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Development of a Fourth Generation Predictive Capability Maturity Model

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Abstract

The Predictive Capability Maturity Model (PCMM) is an expert elicitation tool designed to characterize and communicate completeness of the approaches used for computational model definition, verification, validation, and uncertainty quantification associated for an intended application. The primary application of this tool at Sandia National Laboratories (SNL) has been for physics-based computational simulations in support of nuclear weapons applications. The two main goals of a PCMM evaluation are 1) the communication of computational simulation capability, accurately and transparently, and 2) the development of input for effective planning.

As a result of the increasing importance of computational simulation to SNL's mission, the PCMM has evolved through multiple generations with the goal to provide more clarity, rigor, and completeness in its application. This report describes the approach used to develop the fourth generation of the PCMM.

Acknowledgments

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CONTENTS

FIGURES

EXECUTIVE SUMMARY

The credibility of a computational simulation (CompSim) analysis has historically been based largely on the experience of the CompSim analyst using a CompSim tool and judgment by that analyst on the suitability of the results produced for a particular application. The first generation of the Predictive Capability Maturity Model (PCMM) was developed to provide more structure and formality in assessing the credibility of a CompSim analysis for a target application, to reduce the ambiguity in such assessments, and to provide specificity as to what should be assessed and communicated to the analyst's customer. PCMM evaluations have the potential to provide information for effective planning as well as for communication. This first generation was based on six evaluation dimensions, or ***elements***, that are deemed fundamentally important to the quality of a CompSim analysis. These elements address 1) the fidelity in representing physics, including the material models; the 2) the geometric fidelity in representing the system or subsystem element being modeled; 3) the completeness in addressing whether the computational simulation code has been verified from a software assurance point of view and 4) verified from a solution convergence point of view; 5) assessments against experimental data; and 6) the evaluation of uncertainty in the CompSim results due to uncertainties such as the input information used to characterize the specific geometry, environment, and material properties for the application.

With increasing dependence on CompSim results for Nuclear Weapons (NW) work at Sandia National Laboratories (SNL), the importance of characterizing credibility in CompSim results has only increased in the years since the development of the first generation PCMM. As a result, the PCMM has evolved through several generational changes. The first change (to Generation 2) added depth and clarity to the items addressed by the six main elements. The second change (to Generation 3) recast the concept of CompSim maturity into a more overtly evidence-based assessment process, and demanded evaluation of evidence quality. However, even with these changes, concerns with significant inconsistencies between the approach and rigor between different PCMM assessments, and concerns with the apparent lack of impact of such assessments, persist. As a result of these observations and the perceived increased importance of the PCMM for NW work at SNL, a comprehensive review of the PCMM, its process, its management, and its impact was performed in Fiscal Year (FY) 2012. The results of this review are described in this report.

Specifically, we formed a team of PCMM SMEs (subject matter experts and the authors of this report) with significant experience in developing, coordinating, and utilizing previous versions of the PCMM as well as other PCMM-like assessments, to perform a top-down review and revision of the PCMM, with the end goals of (1) increasing implementation process rigor (including quality, breath, and depth), (2) increasing consistency across varied assessments, and (3) increasing relevance to the customer for the CompSim analysis. The following multiple step process defined the course of this work.

1. Revise the PCMM to increase consistency and relevance across multiple PCMM evaluations based on the experience of the team with previous PCMM evaluations. Specific modifications include:
   a. A restructuring of a spreadsheet tool originally developed by Dean Dobranich in FY12 to help insure consistency across multiple PCMM evaluations and across multiple CompSim applications,
   b. Clarification and expansion of the explanatory information provided with each element description ("descriptor") in the PCMM tool,
   c. Reorganization and realignment of the tool and descriptors to be more consistent with the workflow of CompSim analysts,
   d. Inclusion of lessons learned and impact fields in the spreadsheet to help align and clarify the impact of an assessment on the needs of Sandia mission program planners and customers,
   e. Specification of a more inclusive team-based SME elicitation process designed to improve PCMM quality, breadth, and depth. The PCMM evaluation teams should be comprised of customers, analysts, developers, experimentalists, and a PCMM SME, and
   f. Replacement of the phrase 'Maturity Level' in the column headers with the term 'Level'. 'Maturity Level' implies a grading system, whereas 'Level' is intended to represent categories.
2. Trained a pool of PCMM SME's to participate as assessment team members to increase consistency between assessments. Utilized feedback from this pool to further refine the modified version of the PCMM. Members of this pool participated as team members for the prototype assessments listed in item 3.
3. Test and prototype the revised PCMM/ PCMM spreadsheet tool through application to 4 SNL focus areas of high importance to the Sandia ASC program. These focus areas were:
   a. Neutron tube
   b. Gravity/spin rocket motor/B61 Captive Carry
   c. Thermal-mechanical integrated safety theme
   d. Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) program
4. Obtain feedback based on the modified PCMM version from
   a. PCMM Level 2 milestone Review Panel in a mid-year review of the project
   b. Each of the 4 focus area leads and team members, and
   c. The PCMM SMEs who supported each focus area team
5. Based on input from item 4, plus input obtained by the authors but not addressed in the previous PCMM modification, the PCMM was further modified to include:
   a. The definition of an outer process management loop specifying required preconditions for the evaluation of a PCMM.
   b. A streamlined elicitation process designed to more efficiently accommodate different viewpoints of the PCMM evaluation team members.
   c. The addition of an evaluation element assessing understanding and specificity of the customer requirements and needs.
   d. Further revision of PCMM element descriptions for increased clarity.

e. Expanded and reorganized the PCMM validation element to address the validation hierarchy fundamental to ASC V&V methodology, with increased detail for the individual elements of this hierarchy.
f. Added elements to address experimental data issues associated with data used for material model calibration and data used for validation.

6. A final set of PCMM modifications was made in response to the final review of the milestone review Panel.

The deliverables of these efforts include 1) this report that describes the motivation, process, feed-back, resulting changes, and recommended future changes to the PCMM, 2) a presentation summarizing the content of this report, 3) PCMM assessments for four application areas using an intermediate version of the modified PCMM tool, and 4) a revised and self-contained spreadsheet tool that defines the PCMM process, including the preconditions, team approach, and the expected output from an assessment. The organization of the tool is designed to assist in executing PCMM evaluations.

1. INTRODUCTION

1.1. Background

The Predictive Capability Maturity Model (PCMM) is an assessment and communication tool that addresses the 'Maturity' of a computational simulation (CompSim) for an intended application. The term 'Maturity' is meant to convey the completeness and rigor of the approaches used for computational model definition, evaluation, and use. The first generation PCMM was developed by Oberkampf, et al. (2007) and was in the form of a table with the table entries containing descriptions of requirements to be met for maturity levels of 0 through 3 for each of 6 elements deemed important to the credibility of a CompSim. A maturity level of 0 represents a low consequence application with minimal CompSim impact. A maturity level of 3 represents a high consequence application with the decision making heavily dependent on the CompSim results. The elements are 1) Representative and Geometric Fidelity, 2) Physics and Material Model Fidelity, 3) Code Verification, 4) Solution Verification, 5) Model Validation, and 6) Uncertainty Quantification and Sensitivity Analysis and are arranged by row. The corresponding maturity levels are arranged by column, with higher maturity levels requiring more complete and rigorous approaches to assessing the confidence in the CompSim.

Martin Pilch developed a second generation of the PCMM (unpublished) beginning in 2008. This generation is based on the six elements of the first generation documented by Oberkampf et al. but is expanded to include more detail in the form of multiple sub-elements for each of the main elements. The sub-elements include more complete description of the issues that should be addressed in assessing credibility each of the main elements. This generation is available in the form of an undocumented spreadsheet.

A third generation PCMM was developed by Pilch et al. (2011), with a focus on 'maturity' defined in terms of quality of 'the evidence' that various items described in the sub-elements are addressed in an evaluation. Pilch et al. (2011) provides an extensive discussion of the PCMM, along with a detailed example demonstrating evaluation of the PCMM for a notional application. An important addition to the third generation PCMM is the independent development of a spreadsheet 'tool' by Dean Dobranich (unpublished). This tool has been used by several different teams at Sandia for a series of applications and has been well received.

Each successive generation of the PCMM was developed with one or more of the following goals:

1. Increase the rigor and completeness of the credibility assessment.
2. Revise the descriptions provided in each cell of the spreadsheet to clarify intent.
3. Better align the use of the PCMM with the needs of computational analysts and their NW customers.

While each of these generations of the PCMM represents conceptual evolution, experience with PCMM evaluations, including the Generation 3, indicates that the approach to the evaluation, the interpretation of the element descriptions, the perceived purpose, and the impact of the evaluation vary significantly from team to team and from application to application. Increased consistency and rigor in the use of the PCMM is required for the resulting information to be useful for CompSim-informed decision making across the NW CompSim application space at Sandia.

The solution to increased consistency and rigor is not necessarily 'just' another version of the PCMM. A more systematic approach to the process of management, evaluation, as well as modifications to the PCMM itself, is required. A team of PCMM subject matter experts (the authors of this report) was assembled to perform a top-down evaluation of the PCMM and the processes associated with its evaluation. Members of this team were selected based on their experience with the development of the PCMM or PCMM-like frameworks, participating in PCMM evaluations, and their experience with the assessment of the processes and results of evaluations across multiple application domains. This team has engaged the notion of the PCMM on several fronts during its top-down assessment of the PCMM and PCMM process:

- **Purpose** of the PCMM.
- **Content** of the PCMM.
- **Evaluation** using the PCMM.
- **Management** of the PCMM.

These elements are not independent. The best current example of this is our FY13 Level 2 milestone initially having the main goal of developing a useful and coherent PCMM evaluation process based on the most current content definitions as of early FY13 (the so-called Generation 3 content, based on Pilch et al., 2011). Once engaged on this milestone, our team promptly discovered that a systematic exploration of the PCMM evaluation process was not supportable if based strictly on Generation 3 language. The Generation 3 content descriptions were simply not clear enough to allow the milestone effort to focus strictly on evaluation methodology. We ended up creating a Generation 4 PCMM that was better suited to the larger goals of the milestone.

There is a sharp lesson here. Through multiple generations of the PCMM content, systematic and systematically managed evaluation methodology and implementation principles have basically been missing. In retrospect, it is clear that this difficulty is linked to the lack of clarity around formalization (if not institutionalization) of the ***purpose*** of the PCMM. Such formalization cannot be achieved in the absence of a management commitment to control the efficacy and ultimate application of PCMM results. Lack of clear purpose also affects PCMM content, not simply the clarity of the words but the core meaning that drives relevant evaluation.

Pilch et al. (2011) also pointed out the following:

- The PCMM is entirely requirements-driven. The requirements come from customers, that is, at the very least the people who must use the CompSim results to answer questions. In the case of the Sandia NW Annual Assessment cycle, customers are indeed actually paying for PCMM evaluation(s). Their requirements should be explicit and documented as part of the PCMM development and evaluation process. These requirements must include a specification of how the information is to be used.

- The underlying requirements inevitably drive the information that should emerge from the PCMM, that is outputs and outcomes (impact). A defined implementation process states expectations about outputs from the PCMM, and identifies strengths and weaknesses in how that information should be used.

- Evaluation of a PCMM requires a team for computational simulations of the complexity of Advanced Simulation and Computing (ASC) applications. The desirable composition of such a team, and how they should operate, are appropriate for implementation specification. Such a team will also probably require some degree of training to achieve desirable levels of performance.

- Consistency, validity and coherence of PCMM evaluation is important, as previously stated, but unlikely until people gain experience in evaluating it and using it. This experience must be collected and made available to improve the overall implementation process, for example in training evaluation teams. Thus, lessons-learned elements in an implementation are essential.

- In direct proportion to the rigor of the intended application of PCMM evaluations, and also in direct proportion to the degree that multiple PCMM evaluations must be integrated, PCMM evaluations must be formally documented.

- Procedures for gathering the information are needed for evaluating PCMM content and assessing maturity, with some expectation of controlling the quality of this information. These procedures define the inputs for the evaluation. It is possible that the input process, and its quality, can be situation dependent, minimizing the need for uniform procedures in those cases. But for integrated applications where multiple PCMM evaluations need to be aggregated, the consistency of the processes used to provide inputs and control their quality is important.

- A PCMM implementation process places strong constraints on the form of the outputs of the PCMM. We do not favor indexes for summarizing the scoring in the PCMM because too much information is lost and because the index ends up implying a quantitative formality that is likely to be deceptive. The current, somewhat ad hoc, implementation of PCMM outputs is restricted to maturity assessments for the twenty-five detailed content elements (created in the Generation 2 PCMM), and is typically summarized using a ***Kiviat diagram*** (informally called a “radar plot”). The example in Section 4 illustrates this practice. Pfleeger et al. (1992) discuss this diagram in the context of broad approaches to summarizing multiple software evaluation outputs. An implementation process would invite deeper consideration of optimal representations of complex information in the PCMM, not only maturity scores but linkages to the information underlying the scores and meta-data associated with the implementation process. More general representation procedures, such as information dashboards (Few, 2006), might be more desirable from the perspective of formality and coherence across multiple PCMMs.

These issues remain critical at this point in time. Our views here are designed to provide some fresh leverage on them.

As well, we are emphatically focused on supporting the two main goals of effective PCMM application:

- Communication of computational simulation capability accurately and transparently.

- Effective planning input.

The goal of PCMM has really never been to "grade" computational simulation capability, although unclear writing and lack of attention to implementation processes have obscured this fact. The current Level 2 milestone has reinforced our commitment to these goals, however, and this document should be interpreted as an attempt to clarify this emphasis.

1.2. The Level 2 Milestone

The work to revise the PCMM and to apply the revised PCMM to several focus areas (applications) of high importance to SNL ASC program was supported as a FY13 Level 2 Milestone through the ASC V&V Program portfolio. The Milestone title, goals, and products are listed below:

Milestone Title: ASC V&V Project Credibility Assessment using PCMM Methodology

Milestone Statement: Improve PCMM evaluation process and apply the process to 3 SNL focus areas. Perform a post analysis to assess the effectiveness of the process, provide lessons-learned, and suggested further improvements in the PCMM evaluation process.

Key Goals of Milestone:
1) Develop improved PCMM evaluation process to increase consistency, understanding, and usefulness to stakeholders of PCMM assessments.
2) Use improved process to evaluate PCMMs for 3 focus areas of high importance to SNL ASC V&V.

Deliverables
1. Modification of the PCMM spreadsheet tool to increase consistency and relevance across multiple PCMM evaluations
2. Specification of the SME elicitation process used to evaluate the PCMMs, to improve PCMM quality, breadth, and depth
3. Application of modified tool and improved process to 3 SNL focus areas

4. Post assessment of the effectiveness and quality of the resulting focus area PCMM evaluations

L2 Panel Assessment
Completion of above products

1.3. Additional deliverables

Although not specified in the original Milestone statement as deliverables, additional products have been developed under this project.

1. The modified tool (see Product 3) was applied to a fourth focus area.
2. The PCMM and the PCMM framework was further revised as a result of the observations and feedback from the application of the PCMM to the focus areas and as a result of the feedback obtained from the mid year review by the L2 Milestone Panel. The production of this improved PCMM framework for broader applicability, increased effectiveness and communication was suggested as an additional product of the current effort during the L2 Panel kick-off meeting.

1.4. Overview of the Approach Used to Develop Milestone and Additional Products

This section provides an overview of the approach used to develop the milestone and additional products. More complete descriptions are provided in the following chapters.

The timeline followed for the project is illustrated in Figure 1.1. We begin with an overview of the approach used to address the Milestone Product 1.

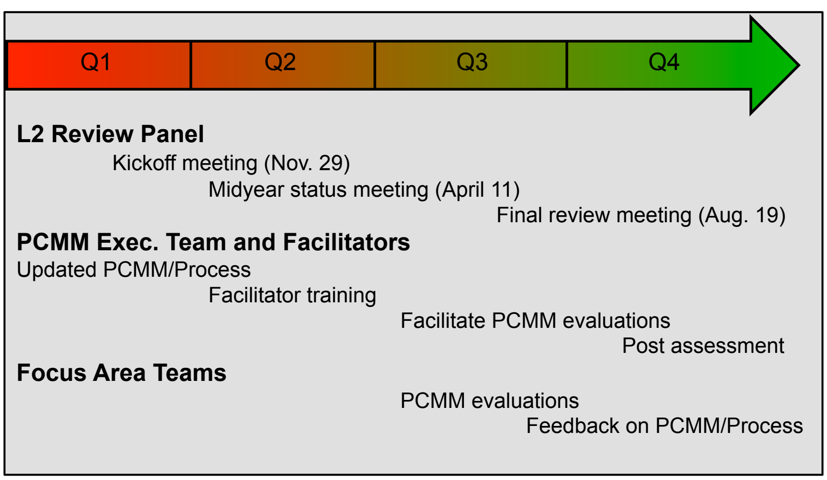

Figure 1.1. Timeline for PCAP Modification and Implementation

1.4.1. Modify and Improve (Deliverable 1)

The first step was to perform a top down review of the PCMM by an experienced team (the authors of the present report). All members of the team had experience with one or more of the following

- Served as a V&V/UQ SME team member for the evaluation of PCMMs for one or more applications
- Participated in the development of earlier versions of the PCMM
- Lead the development of PCMM-like frameworks for non ASC/NW applications
- Served as panel reviewers of SNL ASC/NW projects for which the PCMM was an integral product.

At the beginning of this project, the PCMM project team members had significant concerns about the previous versions of the PCMM based on these experiences. Some of these concerns include

- The descriptions provided in the table cells of the PCMM are sometimes vague (even to V&V SME's), with several different interpretations possible.
- The process used to evaluate a PCMM is not consistent from application to application. The process varies from one analyst quickly completing a PCMM; to teams that include analysts, developers, and experimentalists who reach consensus PCMM scores as a result of a series of meetings.
- The primary impact of past PCMM assessments has been to increase communication between assessment team members, ***when teams rather than individuals performed the assessments***. Other impacts, such as increased communication with the customer of the credibility of the analyst's product, or programmatic changes as a result of issues identified from the evaluation, have occurred for only a limited number of application areas.
- Attitudes toward the value of PCMM assessments varied from 'I'm glad we did this, as I learned a lot' to 'this was a waste of my time, my customer trusts me'. Generally, the experience of PCMM assessment teams was more positive than that of team members performing assessments independently.
- The concept of 'Maturity' as a score is an ambiguous concept and is difficult to convey to the computational analyst and to the customer.
- Assigning maturity levels to multiple physics applications can be difficult when some of the physics is well modeled, while other physics is not. How does one aggregate these results into a single maturity number?
- The relationship between scored maturity levels and supporting the needs of the customer is tenuous. As a result, it is difficult to define and to communicate. For example, the seemingly unwritten rule that computational analysis should reach a Maturity Level of 2 to support the nuclear weapons program is not correct. Results from computations that contain elements with Maturity Levels less than 2 can, and often do, provide very useful information to the decision maker. The purpose of the PCMM is to provide information, not make decisions.

To better understand the concerns analysts might have with previous versions of the PCMM, the project team actively sought the opinions of others that had been involved in past PCMM assessments, including some of the most vocal skeptics of the PCMM. As a result of the past experience of the project team members and the input obtained from others during and prior to this project, the team made the following changes to the PCMM and the PCMM process:

- Clarify the flexibility a team has in defining the desired levels (no longer called Maturity Levels) required for each element or sub-element. There is no requirement that the desired levels be the same for all elements or all sub-elements.
- Perform a revision of sub-element content and descriptions, including removal and addition of content, additional content describing incremental changes in evidence or completeness in transitioning from one level to another, and additional content in terms of general information and definitions
- Perform a re-organization of the format of the previous versions of the PCMM, utilizing the spreadsheet PCMM tool developed by Sandia analyst Dean Dobranich (undocumented) as a starting point.
- Add a worksheet to the tool to provide a recommended expert elicitation process (see the following section).
- Add worksheets to the tool to include team developed summaries of lessons learned, and impact of the PCMM results.

The Modified PCMM was provided to the L2 Review Panel as part of the Milestone mid-year review. It is the opinion of the PCMM project team that the modifications addressed in the above bullets satisfy the requirements for the completion of the Milestone Product 1. More detail on this product is provided in Chapter 2 and evidenced by the PCMM spreadsheet tool.

1.4.2. Specify Consistent Elicitation Process (Deliverable 2)

The approach to provide more consistency between PCMM evaluations was several-fold.

- The revised descriptions and additional descriptive content was designed to reduce the ambiguity of the element descriptions.
- The PCMM evaluation team composition was specified to include at least one each of an analyst, customer, developer, experimentalist, and a SME on the PCMM.
- A recommended elicitation process to be used by the team to assess the PCMM for an application was provided.
- A pool of PCMM SME's were trained (through several training sessions) on the use of the modified version of the PCMM and the PCMM process. Members of this pool participated as the PCMM SME team members for the application of the modified PCMM to focus areas listed in the following section.

It is the opinion of the PCMM Milestone team that the modifications addressed in the above bullets satisfy the requirements for the completion of Milestone Product 2. The elicitation process is documented by a worksheet in the PCMM spreadsheet tool.

1.4.3. Apply and Test (Deliverable 3)

After completion of the modifications to the PCMM and the PCMM SME training sessions, the PCMM and the PCMM process were applied to 4 focus areas (note that 3 focus areas were specified in the original milestone description). The areas and the identified area leads were

- Neutron Tube – Larry Musson
- Gravity/spin rocket motor/B61 Captive Carry – Matthew Barone
- Thermal-mechanical integrated safety theme - Kevin Dowding
- QASPR – Joe Castro (additional area)

It is the opinion of the PCMM project team that the assessments performed by the focus areas in the first three bullets satisfy the requirements for the completion of Milestone Product 3. More detail on focus area assessments is provided in Chapter 3. The actual assessments are provided in Appendix C.

1.4.4. Post Assessment (Deliverable 4)

Feedback on the modified PCMM and process was obtained from the PCMM SME's during training, from the focus area teams, and from the L2 Review Panel as a result of the panel's midyear review. Specific feedback from the focus area teams and post assessment is documented in Chapter 3. The L2 review panel's midyear feedback (post assessment of the revised tool) is documented in a memo (Pilch et al., 2013).

It is the opinion of the PCMM project team that the feedback obtained from these sources and the post assessment provided in Chapter 3, L2 Review Panel's midyear review memo and response memo from Mary Gonzales (2013) provides sufficient evidence that requirements for the completion of Milestone Product 4 were met.

1.4.5. Improve: Additional modifications to PCMM (Deliverable 5)

In addition to modifications made to the PCMM for use during training and for use during the "apply and test" phase (Product 3), modifications were made to address feedback obtained from the focus area evaluations, from the midyear review of the L2 panel, and from other sources.

For example, there was much discussion (based in part on feedback from participants in a FY12 Level 2 milestone involving mechanical failure (Corona et al., 2012)) that there should be fundamental prerequisites to an evaluation of a PCMM. The Milestone team refers to these prerequisites as Gatekeepers. Figure 1.2 illustrates the Gatekeeper concept and lists specific gatekeepers and their place relative to the entire PCMM process. Many of these gatekeeper items are self-evident (e.g., must have the ability to assemble an assessment team and identify the team lead). Likewise, there should be some preliminary evidence that the CompSim can produce results that are consistent with reality, as measured using reliable experimental data, before incurring the expense of a comprehensive PCMM analysis. A detailed discussion of the Gatekeeper concept and the management of the PCMM process are provided in Appendix A.

An overall understanding of what the customer requires is necessary to understanding what physics should be modeled, and the desired level of fidelity in modeling the physics leading to the quantities of interest. Because the evaluation of the PCMM is for an intended application (or family of intended applications), knowledge of what this application entails, and what the customer expects from a computational simulation, is considered a Gatekeeper.

The remaining Gatekeeper listed in Figure 1.2 is the existence of a Phenomena Identification and Ranking Table (PIRT) for the customer application. A PIRT identifies and rates the importance of the relevant physical phenomena that is required to model the customer's application, and performs a high level gap analysis on how well this phenomena/physics can be modeled using a selected CompSim tool (code). The PCMM should be aligned with the phenomena/physics identified in the PIRT, since these are the ones deemed important for the computational simulation in support of the customer's application. If a PIRT doesn't exist the PCMM can't be evaluated.

In addition to the outer loop and the Gatekeeper PCMM process modifications, several other process and tool modifications were made. These include

- Revised the elicitation process defined for Milestone Product 2, to incorporate the outer loop, and to streamline the consensus building process for defining the achieved PCMM levels. The revised elicitation process is provided as a worksheet in the PCMM tool.
- Added elements and sub-elements to the PCMM to characterize the current understanding of customer requirements, to characterize the completeness of the data uses for calibration and data used for validation, expanded the validation element to include more information on the planned and achieved validation hierarchy, and to include the PMMF element of the previous versions of the PCMM as a component in the validation hierarchy.
- Radar plots were reinstated in the PCMM tool, but modified to depict low, mean (or median), and high levels obtained from PCMM evaluation team members when consensus levels were not achieved.
- An additional element that was defined by the project team, but not included in the updated version of the PCMM, was an element characterizing the expertise of the analyst utilizing the computational code for the application. Such an element is relevant, for example, when analysis is outsourced and should be considered in future versions of the PCMM. This element is presented in Chapter 4.

It is the opinion of the PCMM project team that the additional modifications made to the PCMM tool, and the definition of the outer-loop (documented as a worksheet in the tool), fully addresses the delivery of the added products.

1.5. Future Modifications

Caution must be exercised with never-ending changes to the PCMM as such changes represent a moving target for the computational analysts, and a constantly changing interpretation for consumers of the PCMM products. Due to the issues associated with a moving target, the Milestone team ***strongly recommends*** the version of the PCMM, i.e. Generation 4, as defined by the team be frozen for several years[1]. Generation 4 is sufficiently different from previous versions that time is required to gain experience with, and to assess how effective this version of the PCMM is, and to provide a stable target for analysts as to how the PCMM is used.

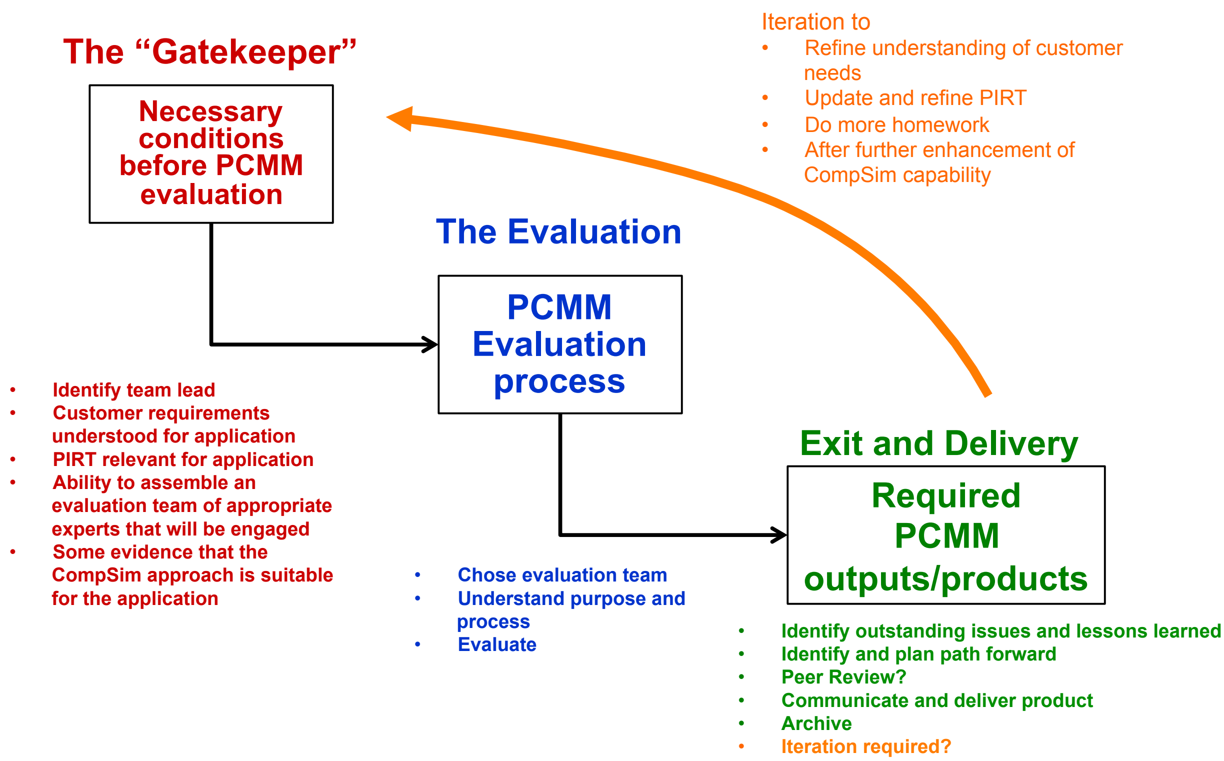

Figure 1.2: Gatekeepers and the Outer Loop of the PCMM Process

[1] However, minor changes, such as spelling and grammatical corrections in the descriptions, and minor changes in their wording to increase clarification but not meaning, should be allowed.

2. MILESTONE DELIVERABLES 1 AND 2

This section addresses Deliverables 1 and 2, which are:

- Modification of the PCMM spreadsheet tool to increase consistency and relevance across multiple PCMM evaluations
- Specification of the SME elicitation process used to evaluate the PCMMs, to improve PCMM quality, breadth, and depth

The Deliverable 1 baseline is the tool that was created by Dean Dobranich (undocumented) in FY12 and the objective of this Deliverable is to increase its usability. Deliverable 2 seeks to deliver a process by which PCMM SME experts, and ultimately users of the PCMM tool, conduct PCMM assessments in a consistent and high quality manner.

2.1. Modifications to the PCMM Tool

The tool's main assessment sheet is shown in Figure 2.1.

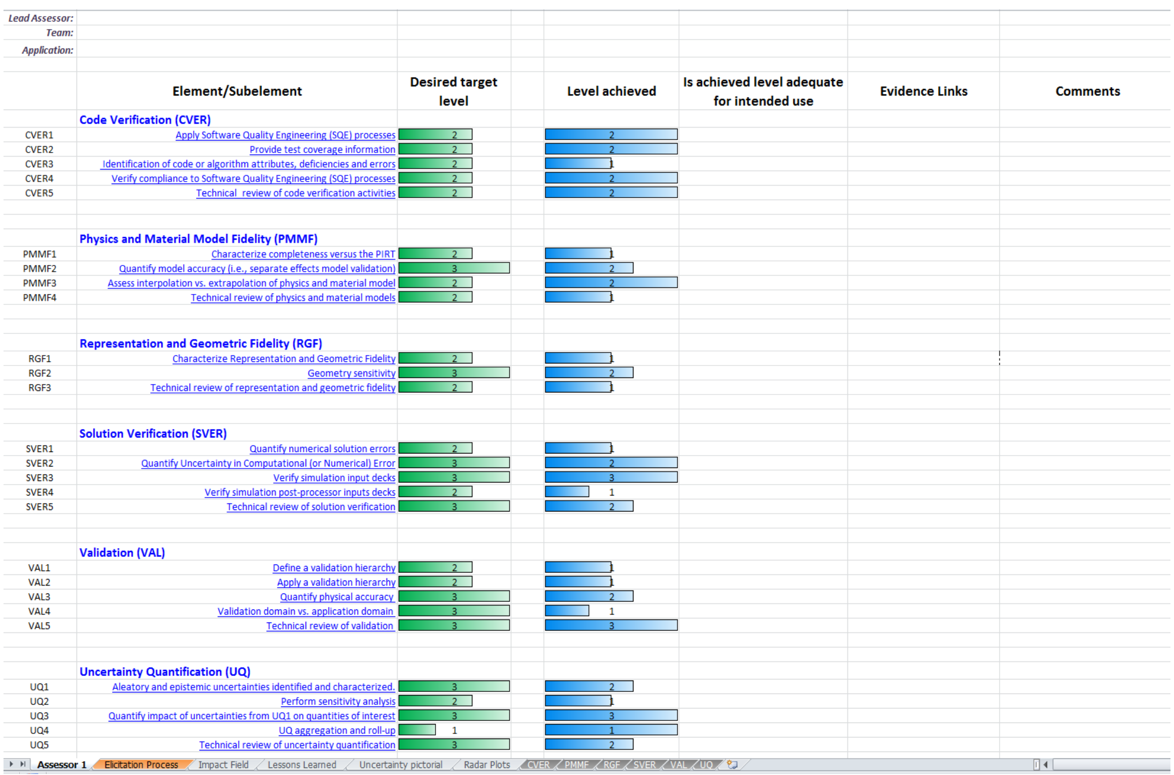

Figure 2.1: PCMM Tool's Main Assessment Sheet

The modifications to the tool can be broadly categorized in 3 areas:

1. Structural changes – how the tool is laid out to improve usability
2. High level changes – how the elements and sub-elements have changed and "Maturity" levels have changed

3. Lower level changes – how the descriptors and related information has changed

2.1.1. Structural Changes

The majority of the structural changes that have been implemented in the tool aim at increasing the usability of the tool and facilitate the assessment. To this end, the tool is designed to be free standing, that is, an assessment should be executed using only this tool. The elicitation process itself is embedded in one of the sheets of the tool and explanatory descriptions of each sub-element and the evidence needed is contained within the tool.

One of the most salient changes to the tool has been the separation of the element and sub-element names and the description of what they are relative to a particular level (i.e. level 0 through 3). The descriptor and other relevant information are now separated into different sheets that are hyperlinked to the main assessment sheet. An example of the CVER descriptor sheet is shown in Figure 2.2.

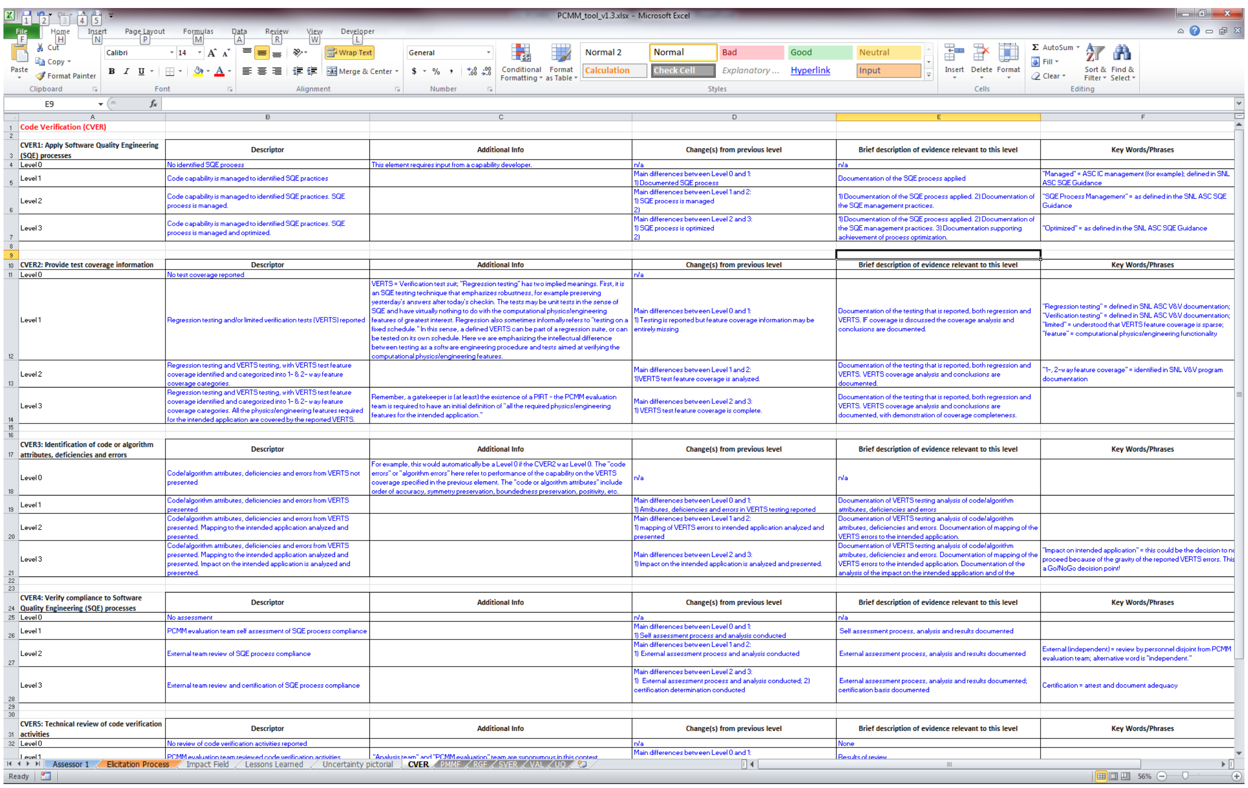

Figure 2.2: Example of CVER Descriptor Sheet

2.1.2. High Level Changes

The modified PCMM tool's elements are arranged in the following way:

1. CVER Code Verification
2. PMMF Physics and Material Model Fidelity
3. RGF Representation and Geometric Fidelity
4. SVER Solution Verification
5. VAL Validation
6. UQ Uncertainty Quantification

This ordering was based on the workflow that an analyst would (or should) follow when starting a CompSim effort.

A second high-level change involves the elimination of the word "Maturity" from the columns identifying the intended use of the CompSim effort. Initially, the column headers were:

Maturity Level 0 =	Low Consequence, Minimal Computational Simulation Impact, e.g. Scoping Studies
Maturity Level 1 =	Moderate Consequence, Some Computational Simulation Impact, e.g. Design Support
Maturity Level 2 =	High-Consequence, High Computational Simulation Impact, e.g. Qualification Support
Maturity Level 3 =	High-Consequence, Decision-Making Based on Computational Simulation, e.g. Qualification or Certification

They are now simply replaced by:

Level 0 = No Words
Level 1 = No Words
Level 2 = No Words
Level 3 = No Words

This is a LARGE CHANGE IN PHILOSOPHY that responds to negative PCMM feedback associated with the implied grading in the word "maturity."

2.1.3. Lower Level Changes

Changes at the lower level consist of changes made to the Level of Maturity of the originally PCMM table and changes in the descriptors of each of the sub-elements. The former changes are shown in the figure below.

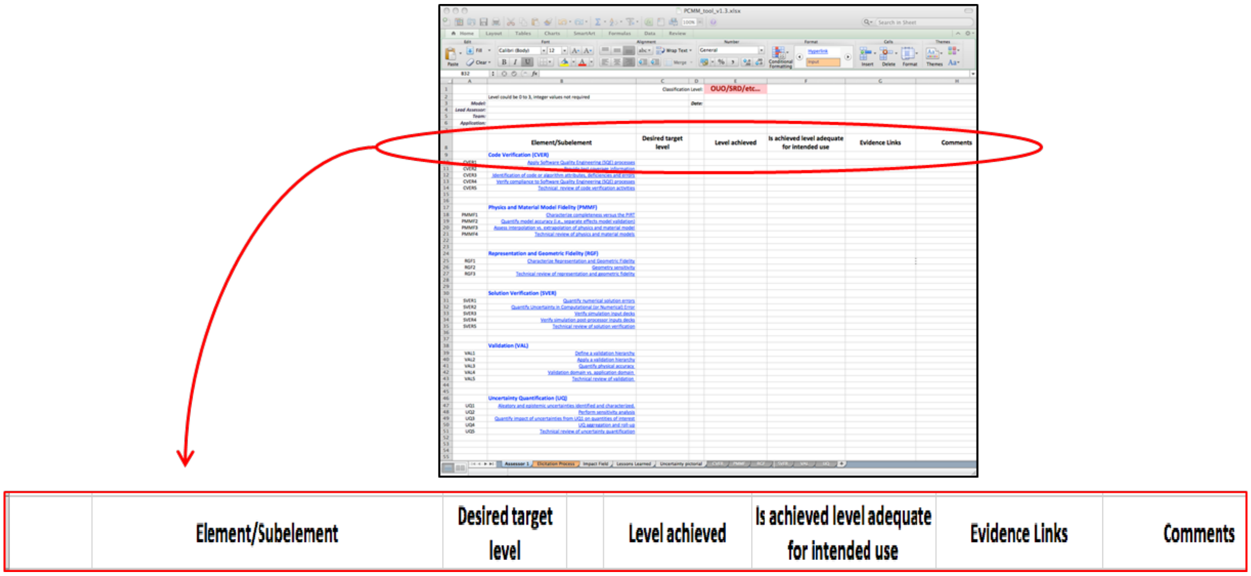

Figure 2.3: Changes to the way levels are specified and assessed

The changes in the descriptor are far more extensive, driven by the intent to increase the usability and reduce the ambiguity in the wording. An example of the evolution of the descriptor changes is shown below:

2009	2011	2013
PMMF1: Science basis for models (how science-based are the models)	**PMMF1:** Characterize the science basis for the separate effects models	**PMMF1:** Characterize completeness versus the PIRT
PMMF2: Model Accuracy (how accurate are the models) i.e., SET validation	**PMMF2:** Quantify model accuracy (i.e., separate effects model validation)	**PMMF2:** Quantify model accuracy (i.e., separate effects model validation)
PMMF3: Extrapolation (what is relevance of the validation database)	**PMMF3:** Assess the relevance of the underlying database	**PMMF3:** Assess interpolation vs. extrapolation of physics and material model
PMMF4: Technical review (confirmation that the validation activities are relevant, adequate, and carried out in a quality manner)	**PMMF4:** Perform technical review	**PMMF4:** Technical review of physics and material models

Figure 2.4: Evolution of sub-element descriptors

As shown above, some sub-element descriptors where not modified and other were completely re-written. It is expected that as we use this new language, further updates and improvement in the descriptors will be incorporated.

A further improvement to the tool was expanding the amount of information that complements the sub-element descriptor. An example of this evolution is shown below:

2009

RGF2:

- Judgment only, numerical errors introduced because of imperfect RGF not addressed

2011

RGF2:

- Judgment only. No evidence of addressing (acknowledging) numerical errors introduced because of imperfect representation of the simulated geometry, part, component, system, etc.

2013

RGF2 Descriptor:	Additional Info:	Change(s) from previous Level:	Brief description of evidence relevant to this level:	Additional evidence from previous level
Simulation sensitivity to major features is not discussed	The computation error referred to means "computational error due to the given level of geometric resolution." The practitioner should understand that this is probably impossible to fully address without having representations at all four levels. This is ONE component is a numerical error; SVER addresses a more integral view of the source of numerical errors.	NA	None	NA

Key Words/Phrases:

Sensitivity = sensitivity of numerical solution to de-featuring. This is not the same thing as quantifying the component of numerical error due to geometry incompleteness. (Issue is how stable a presented solution is to de-featuring.) Major features are defined in element above.) Notice the potential for surprise; major features specified in RGF1, but RGF2 is the real test of how major a feature is!

Figure 2.5: Evolution of level information available to characterize the sub-element

Relative to the original PCMM implementation, the current sub-element descriptor (shown above as the box under "2013") has more information with the hope that this will aid in identifying the desired level in the PCMM. The new columns of information are:

1. Additional Info
2. Changes from previous Level
3. Brief description of evidence relevant to this level
4. Additional evidence from previous level
5. Key words/phrases

Most of these are self-explanatory. One of the most useful contributions of these new columns is the addition of the "Changes from Previous Level" columns. In these columns we describe the additional information, or "delta," that is needed to move from one level to another. It is also provides guidance during the planning phase as to how one will move to a higher level which can then be mapped into cost.

2.2. Specification of SME Elicitation Process

An improvement to the PCMM tool was the addition of a step-by-step elicitation process that is an integral part of the tool. This is shown below:

PCMM Process

Recommended Elicitation Process

Overall Goal:

To increase communication within and outside the product delivery team as to the maturity of a CompSim to support actionable decisions associated with the customer's needs.

Participants:

At least one customer, one or more analysts, one or more experimentalists, one or more developers, and a V&V/PCMM specialist. The number of analyst, experimentalist, and developers should be sufficient to provide subject matter expertise to address the major features of the CompSim that are relevant to the customer's application.

PCMM team lead: Responsible for selecting team members, communicating impact, and delivering final product

V&V/PCMM facilitators: Responsible for facility the overall process, including working with the team lead to insure that momentum is maintained, and to take a lead role during the team meetings. Act as a resource on the use of and interpretation of the items in the PCMM spreadsheet tool.

Other team members: Responsible for providing individual scores and participation in the deliberations for the group evaluations scores

Process:

The following SME elicitation process was designed help insure that both individual opinions and group consensus are characterized by the resulting PCMM document.

The availability of a PIRT for the application is a pre-condition for PCMM evaluations. The PIRT addresses the physical phenomena, which are relevant to a PCMM evaluation.

Step 1: The team meets to discuss the spreadsheet tool, the elicitation process, and the expectations and use of the resulting PCMM product. Copies of the PIRT should be provided to the team at this or prior to this meeting.

Step 2: After the meeting, the team members individually develop an initial evaluation of those features in the PCMM for which they feel comfortable addressing.

Step 3: The team meets to discuss these individual assessments, to share knowledge that affects these assessments, and to reach a team consensus and to document the consensus PCMM scores.

Step 4: After the meeting, the individual team members reflect on the deliberations and update their own scores if appropriate. Note that individual scores do not have to reflect the team scores. These individual scores are used to document diversity of opinion after the deliberation process is completed.

Step 5: Final meeting of the team to discuss the actual or potential impact of the evaluation. The team lead is responsible for providing a summary of the impact in the spreadsheet tool. Impacts can be as specific as planned or recommended programmatic adjustments, or softer impacts such increased understanding of the ability (or lack thereof) of the CompSim to provide the customers with actionable results.

Product:

Completed PCMM spreadsheets by individuals and by team consensus, including completion of the fields on lessons learned and impact in the consensus spreadsheet.

Figure 2.6: PCMM elicitation process

This process spells out the overall goal of the PCMM assessment, the team that needs to be involved with this process and their roles, and the objective of the various meetings that need to be scheduled to perform this assessment. This process also spells out some pre-conditions that are necessary to perform and assessment.

2.3. PCMM SME Training

To carry out the PCMM assessment in a consistent manner, the PCMM SMEs were trained to familiarize them with the new tool and the process to be followed. The relevant features of the training are as follows:

- Training PCMM SMEs to develop consistency
    - 6 sessions for a total of 9 hours of "formal" training
    - Executive team lead training
    - Each session covered roughly one element in the PCMM
    - From each session, valuable feedback from SMEs was incorporated into current version of PCMM tool
    - Changes/decisions were made during training in real time

- Many more hours of "informal" training – off-line questions, hallway conversations, etc.

- SMEs will continue to meet to share lessons learned from each assessment

In addition to this formal training, continuous process refinement was on-going as each of the teams performed their individual assessments and lessons were being past to the other PCMM SME's.

3. MILESTONE DELIVERABLES 3 AND 4

This section addresses Deliverables 3 and 4, which are:

- Application of modified tool and improved process to 3 SNL focus areas
- Post assessment of the effectiveness and quality of the resulting focus area PCMM evaluations

As described earlier in this report, four focus areas were chosen to perform evaluations, followed by post assessments of these evaluations and the lessons learned and feedback collected in the process.

In this section we list the composition of the four assessment teams and we give a brief overview of the process each team followed to conduct the assessments. In addition we provide a compilation of the most common and/or most salient lessons learned and feedback they provided.

3.1. Team and Process

Below is a brief description of the team compositions and the assessment timeline they each followed.

Aeroscience – B61 Captive Carry

- Team
  - Matt Barone, Srini Arunajatesan, Jeff Payne, Justin Wagner
  - Stakeholder: Jerry Cap
  - PCMM SME: Ken Hu
- Assessment timeline:
  - 1 introduction meeting; 1 assessment meeting and individual conversations with team members
- PCMM Experience (prior to this exercise): Medium

Thermal-mechanical integrated safety theme

- Team
  - Kevin Dowding, Sam Subia, Dean Dobranich, Roy Hogan,Nick Francis, Jill Suo Anttila
  - Stakeholder: Jim Nakos
  - PCMM SME: George Orient
- Assessment timeline:
  - 1 introduction meeting and 1 assessment meeting
- PCMM Experience (prior to this exercise): Medium

QASPR

- Team
    - Joseph Castro, Vicente Romero, Biliana Paskaleva, Charlie Morrow, Chuck Hembree, Brian Rutherford, Alan Mar, Henok Abebe, Gary Hennigan, Eric Keiter
    - Stakeholder: Len Lorence
    - PCMM SME: Joseph Castro, Vicente Romero
- Assessment timeline
    - 1 introduction meeting, 1 assessment meeting and a follow-up meeting
- PCMM Experience (prior to this exercise): High

Neutron Tube

- Team
    - Lawrence Musson, Matt Hopkins, Ed Barnat, Matthew Bettencourt, Shawn Dirk, Thomas Hughes
    - Stakeholder: Dan Rader
    - Customer: Allen Roach
    - PCMM SME: Angel Urbina
- Assessment timeline
    - 1 introduction meeting and 2 assessment meetings
- PCMM Experience (prior to this exercise): Medium

3.2. Lessons Learned and Feedback

In this section we summarize the common and/or most relevant lessons learned and feedback that were compiled during each team's assessment. The complete set of "raw" lessons learned and feedback from the evaluation teams are in Appendix C.

Below, we list the high level lessons learned that were common among all the teams. Included in the list are lessons learned that were important enough to be included in this summary but not necessarily mentioned by all teams.

- The overall process
    - Teams saw value in the process.
    - Increased communication within team and with customer.
    - Encouraged the team to think about V&V/UQ aspects of the problem not just CompSim issues.
    - There is a need to communicate clearly that PCMM evaluation is for a specific application. This focus was occasionally lost.
    - Consensus is difficult to reach. Many compromises are needed.
    - Assessment meetings
        - Must have strong commitment from management; key contributors whose input is critical may not be willing participants initially.
        - Scheduling meetings for a large team is a challenge; balanced representation not always achieved.

    - Having a PIRT (Pilch, et al. 2000) is essential but it was not always available. More worrisome is evidence of lack of knowledge of what a PIRT is.

- The customer
    - Customer involvement is absolutely essential for this process to make any sense.
    - May not be willing to state what the desired target level is and will lean to deferring to computational simulation SMEs.
    - Need to find a way to keep him/her/them engaged.
- The spreadsheet tool
    - Generally well accepted.
    - Overwhelming at times.
    - Must spend a full meeting going through it and explain - hard to hold the attention of the audience.

Listed below is the high level feedback that was either common among all the teams or important enough to be included in this summary but not necessarily mentioned by all teams.

- PCMM is recognized as useful for smaller projects as well; need PCMM "lite."
- Consistency and education are key:
    - Glossary of terms is needed.
    - Should PI's be required to attend a V&V Primer type class?
- Managing evidence:
    - Need a formal repository for:
        - Managing evidence of current PCMM.
        - Body of evidence to be referenced in future PCMMs.
- Implementing a very formal credibility assessment is premature.
    - We do not have formal processes for anything else – PIRTs, hierarchy, design of experiments, verification, validation, etc.
- Too complicated, too subjective. How does each sub-element connect back to credibility?
- Different definition for each sub-element is taxing. A more uniform set of criteria is desired.
- Usefulness of PCMM to product teams needs to be demonstrated so that team participants are willing to put in real effort.
- By far, the UQ element is the most challenging to address.

The next logical step after compiling this feedback is to analyze it and act upon it. This is topic of the next section in the report.

4. ADDITIONAL PRODUCTS

This section will cover several important products developed during the final stages of the work driven by the diverse feedback we received over the course of the year. First we will provide a quick discussion of feedback from the L2 mid year review and response as provided in Gonzales (2013). Based on experience in the pilot PCMM reviews we have produced a revised elicitation process. Further clarification and minor modifications were made in the defined "outer loop" for the entire PCMM process.

An overall driver for these changes is the impending freeze in the form of PCMM after this milestone. This motivated defining these changes at this point. All of these changes are a direct result of the milestone work, the associated assessments or the feedback from the milestone reviewers. We are explicitly asking for immediate and direct feedback on these proposed changes. We are proposing several specific changes in the high level structure of PCMM: a Customer Element, (two) Data Elements, and associated restructuring of the existing PMMF element as a combination of the data and validation elements. We have examined, but not adopted, a User/Analyst Element. We note that developments in how computational simulation is being delivered to Sandia programs may make this change more attractive in the near future.

Each of the proposed changes was made because of the seriousness of the related issues surfaced this year. Despite this seriousness, none of the changes is "set in stone" as of yet.

4.1. Brief discussion of Feedback from L2 mid year review and response as defined in Gonzales (2013)

The full documentation of this topic is found in the detailed memos produced by the mid-year review of this milestone. The paraphrased committee comments or questions are italicized, and the response of the team is below each in the standard font.

(1) Include a preamble tab that discusses what the PCMM is and is not. (2) Each of the sub-practices should be expressed in terms of an action verb.

We agree with these recommendations.

The panel recommended that the milestone team re-implement the radar (Kiviat) plot-reporting feature within the basic spreadsheet template for the milestone PCMM.

We agree with this recommendation.

The panel questioned a relatively subtle reordering of the major PCMM elements in the milestone implementation.

The reordering emerged from (1) the milestone executive team itself as it wrestled with improving content clarity and consistency, (2) the PCMM "experts" that were trained as part of the milestone, and (3) feedback from past evaluation attempts.

The panel questioned a major change in philosophy implied by a seemingly simple wording change.

The meaning of the term "Maturity Level" and it's implication toward the assessment of a CompSim's suitability for a particular application has been a major stumbling block in the application of the PCMM as a communication tool.

The panel observed that the subjectivity of some language around sub-practices is virtually impossible (which we agree with), and that subjectivity and potential for confusion of "Quantify physical accuracy" was equal to that of "model accuracy."

We disagree with the latter statement. "Quantify physical accuracy" has been the subject of numerous discussions of validation that have been published by the Sandia V&V program. Emphasizing the need for V&V planning, and particularly the PIRT, in fact creates sharp understanding of what this phrase means.

The panel observed our formulation of the "intended use" column in the milestone PCMM, but the column was not adequately explained during the midyear review.

We agree (see the remainder of this segment of the report for our full response).

The panel observed that we had little or nothing to say about the use of PCMM as a planning tool, and that probing this application might be an important task that is well within the scope of the milestone.

We agree with the importance of use of PCMM evaluations as planning input, and agree that we were opaque about milestone activities that could prototype this application. We plan to address the multiple uses of the PCMM in the outer-loop discussions.

4.2. Revised elicitation process

Based on the feedback from the process and the mid-year review, we have made subtle changes in the elicitation process. These specific changes reflect the aggregated feedback from the pilot PCMM evaluations conducted this year. This process is fully documented in the developed Excel spreadsheet tool. The intent is to avoid the specific modalities of problems encountered this year.

A summary of the revised process is included below. For example the step of examining the specific relevance of the elements in PCMM to customer needs has been included to "vet" the whole examination with the customer. Implicit in this step is a greater communication content from the remainder of the team to the customer. This is paralleled by the addition of a specific customer element in the overall PCMM structure.

The steps are clearly defined:

Step 1. The team assesses the necessary conditions.
Step 2. The team has a kickoff meeting to define the process.
Step 3. Relevance of elements to customer needs is ID'ed.
Step 4. Team members conduct personal assessments
Step 5. Team meets to integrate their individual assessments.
Step 6. Final meeting of the team to discuss impact.

4.3. Outer loop

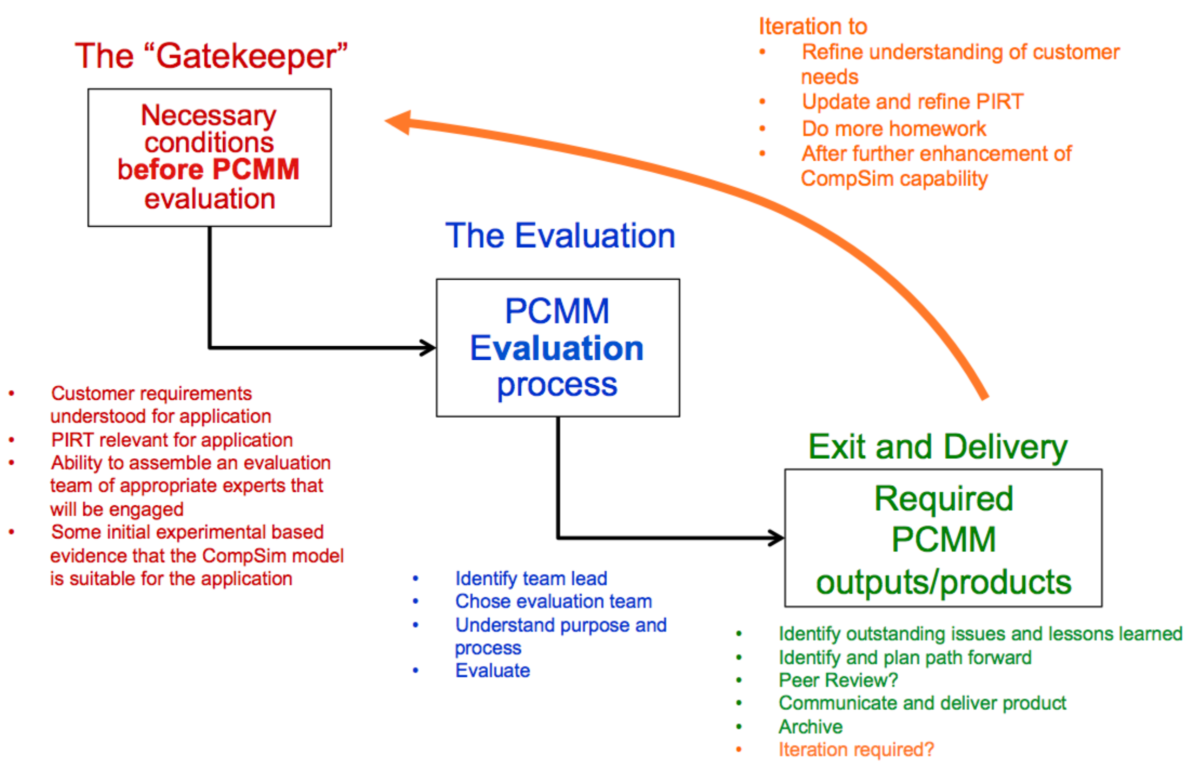

Figure 4.1. The PCMM Process.

Figure 4.1 shows the current outer process as a flow chart. This figure illustrates the PCMM outer loop, and the requisite steps associated with the pre-conditions, the elicitation process, the exit process and any iterative application of the process. The preconditions are clearly defined with a V&V Plan or PIRT being preeminent aspects of work that should precede the process. Initial steps at gathering evidence prior to the more formal heart of the process are discussed. The heart of the process, the actual evaluation, is stable, although the specific steps have been modified per the previous discussion. Finally the existence and delivery of final products is defined with the addition of the potential iterative application of the PCMM. In a sense the iteration is the application of an enhanced set of preconditions to make subsequent evaluations more meaningful and complete.

4.4. Customer Element

This showed up as a significant issue with respect to engaging the customer needs, and providing an inclusive process. Customers did not feel that this process required their engagement. This element is designed to compensate for this point of view.

	Customer Specification Completeness (CSC)
CSC1	Needs
CSC2	Domain of Application
CSC3	Domain of Validation
CSC4	PIRT
CSC5	Technical Review of customer specifications

Figure 4.2. The High Level Structure of the Proposed Customer Element.

4.5. Inclusion of PMMF in validation elements and restructuring and addition of validation elements

These elements reflect the importance of the data itself to any validation activities. The changes parallel the restructuring of the PMMF element.

	Validation - Hierarchy (VALH)
VALH1	Define a validation hierarchy
VALH2	Apply a validation hierarchy
VALH3	Characterize completeness versus the PIRT
VALH4	Validation domain vs. application domain
VALH5	Technical review of validation

Figure 4.3. The High Level structure of the Proposed Validation-Hierarchy Element.

	Validation - Component (VALC)
VALC1	Quantify model accuracy
VALC2	Assess interpolation vs. extrapolation of physics and material models
VALC3	Technical review of component validation

Figure 4.4. The High Level Structure of the Proposed Validation-Component Element.

4.6. Data elements (calibration and validation)

These elements reflect the importance of the data itself to any validation activities. The changes parallel the restructuring of the PMMF element.

	Experimental Data for Model Validation (DATV)
DATV1	Available Data
DATV2	Data Uncertainty
DATV3	Validation Experiment Definition
DATV4	Technical review of data

Figure 4.5. The High Level Structure of the Proposed Experimental Data for Model Validation Element.

	Experimental Data for Constitutive Model Calibration (DATC)
DATC1	Available Data
DATC2	Data Uncertainty
DATC3	Impact of incomplete data for constitutive models
DATC4	Technical review of data

Figure 4.6. The High Level Structure of the Proposed Experimental Data for Constitutive Model Validation Element.

The combination of the validation elements and the data elements constitutes an effectively complete restructuring of the former PMMF element. We emphasize that these changes were made to address some fundamental confusion that arose repeatedly in the use of the former structure. We are endeavoring to reduce the confusion associated with the different aspects of the broad set of activities associated with validation against experimental data.

4.7. Changes considered but not made

We also seriously considered adding an element related to code user/code analyst quality. This change is "too hot to handle" in the near-term frozen implementation of the PCMM, but must be considered for longer-term deployment.

This considered element has a proposed structure:

- Qualification of Code Users – this would encompass the formal and application/code specific training of the users.
- History of Use for Application – This would define the pedigree of the use of the modeling approach (code etc) for the intended use.
- Is the use, rigor and user compatible with the planned activity defined by customer requirements for the analysis. Is the activity aligned with the application use?
- Peer Review – this would be structured just like peer review sub-element in other elements.

Another element that was not seriously considered also merits discussion. The numerical solution is tested via code verification and solution verification, but solution approaches (i.e., numerical methods) are not critically examined. In other words, verification tests whether a formulation is correct, but does not necessarily assess the propriety of the approach for the intended application. It is worth noting that in many applications, the character of the numerical solution has nearly as large an impact as the physical model, or interacts strongly with the modeling. Compelling examples for this effect exist in a number of fields, including turbulence modeling, shock physics, and MHD.

Finally we note that the regulatory environment could become significant for certain safety related applications (experimental facilities, nuclear industry, biomedical engineering, aircraft, etc.). We have had worthwhile interactions with the nuclear engineering world and explored connections to CSAU (Boyack et al., 1990 – a United States Nuclear Regulatory Commission accepted framework) via CASL (Consortium for Advanced Simulation of Light Water Reactors, http://web.ornl.gov/sci/nsed/docs/CASL_Overview.pdf). An increased use of PCMM with the nuclear industry or perhaps computational simulation use for biomedical applications could raise the regulatory issues to sufficient prominence to require a more systematic treatment within the framework.

4.8. Summary

Each of these changes makes a clear difference in the overall process. We have worked to balance our response between a stable PCMM and addressing pressing issues raised during this year's process. We believe that the changes make the overall PCMM better, more responsive, while avoiding divisive issues.

5. DISCUSSION

The need to characterize and communicate credibility of Computational Simulation (CompSim) results developed in support of SNL Nuclear Weapons (NW) work has increased with the growth of use of CompSim for these applications. The Predictive Capability Maturity Model (PCMM) was developed in direct response to this need and can also serve as a planning tool for CompSim development. The PCMM has undergone several generations of evolution. The evolution of the PCMM from Generation 1 to Generation 3 was a result of several drivers including

- The need to improve the characterization of the rigor and completeness of the verification, validation, and uncertainty quantification approaches used for CompSim-based applications
- The need to increase the effectiveness of a PCMM evaluation in terms of the ability to understand and communicate the elements addressed by the PCMM
- The desire to increase its use as an assessment and planning tool

Concerns with significant inconsistencies between the approach and rigor of different PCMM assessments, as well as perceptions of an apparent lack of impact of such assessments, persist. As a result of these observations, a comprehensive review of the PCMM, its process, its management, and its impact was performed in Fiscal Year 2013. The results of this review and the development of resultant Generation 4 of the PCMM in response to these results are described in this report.

As was the case for previous generations of the PCMM, the evaluation of the effectiveness of the latest generation PCMM to address the three drivers listed above requires additional experience through implementation to multiple application domains. Pilch (2013) provided the following questions relevant to the effectiveness of the PCMM, its implementation, and its impact:

- Does the current tool (or any generation) help analysts do better analysis?
- Does the current tool (or any generation) help customer engagement and acceptance of CompSim results?
- Does the current tool (or any generation) help communicate readiness of CompSim capabilities?
- How do we *measure* the benefit of PCMM in the benefit/cost equation?
- What do we codify in the RPP[2] with respect to the PCMM? Is it tangible and sustainable to CompSim activities across the laboratory?

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[2] RPPs (Realized Product Process) are recommended practices that are developed by SNL to support NW work. The RPP cited in the last bullet refers to one developed specifically for CompSim. The CompSim RPP is currently in draft form with completion and deployment expected during FY14. This RPP recommends CompSim processes to support the B61-12 and W88-Alt programs, and specifies that PCMMs be evaluated for CompSim applications

The questions addressed by the present work are those listed in bullets two and three. Specifically, additional elements and content were included in Generation 4 with the intent to increase customer engagement and to improve communication. Experience with the application of the Generation 4 is required before one can assess the effectiveness of these added elements in addressing these questions. The remaining questions asked by Pilch are overarching, and yet to be answered.

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for which CompSim provides a significant contribution to the system qualification or other high consequence decisions.

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APPENDIX A: THE GATEKEEPER AND OUTER LOOP

The Gatekeeper concept and the PCMM process first introduced in Section 1 is an outgrowth of discussions between the project team members and analysts who have had experience with PCMM evaluations. Following is a more complete description of the Gatekeeper concept, including the management of the PCMM process, than was provided in earlier sections of this document.

A.1 Input Requirements

Figure A.1 illustrates a high-level view of a PCMM evaluation process seen in its simplest terms as a ***serially executed process***.

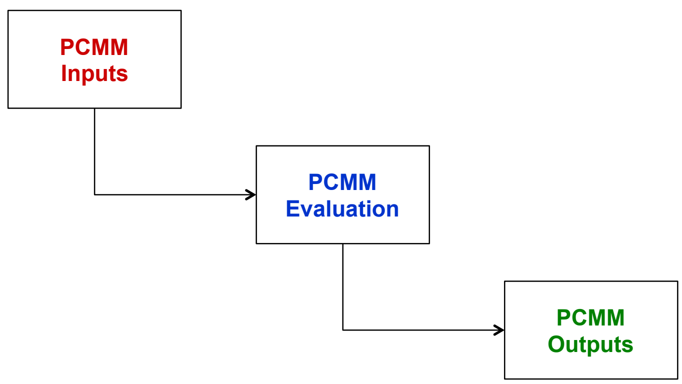


Figure A.1: PCMM Serial Evaluation Process.

A serial view of the PCMM evaluation process is illusory. As soon as some degree of management of PCMM evaluation implementation is enforced, there is the opportunity for a variety of feedbacks in the process that change the simple serial logical flow depicted in Figure A.1. As well, a managed process will define requirements for the implementation. This is depicted in Figure A.2.

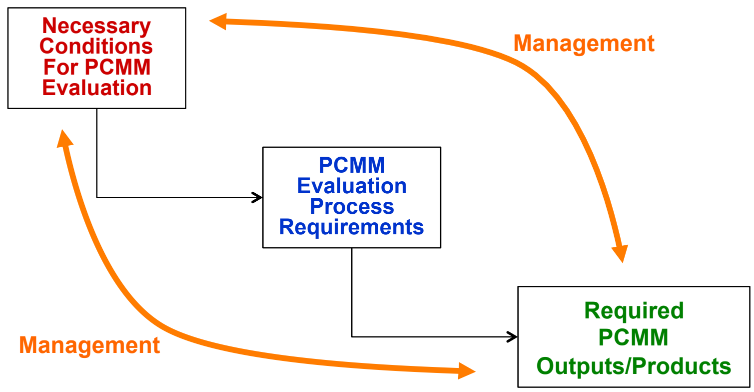


Figure A.2: A Managed PCMM Evaluation Process - with significant feedback loops and potential for iterated requirements specifications.

Once the PCMM evaluation process has a managed implementation, necessary conditions or requirements for executing the evaluation processes and using the resulting evaluation information are specified. These requirements group naturally into the three main phases of the implementation:

- Inputs
- Evaluation execution
- Outputs

Our focus here is on necessary conditions, not on "sufficient" conditions. What sufficiency means in a given PCMM evaluation is highly dependent upon the specific context of the evaluation, and cannot be generally defined.

In this section we concentrate on input requirements. Generally, by "input" we mean the information and context that are required to perform a useful and sensible PCMM evaluation. Our specifications below are based on our experience with PCMM evaluation and feedback from the FY13 Level 2 milestone.

- It is necessary to understand that the ***PCMM is a V&V product***. The PCMM cannot be understood without understanding the V&V context of the evaluation methodology. Specific elements in the PCMM demand comprehension of the vocabulary, philosophy, and principles of the Sandia V&V program. For example, validation is specific to an application. Therefore, because validation is one of the core content elements in the PCMM, the PCMM evaluation is specific to an application of the capability that is being evaluated.

- Ideally, the PCMM is fully connected to the V&V context by starting the PCMM evaluation process with a ***V&V plan*** (Pilch et al., 2000; Trucano et al., 2002). We have decided that we cannot require a documented V&V plan as a necessary condition for the PCMM evaluation, but we can't overemphasize the usefulness of such a plan when performing PCMM evaluations. In the absence of a documented V&V plan, we do require the following, which is a subset of the information that would be created and presented in a full V&V plan:

    - Define the ***intended application*** of the capability that is the focus of the PCMM evaluation.
    - Define the ***customer*** for the intended application of the capability.
    - Define the ***customer requirements***.
    - Define a ***PIRT*** (Phenomenology Identification and Ranking Table; see Pilch et al., 2000 and Trucano et al., 2002).

  The PIRT is particularly crucial. The Generation 4 content element descriptions explicitly depend upon existence of a PIRT.

  We have reinforced the role of the customer in the evaluation process itself with the customer element that we added to the Generation 4 table, which creates the ability to fully respond to the above customer-related bullets.

- There exists minimal confirmation that the capability can actually be evaluated using the PCMM methodology. This includes at least three specific necessary conditions:

    - Problems like the intended application can be ***meshed***.
    - Problems like the intended application can be ***run on available computers***.
    - Some kind of demonstrated ***comparison of computational capability results with physical data***.

  The logic behind these necessary conditions is straightforward. The capability subjected to a PCMM evaluation requires some kind of minimal functionality. Otherwise, the evaluation is a waste of time, because the PCMM assumes that minimal functionality has been achieved as a starting point. If a capability does not have minimal functionality then basically nothing is known about it that is relevant to the PCMM logic. One does not need to perform a PCMM evaluation to draw this conclusion in this event.

- The PCMM evaluation team has done their ***technical homework***. That is, the evaluation team demonstrates enough subject matter expertise in the application domain and the computational capability to be able understand what the PCMM evaluation is telling them as well as to perform the evaluation.

These necessary conditions are "gatekeepers" in the sense that failure to meet one or more of these conditions is a basis for *not executing a PCMM evaluation process*. A softer way of stating this is that the quality and usefulness of a PCMM evaluation performed without achieving all of these necessary conditions can be emphatically questioned.

A.2. PCMM Evaluation Methodology Requirements

PCMM evaluation methodology requirements are presented in this section. Part of this discussion is taken from the full specification of the evaluation process in Urbina et al. (2013) on the PCMM elicitation process. The high level elements of the evaluation process are

Form the evaluation team

- At least one customer, one or more analysts, one or more experimentalists, one or more developers, and a V&V/PCMM specialist. The number of analyst, experimentalist, and developers should be sufficient to provide subject matter expertise to address the major features of the CompSim that are relevant to the customer's application.

Process:

- Assess whether gatekeepers are met
- Team meets to discuss the spreadsheet tool and process
- Team selects those PCMM elements and sub-elements that are relevant to the customer's needs
- After the meeting, the individual team members develop an initial evaluation for those elements for which they possess the expertise
- The team meets to discuss the individual assessments, and attempts to research a consensus on PCMM levels. The consensus scores or the range of scores if a consensus is not met are recorded.
- A final meeting is held to discuss the impact and the lessons learned of the PCMM evaluation. The impact and lessons learned are summarized in the corresponding fields in the spreadsheet tool.

Products:

Products include the PCMM spreadsheet showing single or ranges of scores for the relevant elements, including completion of the fields on lessons learned and impact.

The minimal criteria for exiting the evaluation process are:

- Required table evaluation numbers:
  - Evaluation levels
  - Target levels
  - Weights?
- Metadata supporting, or linked with, the evaluations. This could include references to documented information, for example.

One way to think of the exit status is that a satisfactory degree of completion of the evaluation has been achieved. The next stage, called "Output," is the process of communicating the evaluation and what it means.

A.3. Output Requirements

The communication of evaluation results and their meaning to a targeted audience is extraordinarily sensitive to specific requirements and circumstances of the evaluation. There is no single prescription for a set of necessary outputs from the PCMM evaluation process. As well, this phase could be highly iterative depending on the level of engagement of the targeted audience. For example, communication of some information could (and probably should) generate further requests for more information that clarifies or deepens the understanding of what all of this means.

Here we suggest an array of information that seems, at a high level, to be likely useful in almost all circumstances surrounding the use of the PCMM evaluation for communication and planning.

- Define the recommended or intended ***application*** of the PCMM information.
- Define and deliver the ***required outputs***.
  - Summarized table evaluation numbers:
    - ***Kiviat diagrams*** (radar plots)
    - ***Target-evaluated gaps*** (tabular representation/Kiviat plot)
    - Quantitative ***Dashboards***
  - Metadata
    - Qualitative ***dashboards***
- Required Peer Review?
  - Create/deliver outputs, peer reviewed if required.
  - This information would support higher evaluation levels for "review" sub-elements in the Generation 4 table.
- Define ***archival requirements***.
- Is ***iteration of PCMM evaluation required/desired***?
- ***Lessons learned***.

In general, the outputs that emerge from the final stage of a particular PCMM evaluation process can be grouped as follows:

- Level evaluations (numbers) plus associated metadata
- Supporting evidence plus supporting metadata
  - "The plural of 'anecdote' is not 'evidence'." – Alan Leshner, publisher of Science
- Risk characterization for intended application of capability plus supporting metadata
- QMU support plus supporting metadata

A.4. Flexibility Implies Heterogeneity

When all is said and done, the process diagram for PCMM implementation that reflects necessary conditions looks like:

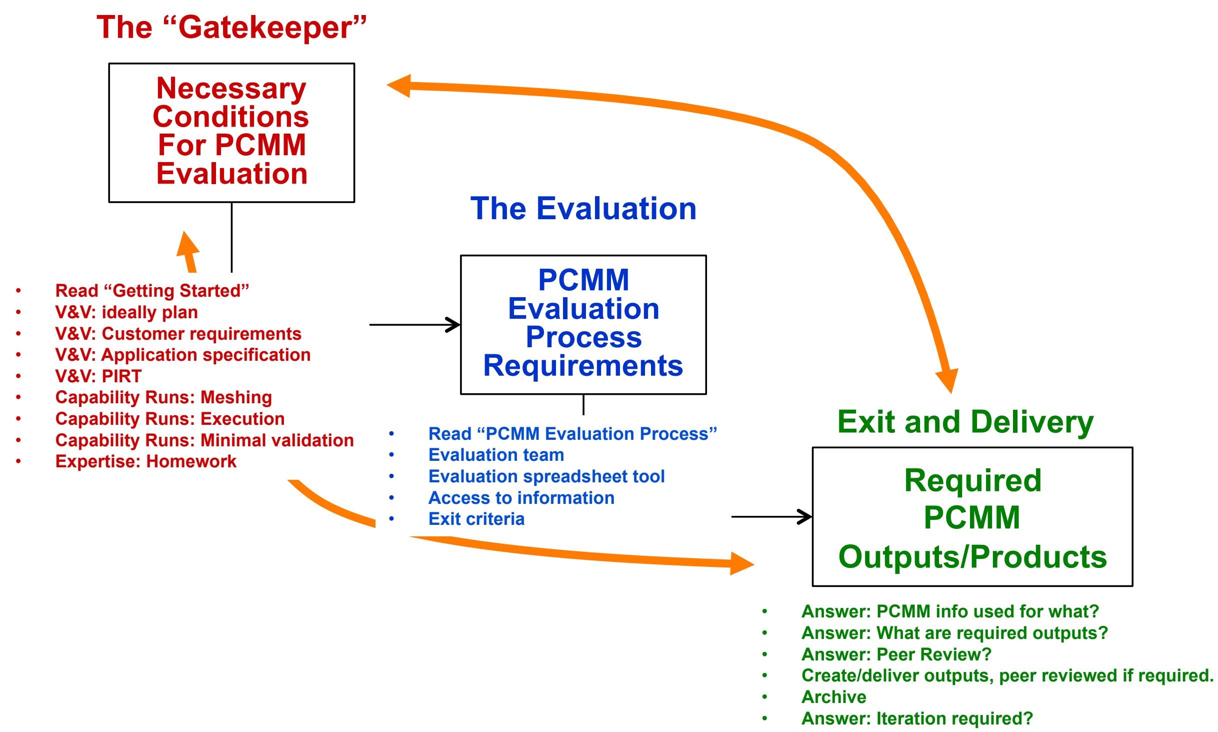


Figure A.3: PCMM Implementation Process with Necessary Conditions at Each Stage.

Nothing about the process suggested in Figure A.3 is dependent upon the specific form of the content of the PCMM. A longstanding issue has been to what extent PCMM content can be flexible, and customized for the purposes of specific applications, projects, and programs. The best current example of this issue is in the QASPR project, where two adaptations of the basic PCMM content (say as defined by Generation 4, Urbina et al., 2013) have been made, one to assess capability of the physical simulation component of QASPR, the other an integrated PCMM representing the combined physical and computational simulation QASPR "system" PCMM (QASPR Systems Engineering Team, 2012).

The process and necessary conditions suggested in Figure A.3 is suitable without modification for any of the PCMMs that QASPR is dealing with.

Content flexibility in PCMMs does raise the issue of heterogeneity of the information and resulting barriers to logical aggregation of that information. We do not state necessary conditions to be applied to this kind of aggregation problem other than to mention that adherence to the necessary conditions discussed in this document contributes to the ability to usefully and coherently aggregate such information. Beyond the formal necessary conditions of a PCMM implementation process, clearly the subject matter of the particular application area, and of the PCMM evaluation details, carries a large burden for successful aggregation.

This is one version of the more general problem of dealing with multiple PCMM evaluations, whether for multiple capabilities, or for multiple time-sequenced evaluations of the same capability. We discuss this problem further in the final section.

A.4. Conclusion: PCMM Evaluation is a Quality Process

The PCMM evaluation process is a quality process. Among other things, this means that it must be managed, that feedback must be collected, and that improvement procedures must be defined and executed. This document defines some necessary conditions for achieving quality in the PCMM evaluation process, but we doubt that these conditions are sufficient. Continued evolution of the quality underpinnings for a managed PCMM implementation at Sandia is the subject of continual experience with meaningful PCMM evaluations and the application of that information within NW.

An overall flow for the evaluation process given the necessary conditions we have suggested looks like that in Figure A.4 (or, alternatively, see Figure 4.1).

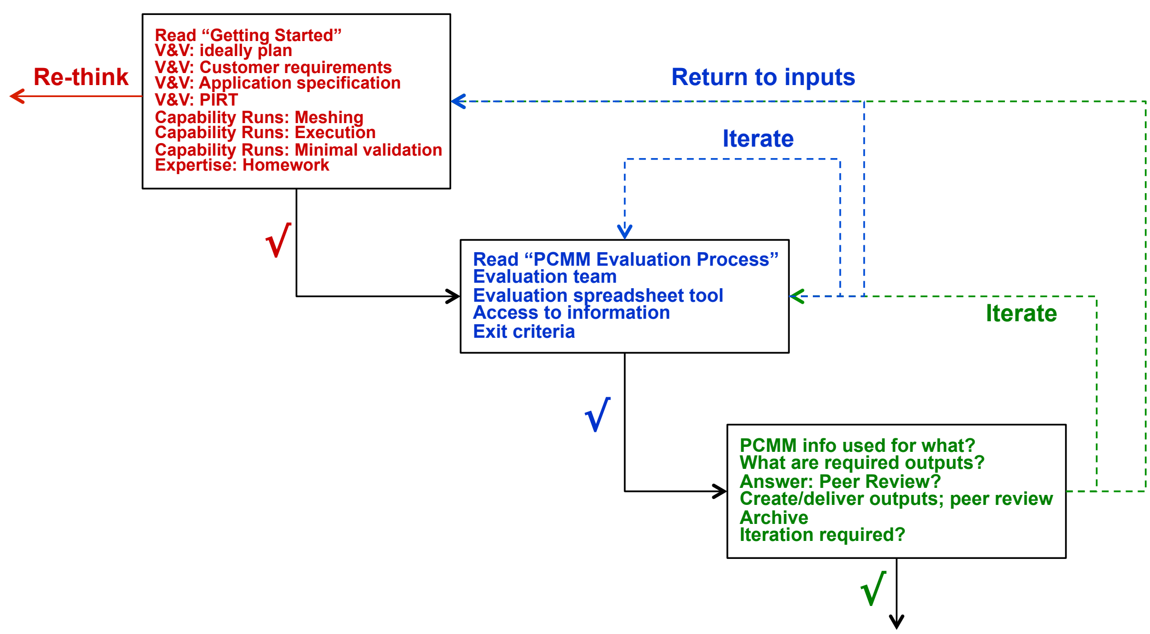


Figure A.4: The Flow of a Requirements-Based PCMM Evaluation Process.

A particular concern that we have not addressed in this document, nor in the broader Level 2 milestone that has triggered it, is the management of diverse PCMM evaluations. There are three natural sources of diversity in PCMMs that serve as a further challenge for managing the implementation process.

- Leveraging the flexibility in the content construct underlying the PCMM. We mentioned QASPR as an example of this phenomenon.
- Projects of sufficient complexity that more than one capability requires evaluation. This naturally arises in complex validation plans for an application like an abnormal environment for a specific tail number.
- More than one evaluation of a single capability. This might arise as at least a pair of evaluations – an "initial" evaluation and a "final" evaluation.

The general issues surrounding aggregating this diversity of PCMMs are complex. Desirable goals for a PCMM implementation include (1) consistent evaluation, (2) consistent communication and (3) consistent application of the results of evaluation. By ***consistent*** we mean roughly that the same evaluation process leads to the same results, the same understanding and the same communication. Underlying this is a further requirement to achieve a certain degree of validity and coherence of these evaluations. ***Valid*** in this context means roughly that the evaluation produces results that are correct, at least in the sense that there is sufficient confidence in them to use the evaluation substantively within the Sandia NW program. ***Coherence*** means roughly that the results of two or more separate evaluations can be meaningfully aggregated, as will be necessary for broad applications.

The necessary conditions we have defined in this document provide some service to achieving consistency, validity and coherence in PCMM evaluations. ***We do not claim that they are sufficient*** in and of themselves to achieve this to a satisfactory degree. More experience with systematic and managed PCMM evaluations will provide insight about this challenge.

Figure A.5 provides one way of looking at the aggregation problem.

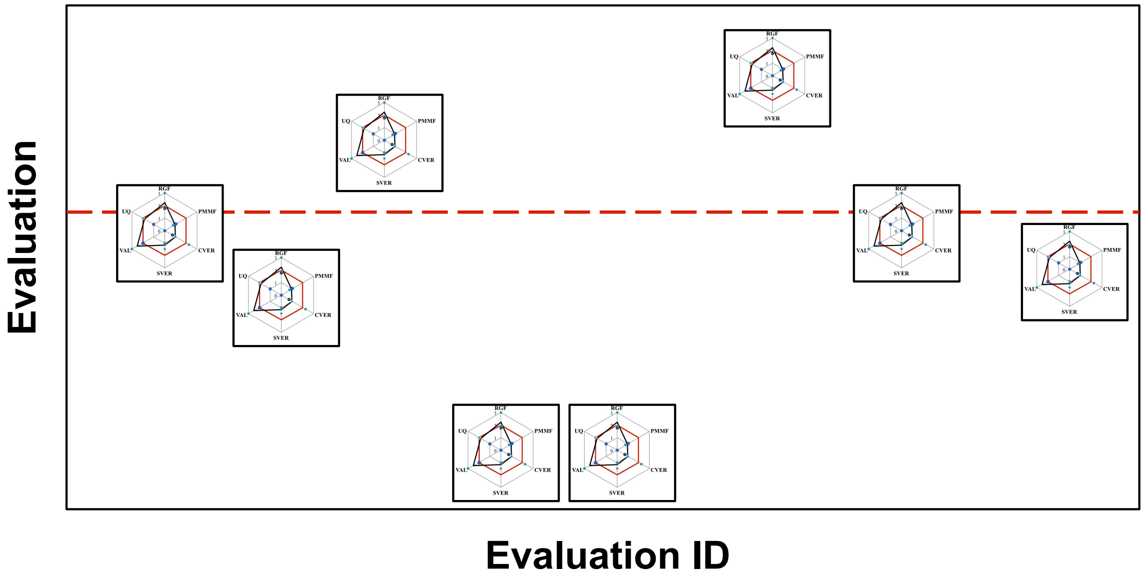


Figure A.5. A Series of Evaluation Outputs may be presented to a project or program. The form and content of this presentation should be driven by requirements of the people and/or programs that are using this information, and by evaluations that are consistent, valid, and coherent.

APPENDIX B: GENERATION 4 PCMM DETAILED ELEMENT DESCRIPTIONS

Earlier, we described the changes between the Generation 3 and Generation 4 PCMM, and the underlying logic. In this Appendix, we provide a list of the detailed descriptions of the Generation 4 table elements. Some users, especially those with greater familiarity of earlier PCMM generations, might find aspects of this summary to be useful in putting our earlier discussion in context.

The highest-level elements in the Generation 4 PCMM are:

CSC: Customer Specification Completeness
CVER: Code Verification
RGF: Representation and Geometric Fidelity
SVER: Solution Verification
VALH: Validation - Hierarchy
DATC: Experimental data for Constitutive Model Calibration
DATV: Experimental data for CompSim model validation
VALC: Validation – Component
UQ: Uncertainty Quantification

Sub-element descriptors for given levels are summarized next.

B.1. Customer Specification Completeness (CSC)

CSC1: Needs Descriptor

Level 0 Needs of customer incompletely and informally defined
Level 1 Needs defined with some feedback (informal) from the customer that the planned product addresses the needs
Level 2 Majority of needs defined with formal feedback from the customer that the planned product addresses the needs
Level 3 All needs defined with formal feedback from the customer that the planned product addresses the needs

CSC2: Domain of Application

Level 0 Domain of application incompletely and informally defined.
Level 1 Domain of application defined with some potential for domain creep for the model during development and analysis
Level 2 Domain of application formally and completely defined. Little potential domain creep for the model during development and analysis
Level 3 Domain of application fully defined with formal feedback for the users that the domain meets customer needs

CSC3: Domain of Validation

Level 0 Domain of validation incompletely and informally defined.
Level 1 Domain of validation defined with some potential for domain creep for the model during development and analysis
Level 2 Domain of validation formally and completely defined. Little potential domain creep for the model during development and analysis

Level 3 Domain of validation fully defined with formal feedback from the customer that the domains meets customer needs

CSC4: PIRT

Level 0 No PIRT exists that is relevant for the domain of application
Level 1 Most major effects/phenomena for domain of application identified and ranked
Level 2 Most major and some secondary effects/phenomena for domain of application identified and ranked
Level 3 All major and significant secondary effects/phenomena for domain of application identified and ranked

B.2. Code Verification (CVER)

CVER1: Apply Software Quality Engineering (SQE) processes

Level 0 No identified SQE process
Level 1 Code capability is managed to identified SQE practices
Level 2 Code capability is managed to identified SQE practices. SQE process is managed
Level 3 Code capability is managed to identified SQE practices. SQE process is managed and optimized

CVER2: Provide test coverage information

Level 0 No test coverage reported
Level 1 Regression testing and/or limited verification tests (VERTS) reported
Level 2 Regression testing and VERTS testing, with VERTS test feature coverage identified and categorized into 1- & 2- way feature coverage categories.
Level 3 Regression testing and VERTS testing, with VERTS test feature coverage identified and categorized into 1- & 2- way feature coverage categories. All the physics/engineering features required for the intended application are covered by the reported VERTS.

CVER3: Identification of code or algorithm attributes, deficiencies and errors

Level 0 Code/algorithm attributes, deficiencies and errors from VERTS not presented
Level 1 Code/algorithm attributes, deficiencies and errors from VERTS presented
Level 2 Code/algorithm attributes, deficiencies and errors from VERTS presented. Mapping to the intended application analyzed and presented.
Level 3 Code/algorithm attributes, deficiencies and errors from VERTS presented. Mapping to the intended application analyzed and presented. Impact on the intended application is analyzed and presented.

CVER4: Verify compliance to Software Quality Engineering (SQE) processes

Level 0 No assessment
Level 1 PCMM evaluation team self assessment of SQE process compliance
Level 2 External team review of SQE process compliance
Level 3 External team review and certification of SQE process compliance

CVER5: Technical review of code verification activities

Level 0 No review of code verification activities reported
Level 1 PCMM evaluation team reviewed code verification activities
Level 2 External (independent) review of code verification activities
Level 3 External (independent) review of code verification activities; certification of code verification activities

CSC5: Technical review of customer specifications

Level 0 No review of customer specifications activities reported
Level 1 PCMM evaluation team reviewed customer specifications activities
Level 2 External (independent) review of customer specifications activities
Level 3 External (independent) review of customer specifications; certification of customer specifications

B.3. Representation and Geometric Fidelity (RGF)

RGF1: Characterize Representation and Geometric Fidelity

Level 0 Model has no major or minor features present. Model is mainly "blobs" or point masses or stick-figure models or a curve fit of data.

Level 1 Relative to the actual system, the meshed model is a de-featured representation of it. Subject matter expertise may define this level of meshing and define the meaning of "major features," relationship to "actual system," etc.

Level 2 Relative to the actual system, the model has most of the major features. Component geometries are accurate meshed, but most fillets are omitted, bolts and holes may or may not be included, etc. Subject matter expertise may define this level of meshing and define the meaning of "major features."

Level 3 Model represents "as built" system including all "major features" and most "minor features." "All" defined by the evaluation team. "Most" defined by the evaluation team.

RGF2: Geometry sensitivity

Level 0 Simulation sensitivity to major features is not discussed

Level 1 Sensitivity of solution to major features is discussed

Level 2 Sensitivity of solution to SOME major features is quantified

Level 3 Sensitivity of solution to ALL major features is quantified

RGF3: Technical review of representation and geometric fidelity

Level 0 No review of representation/geometry reported

Level 1 PCMM evaluation team reviewed representation/geometry

Level 2 External (independent) review of representation/geometry

Level 3 External (independent) review of representation/geometry; certification of representation/geometry

B.4. Solution Verification (SVER)

SVER1: Quantify numerical solution errors

Level 0 Errors due to mesh size not examined

Level 1 Sensitivity, or robustness, of one or more computed quantities of interest (QoI) to mesh resolution and numerical solution parameters is studied and presented. Quantification as a computational "error" is not required or expected. Conclusions may be qualitative.

Level 2 Computational errors, due to mesh resolution and choice of numerical solution parameters, in one or more QoIs are estimated, analyzed and reported. The computational errors are interpreted as error bars on the computed results for the chosen QoIs. The question "What is the validity of these error estimates" is answered.

Level 3 Computational errors, due to mesh resolution and choice of numerical solution parameters, for all QoIs of the intended application are estimated, analyzed and reported. The computational errors are interpreted as error bars on the computed results for the chosen QoIs. The question "What is the validity of these error estimates" is answered.

SVER2: Quantify Uncertainty in Computational (or Numerical) Error

Level 0 Uncertainty in computational error estimate not examined

Level 1 Uncertainty of computational error estimates, of one or more computed quantities of interest (QoI) to mesh resolution and numerical solution parameters is examined and presented. Quantification as an uncertainty in computational "error" is not required or expected. Conclusions may be qualitative.

Level 2 Uncertainty of computational error estimates, due to mesh resolution and choice of numerical solution parameters, in one or more QoIs are estimated, analyzed and reported. The computational uncertainties are interpreted as variation in error bars on the computed results for the chosen QoIs. The question "What is the potential variation of these error estimates" is answered.

Level 3 Uncertainty of computational errors, due to mesh resolution and choice of numerical solution parameters, for all QoIs of the intended application are estimated, analyzed and reported. The uncertainty in computational error is interpreted as variations in the error bars on the computed results for the chosen QoIs. The question "What is the validity of the variations on the error estimates" is answered.

SVER3: Verify simulation input decks

Level 0 Inspection of input deck(s) for intended application not reported

Level 1 Inspection of input deck(s) for intended application by the analyst(s).

Level 2 Inspection of input deck(s) for intended application by one or more people other than the analyst(s). This is an "external" or "independent" review, but need not be performed as a formal "software inspection."

Level 3 Formal inspection of input deck(s) for intended application by an independent inspection team (one or more readers, scribe).

SVER4: Verify simulation post-processor inputs decks

Level 0 Inspection of post-processor input deck(s) for intended application not reported

Level 1 Inspection of post-processor input deck(s) for intended application by the analyst(s).

Level 2 Inspection of post-processor input deck(s) for intended application by one or more people other than the analyst(s). This is an "external" or "independent" review, but need not be performed as a formal "software inspection."

Level 3 Formal inspection of post-processor input deck(s) for intended application by an independent inspection team (one or more readers, scribe).

SVER5: Technical review of solution verification Descriptor

Level 0 No review of solution verification activities reported

Level 1 PCMM evaluation team reviewed solution verification activities

Level 2 External (independent) review of solution verification activities

Level 3 External (independent) review of solution verification activities; certification of solution verification activities

B.5. Validation – Hierarchy (VALH)

VALH1: Define a validation hierarchy

Level 0 No validation hierarchy is defined (presented, specified, identified, acknowledged, etc).

Level 1 One level (i.e. level refers to either material level, component level, subsystem level, etc) of a complete validation hierarchy, or an incomplete validation hierarchy, is defined (etc).

Level 2 More than one level (i.e. level refers to either material level, component level, subsystem level, etc) of an incomplete validation hierarchy is defined (etc).

Level 3 Complete validation hierarchy is defined.

VALH2: Apply a validation hierarchy

Level 0 No identified validation work is aligned with a validation hierarchy.

Level 1 Presented validation work aligns with this level.

Level 2 Presented validation work aligns with these levels.

Level 3 Presented validation work aligns with the complete hierarchy.

VALH3: Characterize completeness versus the PIRT

Level 0 No correlation of relevant material/physics models in the capability with the PIRT for the intended application is presented; alternative view - NO PIRT elements are present in the capability to be applied.

Level 1 Some relevant material/physics models in the capability are correlated with the PIRT for the intended application

Level 2 Most relevant material/physics models in the capability are correlated with the PIRT for the intended application

Level 3 All relevant material/physics models in the capability are correlated with the PIRT for the intended application

VALH4: Validation domain vs. application domain

Level 0 No assessment of the relationship (interpolation vs. extrapolation) of the validation domain to the application domain.
Level 1 Pure extrapolation of validation domain with application domain.
Level 2 Partial extrapolation of validation domain with application domain (i.e. mix of interpolation and extrapolation).
Level 3 Application domain contained by validation domain (i.e. pure interpolation).

VALH5: Technical review of validation

Level 0 No reported review of validation assessment
Level 1 Project team reviews validation assessment
Level 2 External team reviews validation assessment
Level 3 External team reviews validation assessment and certifies the assessment

B.6. Experimental data for Constitutive Model Calibration (DATC)

DATC 1: Available data

Level 0 Little or no data, constitutive model parameters somewhat arbitrarily set to values within reasonable ranges
Level 1 Sufficient data for calibration for major constitutive models, calibration performed using statistical techniques
Level 2 Sufficient data for calibration of major and some minor constitutive models, calibration performed using statistical techniques with estimates of calibration uncertainty
Level 3 Sufficient data for calibration of major and significant minor constitutive models, calibration performed using statistical techniques

DATC 2: Data Uncertainty Descriptor

Level 0 Potential sources and characterization of data uncertainties not addressed
Level 1 Most potential sources of data uncertainty identified with some quantitative characterization of these uncertainties
Level 2 Most significant sources of data uncertainty identified with characterization these uncertainties using statistical techniques
Level 3 All significant sources and types of data uncertainties are quantified using statistical techniques

DATC 3: Impact of incomplete data for constitutive models

Level 0 Impact of incomplete data ignored, associated constitutive model parameters arbitrarily set to values within reasonable ranges
Level 1 Impact of incomplete data based on judgment, associated constitutive model parameters set to values based on experience
Level 2 Impact of incomplete data based on judgment with supporting sensitivity analysis limited to critical constitutive model parameters, other parameters set to values based on experience
Level 3 Impact of incomplete data evaluated through comprehensive sensitivity analysis

DATC 4: Technical review of data

Level 0 No review of data used for constitutive models reported
Level 1 PCMM evaluation team reviewed sufficiently of data
Level 2 External (independent) review of sufficiently of data
Level 3 External (independent) review of sufficiently of data; certification of sufficiently of data

B.7. Experimental data for CompSim model validation (DATV)

DATV 1: Available Data

Level 0 Little or no data for validation

Level 1 Sufficient data for validation of high priority items identified in the PIRT, validation experiment somewhat characterized, validation performed with some estimate of uncertainty in the resulting differences between simulation and measured data

Level 2 Sufficient data for validation of high priority items identified in the PIRT, validation experiment well characterized, validation differences and uncertainty in these differences are characterized

Level 3 Sufficient data for validation of high and medium priority items identified in the PIRT, validation experiment well characterized, validation differences and uncertainty in these differences characterized

DATV 2: Data Uncertainty

Level 0 Potential sources and characterization of data uncertainties associated with the validation data not addressed

Level 1 Potential sources of data uncertainty identified with some statistical characterization these uncertainties

Level 2 Potential significant sources of data uncertainty identified with characterization of most of these uncertainties using statistical procedures

Level 3 All identified significant sources and types of data uncertainties are characterized using established statistical procedures

DATV 3: Validation Experiment Definition

Level 0 Experiment not adequately specified to develop a computation model of the experiment

Level 1 Experiment adequately specified to define a computation model of experiment with some assumptions required and with additional undocumented information required from the experimentalist

Level 2 Experiment adequately specified to develop a computation model of experiment with limited assumptions required and with limited undocumented information required from the experimentalist

Level 3 Experiment adequately defined with documentation adequate to develop the computation model of experiment requiring no additional input from the experimentalist

DATV 4: Technical review of data

Level 0 No review of validation experiments

Level 1 PCMM evaluation team reviewed validation experiments

Level 2 External (independent) review of validation experiments

Level 3 External (independent) review of completeness of validation experiments and results certified

B.8. Validation - Component (VALC)

VALC1: Quantify model accuracy (i.e., separate effects model validation)

Level 0 No validation assessment is performed (A gatekeeper here is familiarity with the SNL V&V program approaches to V&V).

Level 1 Imprecise validation conclusions: qualitative statements, in particular use of vugraph norms, no use of experimental uncertainty, expert opinion-centric validation statements, etc.

Level 2 Quantitative validation characterizations and conclusions. Some, but acknowledged INCOMPLETE characterization of uncertainty in experimental data and/or computational data. Quantitative validation statements are made and supported by presented quantitative

analysis. Pedigree information is presented, but may be incomplete. Expert opinion may also be presented.
Level 3 Quantitative validation characterizations and conclusions. Complete characterization of uncertainty in experimental data and computational data. Quantitative validation statements are made and supported by presented quantitative analysis. COMPLETE pedigree information is presented. Expert opinion may also be presented.

VALC2: Assess interpolation vs. extrapolation of physics and material model

Level 0 Interpolation and/or extrapolation of the application domain to the validation domain is not analyzed or presented.
Level 1 The application domain does not intersect the validation domain, so that the application is a full extrapolation beyond the validation domain.
Level 2 The application domain partially intersects the validation domain. Part of the application domain is therefore an interpolation of the validation domain, while the rest is an extrapolation.
Level 3 The application domain is entirely contained within the validation domain, so that the application is solely interpolation within the validation domain.

VALC3: Technical review of validation

Level 0 No reported review of validation assessment
Level 1 Project team reviews validation assessment
Level 2 External team reviews validation assessment
Level 3 External team reviews validation assessment and certifies the assessment

B.9. Uncertainty Quantification (UQ)

UQ1: Aleatory and epistemic uncertainties identified and characterized.

Level 0 No uncertainties identified/characterized
Level 1 Some uncertainties identified/characterized. Aleatory/epistemic separation (segregation, etc) not performed.
Level 2 Some uncertainties identified/characterized. Aleatory/epistemic separation (segregation, etc) is performed for these uncertainties.
Level 3 All significant uncertainties identified/characterized except for unknown/unknowns. Aleatory/epistemic separation (segregation, etc) is performed for these uncertainties.

UQ2: Perform sensitivity analysis

Level 0 No sensitivity analysis of uncertainties performed
Level 1 Qualitative sensitivity analysis of some uncertainties is performed
Level 2 Quantitative sensitivity analysis of some uncertainties is performed
Level 3 Quantitative sensitivity analysis performed for all characterized uncertainties

UQ3: Quantify impact of uncertainties from UQ1 on QoIs

Level 0 Impact reported for uncertainty characterization
Level 1 Impact reported for some uncertainty characterizations without aleatory/epistemic separation
Level 2 Impact reported for some uncertainty characterizations with aleatory/epistemic separation
Level 3 Impact reported for ALL uncertainty characterizations with aleatory/epistemic separation

UQ4: UQ aggregation and roll-up

Level 0 No aggregation or roll-up performed
Level 1 Aggregation or roll-up performed for some of the major uncertainties
Level 2 Aggregation or roll-up performed for most of the major uncertainties
Level 3 All significant sources of uncertainty are aggregated and rolled-up

UQ5: Technical review of uncertainty quantification

Level 0 No review of UQ is reported
Level 1 PCMM evaluation team reviewed UQ
Level 2 External (independent) review of UQ
Level 3 External (independent) review of UQ; certification of UQ

The current version of the PCMM tool that incorporates the elements described above is shown below:

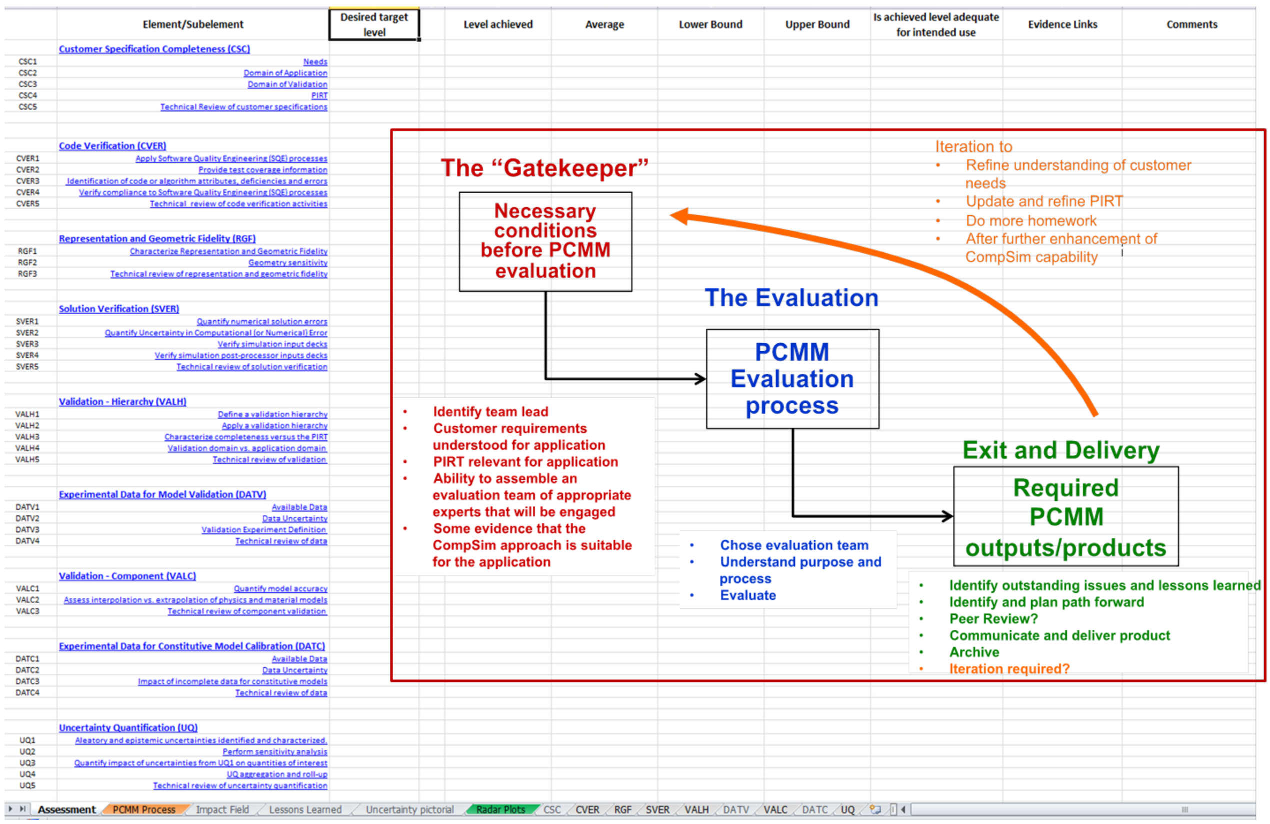


Figure B.1. Conceptual Summary of Current Version of PCMM Tool

APPENDIX C. PCMM ASSESSMENTS AND RAW FEEDBACK FROM FOCUS AREA EVALUATIONS

Chapter 4 provides a summary of PCMM assessments as well as the feedback obtained from the focus area evaluations. This appendix documents the feedback obtained on an application-by-application bases, as provided by the teams.

C.1. Aerosciences – B61 Captive Carry

Team

- Matt Barone, Srini Arunajatesan, Jeff Payne, Justin Wagner
- Facilitator – Ken Hu
- Stakeholder – Jerry Cap

PCMM Impact

- On the project:
  - Revealed a gap in the validation hierarchy
- On the way 1515 works:
  - Revealed the need for better documentation in all aspects of the project
    - Every activity has an owner – team needs to own docs
  - Forced team to think about important uncertainties
    - Served as a high quality project review
  - Improved communication within the team

PCMM Lessons Learned

- Team sees value in the process
- Concern that results are not "standardized"
  - Subjective – hard to compare projects
  - Inconsistent between elements/sub-elements
- Implementing a very formal credibility assessment is premature
  - We do not have formal processes for anything else – PIRTs, hierarchy, design of experiments, verification, validation, etc.

Feedback – Impressions

- Helpful in guiding discussions & self-assessing
- Consistency and education are key
  - Already too late for FY14 projects
  - Constant changes have really hurt adoption
- Too complicated, too subjective. How does each sub-element connect back to credibility?

Feedback – Process

- Grading scale is too coarse, especially at bottom
  - Does 0 mean nothing done, or nothing worthwhile?
  - Very discouraging

- Stakeholder needs a higher level view
    - Not enough interest/knowledge to set targets

Application:	Captive Carry Aerodynamics			*Dates:*	4/3/2013, 4/22/2013	
Team:	Arunajatesan, Barone Cap, Hu, Payne, Wagner					
	Element/Subelement	**Desired target level**	**Level achieved**	**Adequate for intended use**	**Evidence Links**	**Comments**
	Code Verification (CVER)					
CVER1	Apply Software Quality Engineering (SQE) processes	1	0.5			Close to 1, need documentation
CVER2	Provide test coverage information	1	0.5			
CVER3	Identification of code or algorithm attributes, deficiencies and errors	1	0.5			Need documentation
CVER4	Verify compliance to Software Quality Engineering (SQE) processes	1	0.5			Need documentation
CVER5	Technical review of code verification activities	1	0			
	Physics and Material Model Fidelity (PMMF)					
PMMF1a	Quantify model accuracy - RANS model predictions of unit level tests	2	1.5		Based on literature review	need documentation, no M&S UQ planned, Limitations of RANS are well known.
PMMF2a	rpolation vs. extrapolation - RANS model predictions of unit level tests	2	2		Geometries are different, but still relevant to application domain	
PMMF1b	Quantify model accuracy - LES model predictions of unit level tests	2	1.5		Based on literature review	Many LES studies of unit level problems.
PMMF2b	nterpolation vs. extrapolation - LES model predictions of unit level tests	2	2		Geometries are different, but still relevant to parts of the application domain	
PMMF1c	Quantify model accuracy - Rectangular empty cavity flow	2	1			No way to get to 3
PMMF2c	Assess interpolation vs. extrapolation- Rectangular empty cavity flow	2	2			
PMMF1d	Quantify model accuracy - Rectangular cavity with model elastic store	2	0			No way to get to 3
PMMF2d	polation vs. extrapolation - Rectangular cavity with model elastic store	2	2			
PMMF1e	Quantify model accuracy - Actual bomb bay empty cavity flow	2	0			Achieved levels to increase soon with CFD, no way to get to 3
PMMF2e	ess interpolation vs. extrapolation - Actual bomb bay empty cavity flow	2	2			
PMMF3	Technical review of physics and material models	2	1			
	Representation and Geometric Fidelity (RGF)					
RGF1	Characterize Representation and Geometric Fidelity	2	2			
RGF2	Geometry sensitivity	2	2		Specific to the F35, based on Srini's experience, did M&S w & w/o major features	
RGF3	Technical review of representation and geometric fidelity	2	1			Need feedback from Jerry Cap --> 2
	Solution Verification (SVER)					
SVER1	Quantify numerical solution errors	1	1			Active research area
SVER2	Quantify Uncertainty in Computational (or Numerical) Error	1	1			Active research area
SVER3	Verify simulation input decks	2	2		Checked by other team members	For troubleshooting, not a formal practice.
SVER4	Verify simulation post-processor inputs decks	1	1		Have done code-to-code comparison	Code is very simple
SVER5	Technical review of solution verification	2	1			
	Validation (VAL)					
VAL1	Define a validation hierarchy	3	2			
VAL2	Characterize completeness versus the PIRT	3	3			
VAL3	Apply a validation hierarchy	3	3			
VAL4	Validation domain vs. application domain	2	2			
VAL5	Technical review of validation	2	1			
	Uncertainty Quantification (UQ)					
UQ1	Aleatory and epistemic uncertainties identified and characterized.	2	1			
UQ2	Perform sensitivity analysis	1	0.5			
UQ3	Quantify impact of uncertainties from UQ1 on quantities of interest	1	0			
UQ4	UQ aggregation and roll-up	1	0			
UQ5	Technical review of uncertainty quantification	2	0			

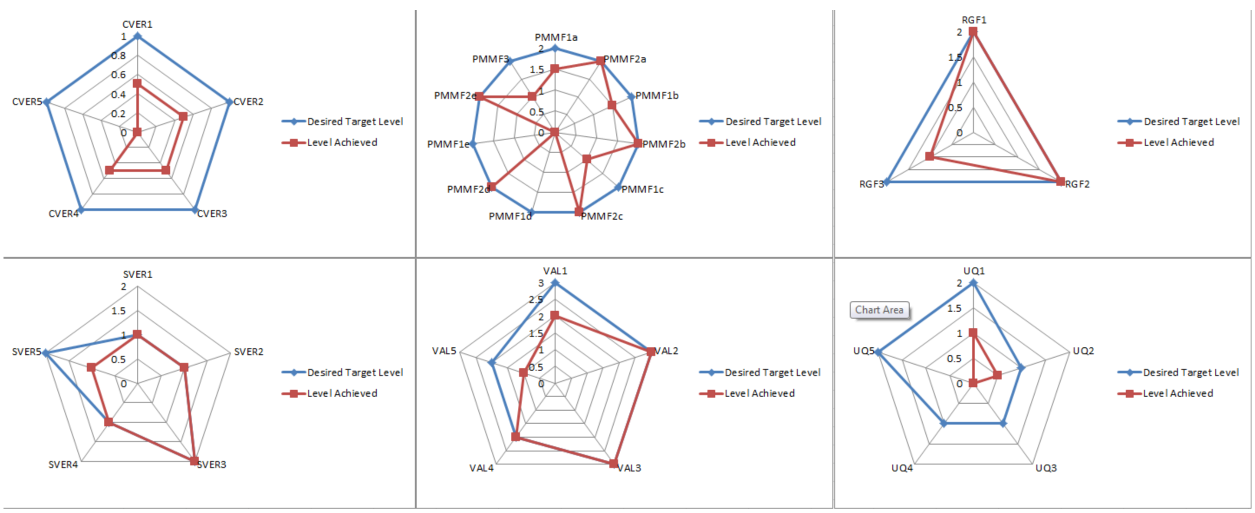


Figure C.1: Aeroscience-B61 Captive Carry: PCMM Assessment Sheet and Kiviat Plots.

C.2 Thermal-Mechanical Integrated Safety Theme

Team

- Project Lead: Kevin Dowding (1544)
- Stakeholder: Jim Nakos (2129)
- Code Developer: Sam Subia (1541)
- Analysts: Dean Dobranich (1514), Roy Hogan (1514), Nick Francis (1514)
- Experimentalist: Jill Suo-Anttila (1532)
- PCMM SME: George Orient (1544)

Project Summary: Analysis of full system safety for thermally-driven events

Lessons Learned

- Managing evidence
  - Not achieved during the exercise
  - Need a formal repository for
    - Managing evidence of current PCMM
    - Body of evidence to be referenced in future PCMM's (… we know this CompSim process model works…)
- Need to communicate clearly that PCMM is for a particular application. This focus was occasionally lost
- Multi-physics and multi-component applications
  - Difficult to aggregate resulting in numerical scores with low confidence. More formality may be required (which is contradictory to the general desire for simplification)
  - Alternative: group of 2-3 phenomena and/or components; perform multiple PCMMs
- Scheduling, conducting meetings
  - Must have strong commitment from management; key contributors whose input is critical may not be willing participants initially
  - Scheduling meetings for a large team is a challenge; plan ~ 1 month lead time
  - Even with the meetings on the calendars balanced representation not always achieved
- The customer
  - May not be willing to state what the desired target level is; deferring to SME
  - Need to find a way to keep him/her engaged
- The spreadsheet tool
  - Generally well accepted
  - Must spend a full meeting going through it and explain - hard to hold the attention of the audience
- PIRT with sufficient granularity and currency may not exist even for applications that would otherwise warrant a PCMM. Resources may need to be allocated to generate a good PIRT before PCMM

- Different definition for each sub-element is taxing. A more uniform set of criteria is desired
- Numerical scores need verbal representations uniform across the elements/sub-elements
- Found relatively large scatter in scores for sub-elements evaluated by multiple team members. Due to team dynamics and/or the large number of sub-elements consensus was reached in an ad hoc fashion
- Some confusion why we need PCMM when we already have PIRT identifying gaps

Suggested Improvements

- PCMM is recognized as useful for smaller projects as well; need PCMM “lite”
- Bring back the spider chart in some form. The team liked its visual impact
- Include links to referenced documents (SNL ASC SQE Guidance, for example)
- The SVR elements seems weak; includes sub-elements that are at much lower granularity of the CompSim workflow than those of other elements

Path forward

- We need real case studies where the PCMM is used both as a planning tool and as an assessment of current state
- The usefulness of PCMM to product teams needs to be demonstrated so that team participants are willing to put in real effort
- Opinions about PCMM are quite polarized; didn’t see too many people that were neutral.
    - Consider a PCMM showcase newsletter or other mechanism to spread the word
    - Organize short PCMM training available to everyone

Application:	Abnormal Thermal Environment, WL-SL Race					
	Element/Subelement	**Desired target level**	**Level achieved**	**Is achieved level adequate for intended use**	**Evidence Links**	**Comments**
	Code Verification (CVER)					
CVER1	Apply Software Quality Engineering (SQE) processes	2	2	yes	- From Sierra developer team	
CVER2	Provide test coverage information	2	1.5	yes	feature coverage tool	
CVER3	Identification of code or algorithm attributes, deficiencies and errors	2	0	no	- Memo from Sam S.	
CVER4	Verify compliance to Software Quality Engineering (SQE) processes	2	2	yes		
CVER5	Technical review of code verification activities	2	0	no		
	Physics and Material Model Fidelity (PMMF)					
PMMF1	Characterize completeness versus the PIRT	2	1.5	yes	-SAND2012-0919	
PMMF2	Quantify model accuracy (i.e., separate effects model validation)	2	1.25	yes	-Foam can experiments and models	
PMMF3	Assess interpolation vs. extrapolation of physics and material model	2	1.5	yes	All small-scale, not system level	
PMMF4	Technical review of physics and material models	1.5	0.5	yes		
	Representation and Geometric Fidelity (RGF)					
RGF1	Characterize Representation and Geometric Fidelity	2	1.75	yes	experience	
RGF2	Geometry sensitivity	1	1	yes		
RGF3	Technical review of representation and geometric fidelity	1.5	0.75	yes		
	Solution Verification (SVER)					
SVER1	Quantify numerical solution errors	2	1.5	yes	Model under development, on-going	
SVER2	Quantify Uncertainty in Computational (or Numerical) Error	1	0	no	work documents	
SVER3	Verify simulation input decks	1.5	1	yes		
SVER4	Verify simulation post-processor inputs decks	1	0.5	yes		
SVER5	Technical review of solution verification	2	0	no		
	Validation (VAL)					
VAL1	Define a validation hierarchy	2	2	yes	- SAND2012-0919	
VAL2	Apply a validation hierarchy	2	0.5	yes	- Qalification plan completed, tests	
VAL3	Quantify physical accuracy	2	0.5	maybe	on-going	
VAL4	Validation domain vs. application domain	3	0.5	yes		
VAL5	Technical review of validation	2	0.5	yes		
	Uncertainty Quantification (UQ)					
UQ1	Aleatory and epistemic uncertainties identified and characterized.	2	1	yes		
UQ2	Perform sensitivity analysis	2	0.5	no		
UQ3	Quantify impact of uncertainties from UQ1 on quantities of interest	2	0.5	maybe		
UQ4	UQ aggregation and roll-up	2	0.5	yes		
UQ5	Technical review of uncertainty quantification	2	0.5	no		

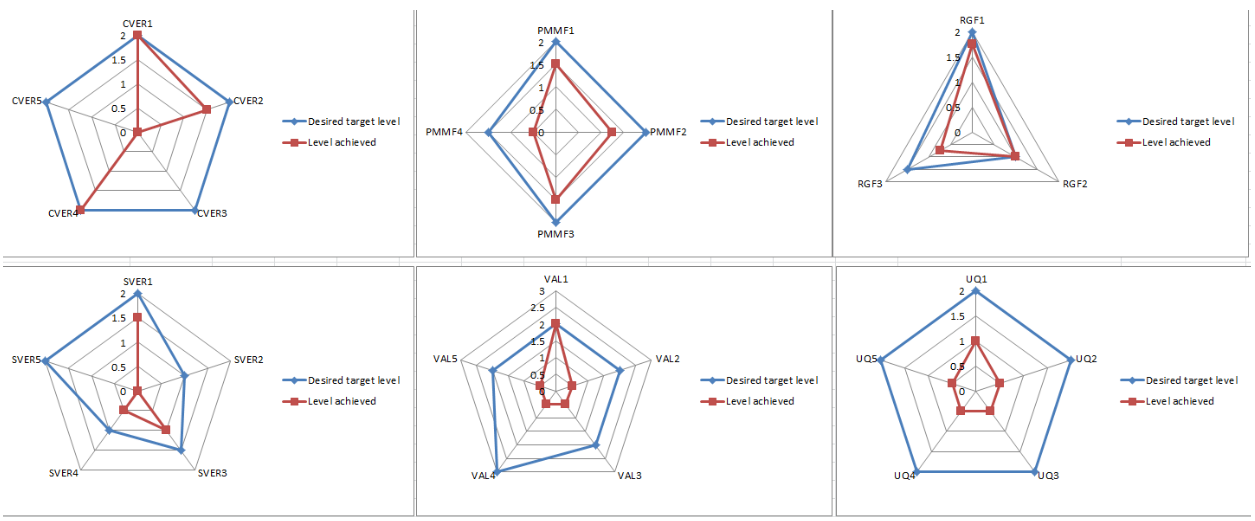


Figure C.2: Thermal-Mechanical Integrated Safety: PCMM Assessment Sheet and Kiviat Plots.

C.3 QASPR: Xyce & Charon

Capability

Assessing the maturity of the III-V Npn model predictability within a threat environment for the Xyce and Charon codes. In particular, the device model for the MESA developed Npn InGap/GaAs 10x50 discrete

Team

- For an assigned element, participant may not be required to give feedback on every piece of that element - Code team or experiments specified in parenthesis
    - Len Lorence – stakeholder
        - None
    - Joseph Castro – PCMM assessor/moderator
        - (Xyce/Charon) All in assessor/moderator role
    - Vicente Romero – PCMM SME
        - (Xyce/Charon) UQ, VAL (All in SME role)
    - Brian Rutherford – UQ SME/analyst
        - (Xyce/Charon) UQ, VAL
    - Biliana Paskaleva – V&V analyst
        - (Xyce/Charon) UQ, VAL, SVER, PMMF, CVER
    - Charlie Morrow – Experimentalist Liaison
        - (Experiments) UQ, VAL
    - Chuck Hembree – Circuit Analysts
        - (Xyce) UQ, VAL, SVER, PMMF
    - Alan Mar/Henok Abebe – Calibration Analysts
        - (Xyce) UQ, VAL, SVER
    - Gary Hennigan – Charon code lead/developer
        - (Charon) All
    - Eric Keiter – Xyce code lead/developer
        - (Xyce) All

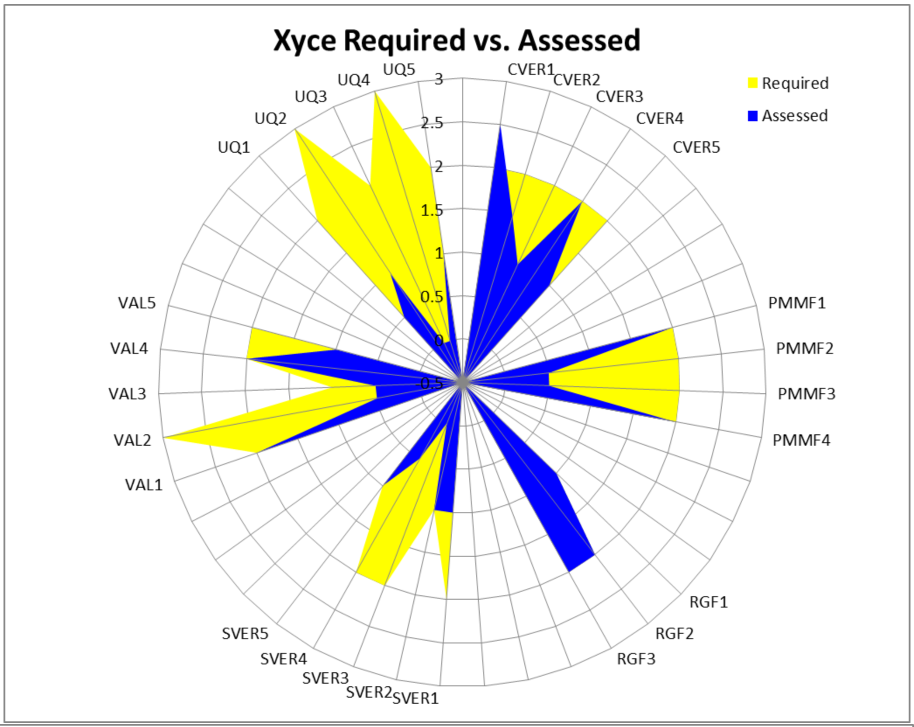
Feedback

- There needs to be further clarification of some of the sub-element descriptions
    - Particularly within the UQ section
    - Some elements seemed to overlap one another
    - Specifics were sent to the PCMM L2 milestone team
- Overall the Excel Tool was judged to be very beneficial
    - Captures a great deal of detail
    - Can be overwhelming at times during the assessment – may create a reduced version for real time assessment
    - Great organization tool for the assessor
- PCMM assessment generated discussion across different teams
    - Team consisted of analysts, developers, and experimentalists
    - Example discussion: For qualification, solution verification will be critical (e.g., input/output file verification) and will need to be better formalized –

analysts are now aware of this and QASPR will need to better formalize this workflow
    - Need another assessment iteration to determine value of some members on the larger team
    - Experimentalists seemed to be the odd man – but may be due to QASPR development of Physical Simulation PCMM which may have captured the experimental elements

Path Forward

- We'll review PCMM elements with PCMM SME prior to assessment to insure all the descriptors are well understood
    - This was done in real time during the assessment which caused delays
- The Excel Tool will be used for future assessments
    - Again, great organization tool for the assessor
    - If QASPR creates web forms of it's other assessment tools – may do the same with this tool
- Evidence may be moved and maintained on a SharePoint site
    - Currently on dpnet2 and only accessible to QASPR team members
    - May link to web tool, if developed
- Will do another iteration of the assessment with the larger group
    - Continue to schedule review to minimize the time required by participants based on roles
- Next assessment will focus on PnP devices and potentially circuits
    - An update of the Npn capability should also be done



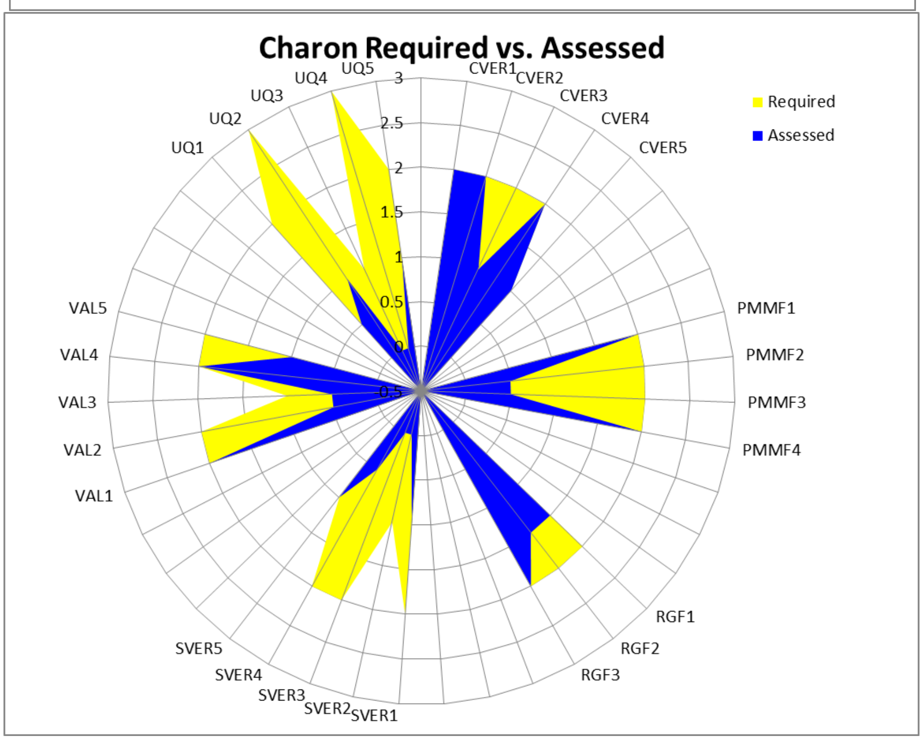


Figure C.3: QASPR: Kiviat Plots.

C.4 Neutron Tube

Team

- Project Lead: Lawrence Musson (1425)
- Stakeholder: Dan Rader (1513)
- Customer: Allen Roach
- Code Developer: Lawrence Musson (1425) analyst/developer
- Analysts: Matt Hopkins (1516) analyst/developer
- PCMM SME: Angel Urbina (1544)

PCMM Lessons Learned

- Team sees value in the process
- Customer involvement is absolutely essential for this process to make any sense.
- PCMM tool is critical to doing assessment.

Feedback

- Lack of clarity – some of the wording still ambiguous
- Glossary of terms is needed
- Should PI's be required to attend a V&V Primer type class
- Too complicated, too subjective. Some examples of what is being asked to assess could be useful
- Too much rigor for the intended use/value of this effort
- Too costly to be implementable across the board.

Dan Rader (ASC/RTBF Stakeholder)	Classification Level:				
Level could be 0 to 3, integer values not required					
Aleph	Date:	6/5/2013			
Angel Urbina					
Ion Extration/Beam Focusing					
Element/Subelement	**Desired target level**	**Level achieved**	**Is achieved level adequate for intended**	**Evidence Links**	**Comments**
Code Verification (CVER)					
Apply Software Quality Engineering (SQE) processes	1	0.5		version control, regression testing, not documented	
Provide test coverage information	2	1.5		regression testing, some verts	
Identification of code or algorithm attributes, deficiencies and errors	1	1			
Verify compliance to Software Quality Engineering (SQE) processes	1	1			
Technical review of code verification activities	1.5	1			
Physics and Material Model Fidelity (PMMF)					
Characterize completeness versus the PIRT	0	0		prt (dated) exists somewhere	
Quantify model accuracy (i.e., separate effects model validation)				SAND2011-7969	
Assess interpolation vs. extrapolation of physics and material model	3	2			
Technical review of physics and material models	2	1.5			
Representation and Geometric Fidelity (RGF)					
Characterize Representation and Geometric Fidelity	3	2.5		Geometry is simple. Model contains sharp corners. Corners were studied previously. SAND2011-7969	
Geometry sensitivity	2	1		SAND2011-7969	
Technical review of representation and geometric fidelity	2	1			
Solution Verification (SVER)					
Quantify numerical solution errors	3	2.5		Has been done for sheath--presented at ICOPS	
Quantify Uncertainty in Computational (or Numerical) Error	2	2			
Verify simulation input decks	2	2		Has been shared amongst analysts	
Verify simulation post-processor inputs decks	2	2			
Technical review of solution verification	2	2			
Validation (VAL)					
Define a validation hierarchy	2	2		Plan to make a plan	
Apply a validation hierarchy	3	3		activities assigned	
Quantify physical accuracy	2	1			
Validation domain vs. application domain	3	3		consultation coming	
Technical review of validation	2	1.25		in planning	
Uncertainty Quantification (UQ)					
Aleatory and epistemic uncertainties identified and characterized.	2	1			
Perform sensitivity analysis	2	2			
Quantify impact of uncertainties from UQ1 on quantities of interest	2	1			
UQ aggregation and roll-up	2	1			
Technical review of uncertainty quantification	2	0.5			

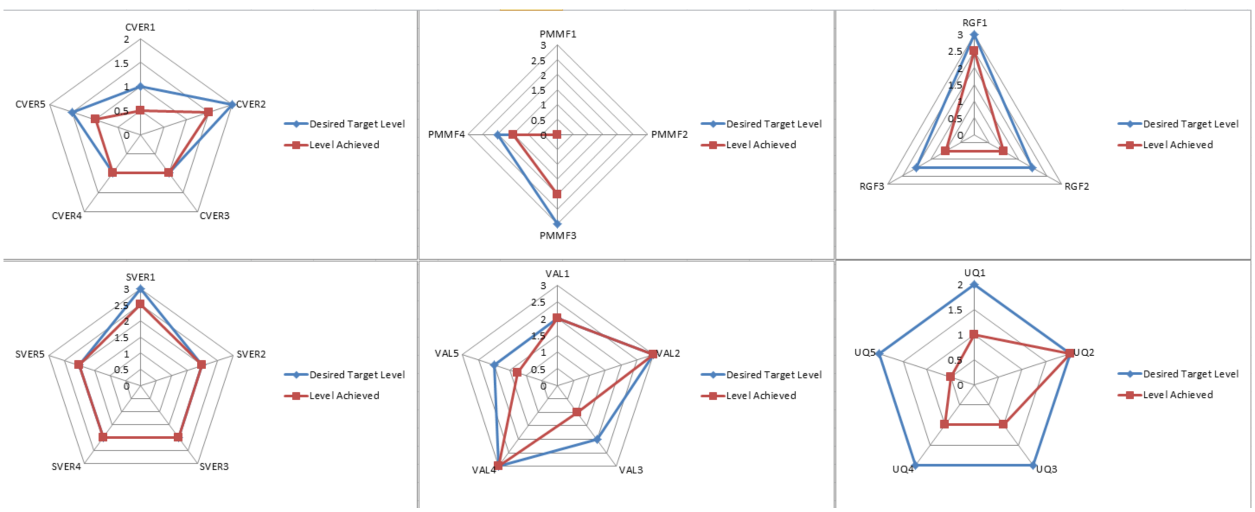


Figure C.4: Neutron Tube: PCMM Assessment Sheet and Kiviat Plots.

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