Approved - 6 Aug 01

Minutes of the USACM Committee on Verification and Validation in Computational Solid Mechanics

Disney World Dolphin Hotel, Orlando FL
Friday 10 November 2000

Highlights

The meeting was called to order at 9:00 AM by Len Schwer. Also in attendance were Ren-Jye Yang, Dale K. Pace, Jim Gran, Tinsley Oden, Tom Paez, Mark Shephard, Ted Belytschko, Tim Hasselman, Paul Senseny, JN Reddy, Don Simons, John Fortna, Bill Oberkampf, Mike Giltrud, Hans Mair, Alan Browne (for Bob Lust) , and Umesh Chandra (as a guest).

Len Schwer gave an introductory presentation. He described the presentation he and Bill Oberkampf made to the ASME Board on Performance Test Codes (BPTC) the previous day, and reported that the Board had approved the petition to make the V&V in CSM Committee an ASME Standards Committee.

Bill Oberkampf gave a brief review of the process leading to the publication of the AIAA guidelines for V&V in CFD.

The remainder of the meeting was led by Hans Mair. He went through the most recent draft outline (Version 2.1) for the Guide for V&V in CSM. Numerous comments and discussions ensued. A copy of the outline appears below, with comments included as annotations in italics.

The meeting adjourned at 1:00 PM.

Action Items

1. **Tinsley Oden** will prepare a brief description of the applicability, maturity, and directions of a posteriori error estimation, as would apply to a guideline document for V&V.

2. **Dale Pace**: will discuss an updated version of the Sargent Circle with Sargent. We need a very simple graphic that illustrates the verification and validation processes, and their relationship to the real world, the mathematical model, and the computerized realization of that model. More detailed graphical representations should be based on the most simple version. Another version of the graphic would include the calibration and prediction processes.

3. **Len Schwer** will propose an official name for the Committee.

4. **Len Schwer** will discuss with Jack Burns, our liaison to the BPTC, if a new category of documents (Series Number) is needed, since it is not clear that the product of the Committee's work should be under an existing publication series.

5. **Len Schwer** will draft and submit to BPTC a recommended charter for the Committee.

6. **Hans Mair** will update the draft outline in accordance with the comments made during the meeting, and summarized below, and distribute the revised version to the Committee members.

7. **Mike Giltrud** will assemble a Committee Task Group to collect examples of V&V exercises.

8. **Tinsley Oden** will assemble a Committee Task Group to collect examples of calculation benchmarks.

Draft Outline Version 2.1, Guide for Verification and Validation in Computational Solid Mechanics (*with annotations of comments made during the meeting.)*

1. Introduction

- 1.1. Background
- 1.2. Scope and Outline

Discussion of CSM - static deflection, dynamic deflection, vibration, fatigue, creep, large plastic deformation, fracture dynamics, constitutive, properties of complex materials, shock dynamics, high speed impact, etc.

Introduction to "Validation Science" - the roles of theoretical, experimental, and computational solid mechanics. Are the divisions between these disciplines artificial? Is validation science a merger?

Scope should include both existing (legacy) and newly developed codes. Wherever a specific recommendation applies only to one it should be noted (Simons).

Is it necessary to spell out all the individual, specific applications of continuum solid mechanics that are to be covered? (Simons)

Should we discuss the process of invalidation?

Should we go to the atomistic level? Majority opinion seemed to be no.

Should the treatment of stochastic or probabilistic approaches be from the standpoint of intrinsic uncertainties in data and methods, methods for implementing known uncertainties in computational methods, or both?

Include principles of software quality assurance (SQA).

Include discussion of data quality assessment.

The term "Validation science" seems to exclude verification, so it should be replaced with "Validation and verification science." (Dale Pace)

There was some objection to the idea that validation and verification science is a ***merger*** *of experimental, theoretical, and computational science. Rather it should be regarded as a set of processes that relate the three to each other.*

Are decision-makers in the intended audience? They are the ones who need to understand the importance of experiments specifically tailored to V&V.

2. Terminology

* 2.1 Modeling and Simulation

Consider updating the "Sargent Circle" with as-yet undetermined figure (e.g., new SNL document). Replaces "model qualification" with "conceptual model validation"?

Maintain correspondence between the new diagram, and the sections of the guide, i.e. the diagram acts as a visual queue to the text.

* 2.2 Conceptual Model

- 2.2.1. Requirements

e.g., "validation referent", deterministic or stochastic?, stable solution?

Dale Pace elaborated here: Conceptual model must include a context (the applicable laws of physics), a representation (mathematics), and controls (computing hardware & software).

2.2.2. Conceptual Model Development

e.g., identification of physical/experimental basis, including limitations of validation data

- 2.2.3. Conceptual Model Validation

* 2.3. Uncertainty and Error

- Includes stochastic/probabilistic

Probability Density Functions are a way of quantifying uncertainties.

Maintain the distinction between randomized known situations, and more fundamental uncertainty in physical processes themselves.

* 2.4 Prediction and Levels of Credibility

* 2.5 Calibration

- Strong focus on Calibration; much more than CFD.

* 2.6 Verification and Validation

Relate V&V to an orderly development process: requirements (what the M&S is supposed to be capable of doing) drive a conceptual model (however described) which gets implemented in M&S, with various tests of pieces and the whole M&S system to demonstrate what it can do.

* 2.7 Theoretical, Experimental and Computational Mechanics

- Development of "Validation Science" for CSM

Change to "Verification and validation science"

* 2.8 Stability ? Optimization ?

Keep stability, drop optimization (Oden)

Discuss how these affect credibility (Pace)

3. Verification

* 3.1 Verification Phases

- Grid Convergence, Time-Step Convergence, Iterative Convergence, Consistency Tests, Code-to-Code Comparisons, Software Quality Engineering (SQE, including Configuration Management).

* 3.2 Verification Tests

- Particularly important for assessments involving complex material models (e.g., nonlinear elasticity, history dependence, heterogeneous solids, rate-dependent plasticity), few of which can be adequately represented by well-characterized benchmarks.

General discussion, and specific cases, of analytical solutions and numerical benchmarks

* 3.3 Acceptance Criteria

Change "acceptance" to "verification."

- The Verification Metric.

* 3.4 Verification Products, including Documentation

Oden will recommend how to include a posteriori error estimation in this section.

4. Validation

* 4.1. Validation Phases

Include conceptual validation or conceptual model validation (Pace).
In Oberkampf's presentation to the BPTC he had replaced "conceptual model" with "mathematical model," where it appeared in the Sargent circle.

* 4.2 Computational Solid Mechanics - "as is"

\- 4.2.1 Current practices

* Generalization is not possible, as no accepted procedures in place. Extent of validation can range from none to extensive; mission-critical simulations, and systems with significant legal liabilities, tend to focus more on validity.

* Current limitations - focused on strong dependence on analyst expertise, which forces the analyst, not the developer, to be responsible for validation.

Role of the analyst?

There was a long discussion here about need to have a specific model to validate. Can you even validate a code?

\- 4.2.2 Calibration

* Numerical approximations (e.g., artificial viscosity)

* System approximations (e.g., sub-models for joints, etc.)

* Physical approximations (e.g., constitutive models)

* Modeling approximations (i.e., analyst-implemented limitations like boundary conditions, lack of mesh convergence, etc.)

Majority opinion seemed to be that there should be a separate section on calibration, at the same level as sections on verification and validation.

Calibration is part of model development and must be finished before validation is begun (Senseny)

Insert a section on hierarchical models (Oden)

Validate models, not codes.

Need to ***recognize*** *when you are calibrating (Oberkampf).*

When performing parameter estimation, e.g. for properties of bolted or riveted joints, does this type of calibration based on one structure apply to any others?

\- 4.2.3 "Trend Validity"

* 4.3 Experimental Data

\- Generalization of AIAA Guide 4.3

* 4.4 Systems View of Validation - PIRT

\- Sub-model validation and calibration, followed by system-level validation.

\- Applies PIRT (Phenomena Identification and Ranking Tables)

* 4.5 Computational Solid Mechanics - "to be"

\- "Validation Science" - the roles of theoretical, experimental, and computational solid mechanics.

* 4.6 Acceptance criteria - the Validation Metric

* 4.7 Validation Products, including Documentation

5. Summary

Appendices

Appendix 1 - "How much V&V is enough?"

* Focuses on consequences of LACK of validation.
* Proposes multi-tiered structure to avoid "science project" label; describes levels of effort.
* Not an in-depth discussion, which would be more appropriate for a document aimed at decision makers in support of "accreditation".

Need examples of breakdowns in the process.

Appendix 2 - "What V&V is not (yet)"

* Development requirements for Validation Science (a summary of issues mentioned in the main body).

Appendix 3 - Resources

* Provides guidance about special resources (such as software packages) required for use of various V&V techniques and methods – and possibly suggestions for how to employ various V&V methods (such as SME or code reviews) effectively and efficiently.

References

* AIAA, "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations" (AIAA G-077-1998)
* Roache, "V&V in Computational Science and Engineering"
* Phenomena Identification and Ranking Tables (PIRT): Wulff, "Scaling of thermohydraulic systems," Nuclear Engineering and Design 163 (1996), 359-395.
* Trucano and Moya, "Guidelines for Sandia ASCI Verification and Validation Plans - Content and Format: Version 1.0," SAND99-3098, Dec 99 [Version 2.0 is due out soon]
* Oberkampf, et. al, "Estimation of Total Uncertainty in Modeling and Simulation," SAND2000-0825, April 2000.
* Alvin, et. al, "Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation," SAND2000-0515, March 2000.