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Predictive Capability Maturity Model (PCMM)

Angel Urbina, Pat Knupp and Laura Swiler
Sandia National Laboratories
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Outline

- **Overview**
  - Based on concepts developed under DOE's Advanced Simulation and Computing (ASC) Program for Nuclear Weapons
- **An Example – NEAMS-Waste**
- **Our plan to implement PCMM in NEAMS**
- **Summary/Path forward**

PCMM what is it and what is not

PCMM is not a Number or a Score

PCMM *is* a Communication Tool That *Must* Include a Discussion of the Supporting Evidence

PCMM=1.22

PCMM is a Tool for Managing Risk in the Use of Modeling and Simulation

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Predictive Capability Maturity Model (PCMM)

for Computational Modeling and Simulation (M&S)

- **PCMM components:**
  - M&S elements
  - Maturity levels
  - Assessment criteria
- **It is application specific.**
- **It helps assess the current state of predictive capability.**

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SAND2007-5948

A tool for assessing and communicating progress in predictive capability.

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for Computational Modeling and Simulation (M&S)

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Elements are important not because they are on the table.

PCMM Overview

- PCMM is in the service of organizing evidence to help tell the modeling and simulation (M&S) story.
- PCMM table describes what activities within each element are undertaken at each of the levels of maturity.
- Target levels of maturity can be established based on the intended application.

The assessment is to inform what level has been achieved compared to the desired level, to help prioritize the VU activities & to allocate resources.

PCMM Elements

Representation and Geometric Fidelity
What features are neglected because of simplifications or stylizations?

Physics and Material Model Fidelity
How fundamental are the physics and material models and what is the level of model calibration?

Code Verification
Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?

Solution Verification
Are numerical solution errors and human procedural errors corrupting the simulation results?

Model Validation
How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?

Uncertainty Quantification and Sensitivity Analysis
How thoroughly are uncertainties and sensitivities characterized and propagated?

These elements need to be customized for a given application.

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Maturity Levels

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- **Level 0: Minimal M&S impact (e.g., scoping studies)**
- **Level 1: Some M&S impact (e.g., design support or qualification test support)**
- **Level 2: High M&S impact (qualification decision support)**
- **Level 3: Decision making based predominately on M&S (dominant basis for qualification or certification)**

The goal is not to grade.
It is to inform and communicate.

Solution Verification Element

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Solution verification is considered an important element in M&S and thus put on the table.

The criteria associated with this element needs to be relevant to the given application.

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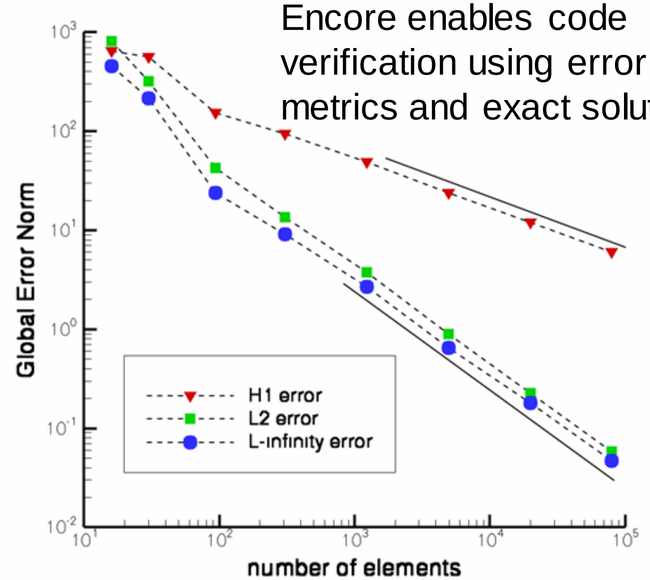
We can be more objective on the verification rows of PCMM through:

- Better error estimators and adaptive schemes,
- Better feature coverage measuring capabilities for code verification
- We developed capabilities in that area



Encore supports the code and solution verification elements in PCMM.

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What does PCMM do?

- **Use PCMM to:**
  - (1) help collect the right kind of evidence,
  - (2) organize the evidence to tell the story

- **VU *evidence* must exist before it can be assessed.**
  - The IPSC's generate the evidence.
    - What evidence will they generate?
    - Will it tell a coherent story?
    - Will it be adequate? (History tells us that probably it will not.)

- **This is where PCMM implementation comes in.**

Implementation of the PCMM for NEAMS

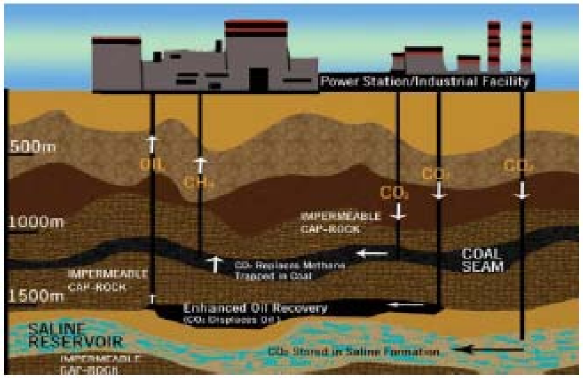
Suggested Implementation Steps:

1. Identify as clearly as possible, the type of evidence that should be generated (for different levels of maturity).
   - See next slides for an example

2. Generate the evidence

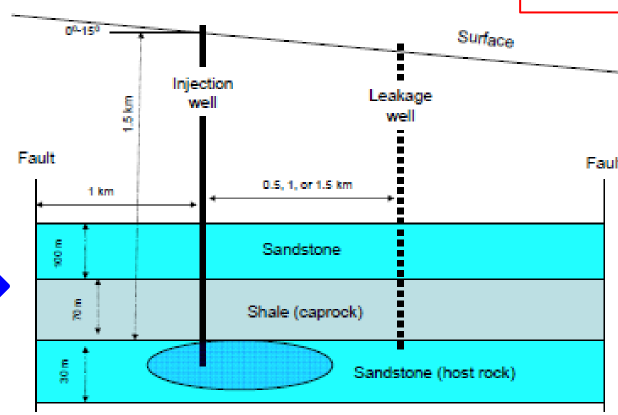
3. Manage the evidence
   - Document it
   - Add it to a evidence management system (just like QA evidence)
   - Report evidence status periodically

NEAMS – Hypothetical Example



Assess this M&S activity using PCMM

Create a model (M1) of application of interest

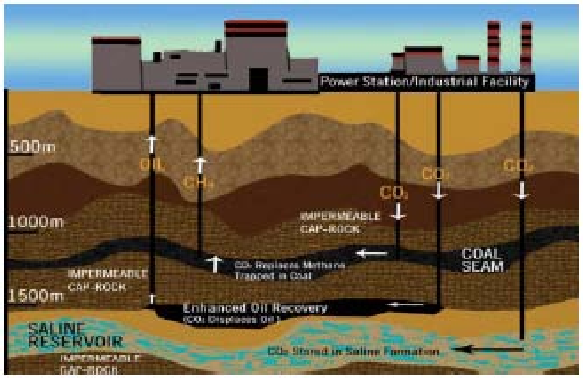


Run model (M1) using TOUGH2 V.2 to get output

Analysis Code: TOUGH2 V.2

Desired output

NEAMS – Hypothetical Example w/PCMM elements



Example courtesy of Wang et al, 2010

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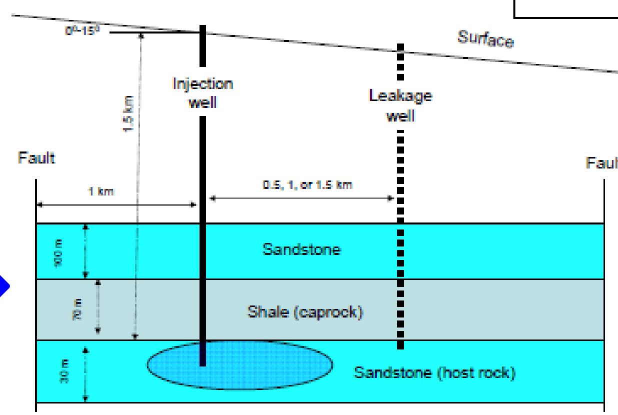

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Example: Assessment Table for the Solution Verification Row

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Practice / M	3
I/O Verifica	esults pendently roduced
Numerical I Parame Sensitiv	stematic stigations RQ sens.
Mesh Refin Study	s definitely mptotic.
Error Estim	mates & r Bars for SRQ's

Example: Assessment Table for the Solution Verification Row

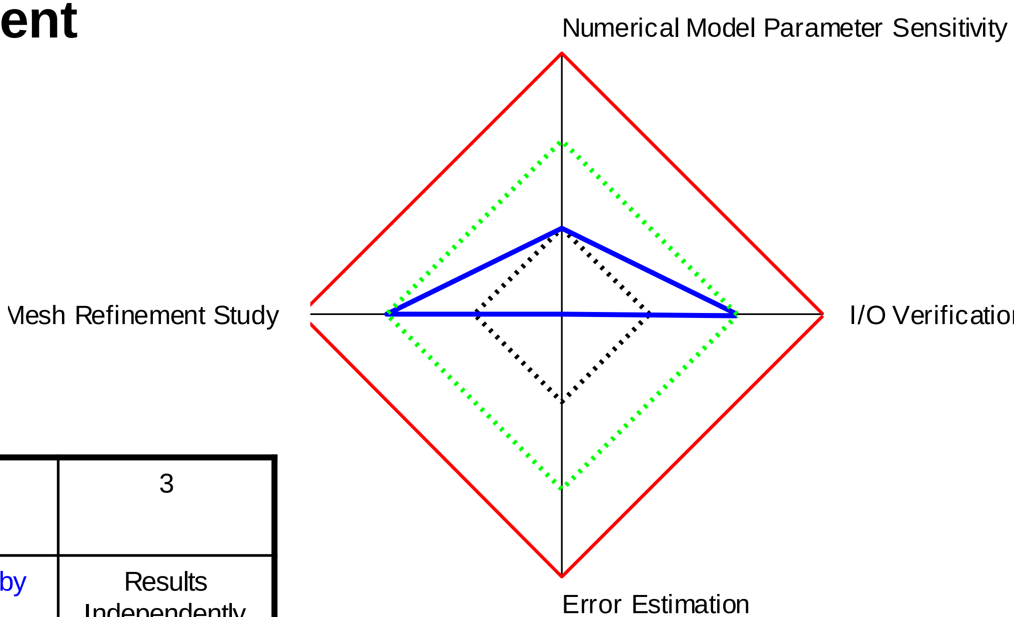
Assess the current "maturity status" of Solution Verification
- for a particular numerical solution related to a NEAMS Problem

Table shows the kinds of evidence needed and the current status

Practice \ Maturity	0	1	2	3
I/O Verification	No Inspection	Inspection by Analyst	**Inspection by Peers**	Results Independently Reproduced
Numerical Model Parameter Sensitivity	Little or None	**Informal Investigations**	Systematic Investigations	Systematic Investigations of SRQ sens.
Mesh Refinement Study	None	In progress or soln. non-asy.	**SRQ's possibly Asymptotic**	SRQ's definitely Asymptotic.
Error Estimation	**None**	Implementation in progress	Estimates for some SRQ's	Estimates & Error Bars for all SRQ's

Example: Assessment Table for the Solution Verification Row

- **Solution verification assessment based on:**
  - Running the model using the TOUGH2 V2 code and
  - Based on a specific numerical solution

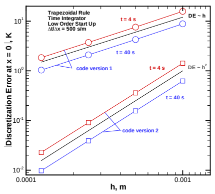


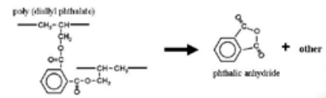
Maturity / Practice	0	1	2	3
I/O Verification	No Inspection	Inspection by Analyst	Inspection by Peers	Results Independently Reproduced
Numerical Model Parameter Sensitivity	Little or None	Informal Investigations	Systematic Investigations	Systematic Investigations of SRQ sens.
Mesh Refinement Study	None	In progress or soln. non-asy.	SRQ's possibly Asymptotic	SRQ's definitely Asymptotic.
Error Estimation	None	Implementation in progress	Estimates for some SRQ's	Estimates & Error Bars for all SRQ's

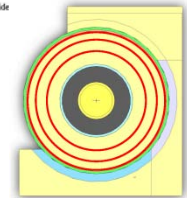
Radar plot is a graphical way to visualize PCMM assessment.

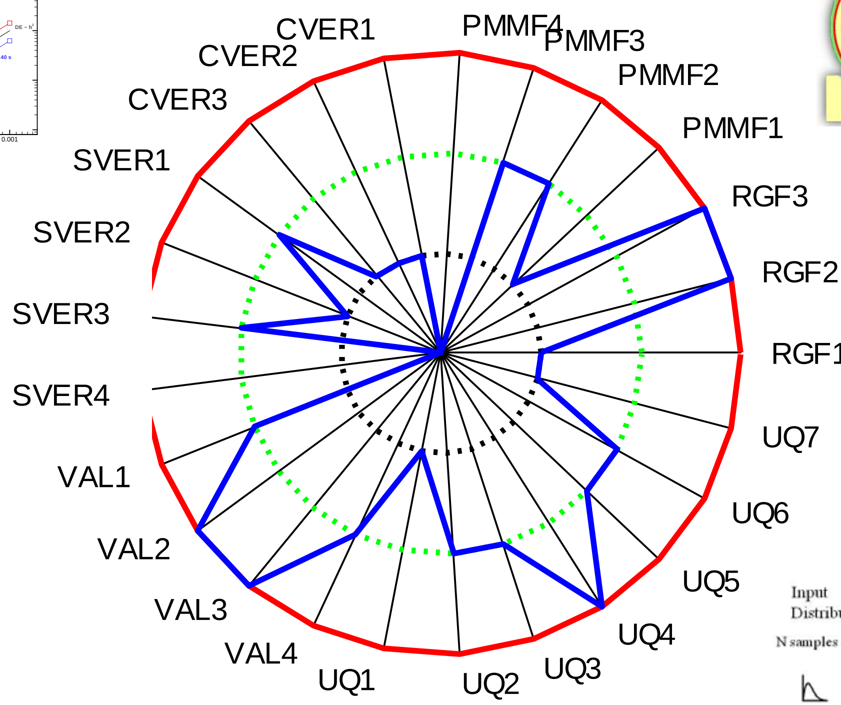
Similar assessment tables are created for the other elements

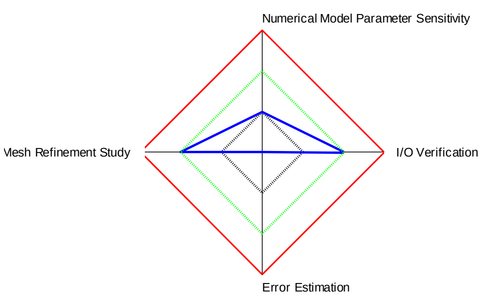
PCMM Must Include the Supporting Evidence

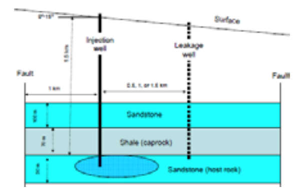


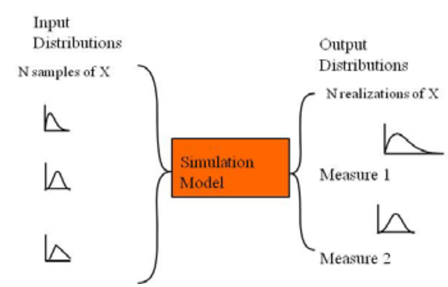












PCMM is intended to make people think about VU in a systematic way and to organize their evidence to tell a story.

How We Will Do This in FY11

1. **Work closely with the Waste IPSC**
   - Develop the PCMM evidence tables for PA, high-fidelity, and sub-continuum simulations,
   - Ensure VU evidence requirements get into Evidence Management Software
   - Focus on the identified Challenge Problem (specific codes, solutions, models)
   - Produce complete collection of VU status tables for Challenge Problem
   - We do not need final Challenge Problem results in order to perform this study
2. **Modify our thinking as we learn more about how this works in practice**
3. **Solicit feedback and communicate with the other IPSC's with eye toward future implementations**
4. **Collaborate with Peter Schultz' PCMM effort on sub-continuum to ensure that this is part of the implementation.**

Summary/Path Forward

- **Presented PCMM as it currently exists and some modifications to make it more NEAMS-applicable**

- **NEAMS-Waste - VU Support**
  - Developing a PCMM-like set of tables & VU evidence generators
  - Coordinating with Waste IPSC evidence management software development effort to ensure that the PCMM approach is integrated into the software
  - Performing an initial VU assessment when one or more Waste IPSC problem effort is “assessable”.

- **Support Reactors IPSC in developing a V&V plan**