsystem to full system levels)?
2. Apply a validation hierarchy
   - What is the methodology for how available experimental data connects the levels of the hierarchy?
   - Have 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 where 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?

Process Outcomes and Conclusions

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 risks

Discuss documentation expectations

- Has the existing evidence been documented?
- Where does it need to go?

Remaining action items (additional activities to perform and documentation):

- Owner
- Path forward