An Industrial Perspective on Materials Modeling Credibility and V&V Standards.

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Who I am?

40 years+ experience in aerospace
Main technical domains: Structure Mechanics & Engineering Simulation

- **Last industry position AIRBUS**
    - **V.P. Engineering, Airbus, Head of Structure Analysis**
- **Present sim concept**
    - **Consulting: Simulation V&V, Governance & Management**
    - **International Committees**
        - **NAFEMS SGMWG, Simulation Governance & Management**
        - **ASME V&V 10 Industrial Review**
    - **Training**

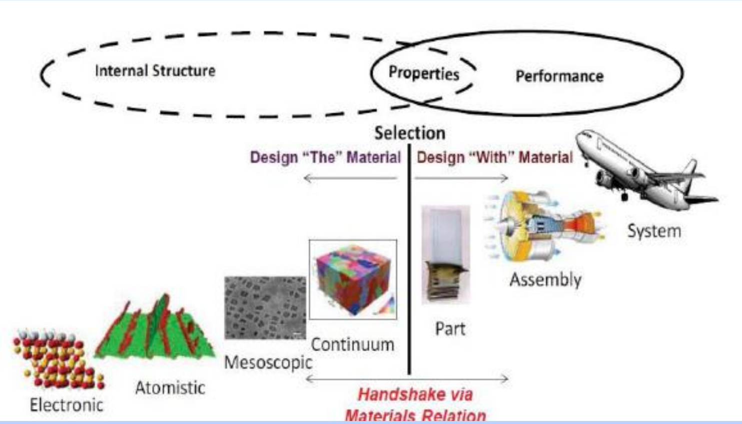
NAFEMS V&V Master Class, 34 courses in Europe

- **Former Professor, Finite Element Analysis at ISAE (SupAero), Toulouse**

Introduction

Digital enterprise transformation.

- Growing simulation importance for industrial decisions
- Strong pressure on lead time and cost reduction including physical testing.
- Decision-makers increasingly require objective evidence of simulation credibility.



Stages of materials and product design
David Cebon, Granta Design, Presentation at EMMC International Workshop, Vienna, 5-7 April 2017

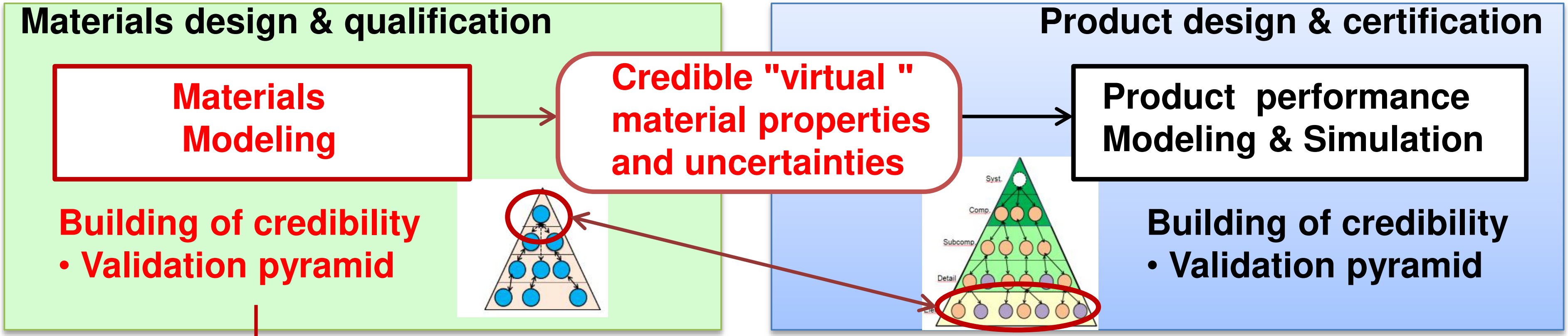
Computational Materials Engineering

- **Huge potential benefits for**
  - **Material technology development**
  - **Product design and development**
- **Materials modeling credibility is essential for industrial acceptance and implementation.**

⇨ **VVUQ**

- **Verification & Validation**
- **Uncertainty Quantification**

Materials Modeling Credibility Requirements



Materials design & qualification

Materials Modeling

Credible "virtual " material properties and uncertainties

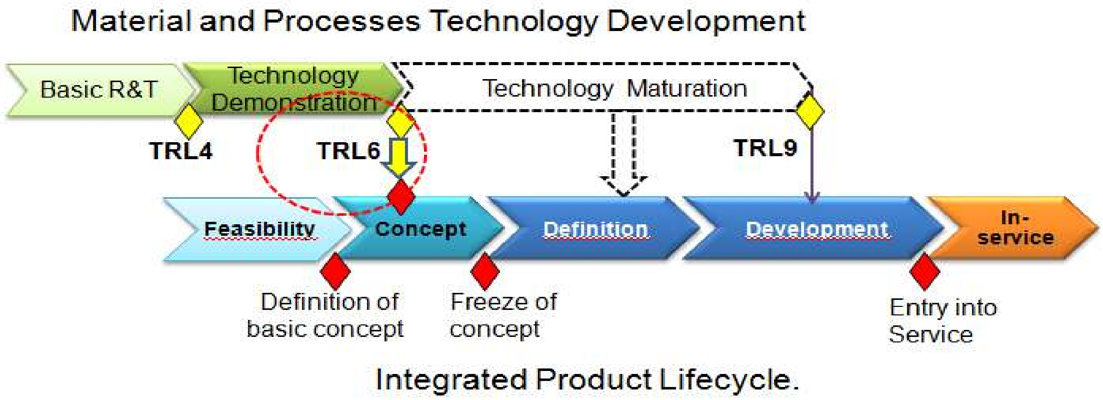
Building of credibility
- **Validation pyramid**

Product design & certification

Product performance Modeling & Simulation

Building of credibility
- **Validation pyramid**

Progressive validation vs.
- TRL progress
- IPD milestones



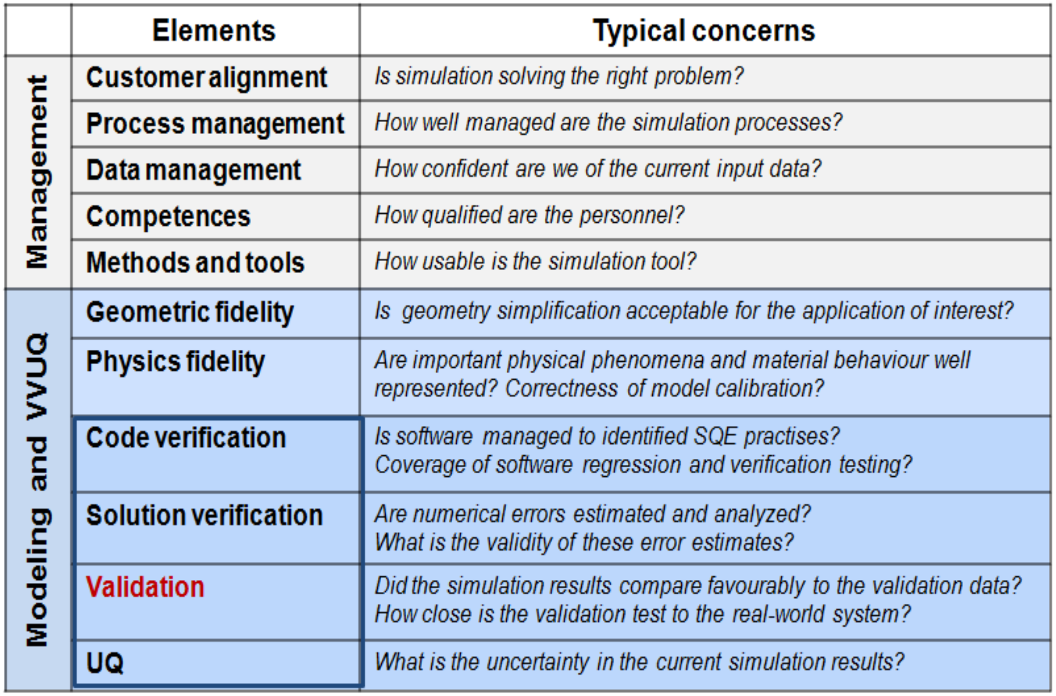
Materials Technology TRL vs. IPD Milestones

The required credibility	**• Increases with Material TRL,** **• Varies with Product Lifecycle application,** **• Ensured by hierarchical VVUQ processes,** **• Demonstrated at key milestones.**

What is simulation credibility?

Trustworthiness of simulation results

- **For an intended application**
- **In order to take risk-informed industrial decisions**

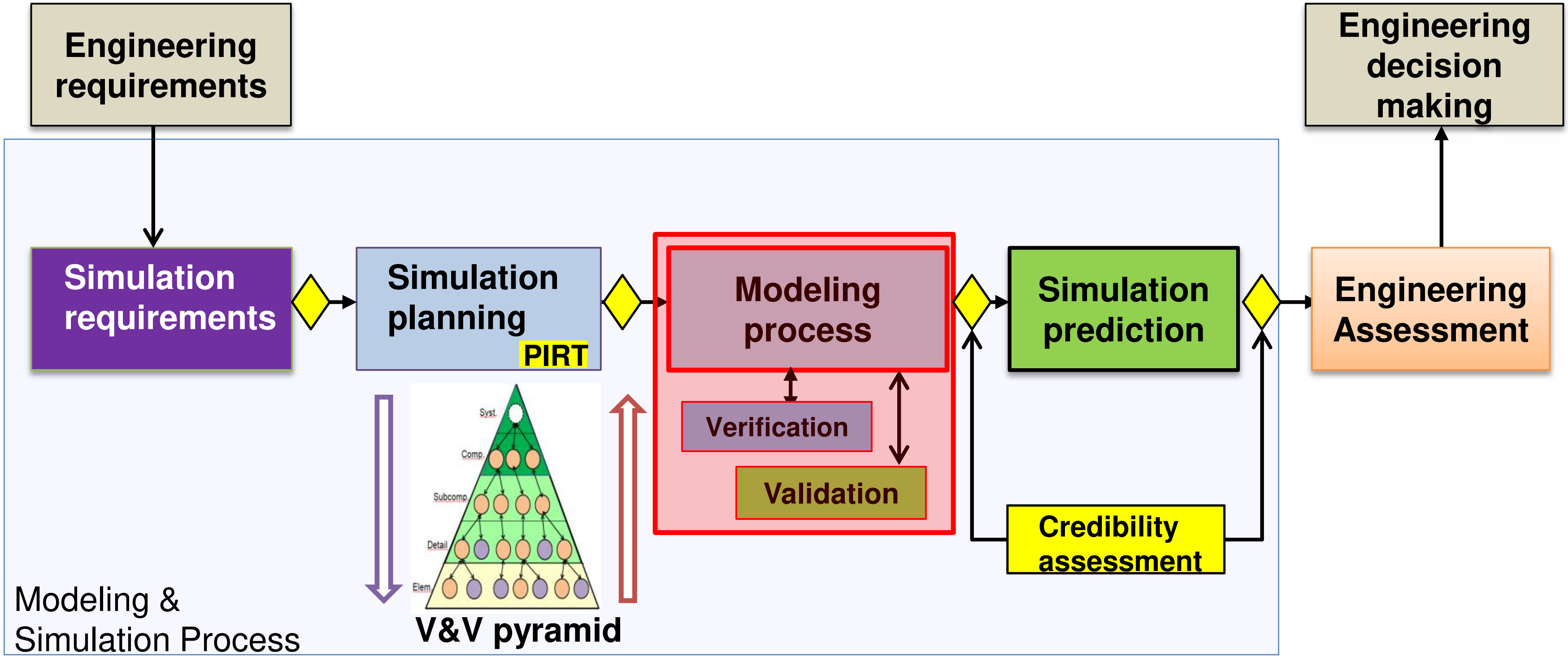


	Elements	Typical concerns
Management	Customer alignment	*Is simulation solving the right problem?*
	Process management	*How well managed are the simulation processes?*
	Data management	*How confident are we of the current input data?*
	Competences	*How qualified are the personnel?*
	Methods and tools	*How usable is the simulation tool?*
Modeling and VVUQ	Geometric fidelity	*Is geometry simplification acceptable for the application of interest?*
	Physics fidelity	*Are important physical phenomena and material behaviour well represented? Correctness of model calibration?*
	Code verification	*Is software managed to identified SQE practises?* *Coverage of software regression and verification testing?*
	Solution verification	*Are numerical errors estimated and analyzed?* *What is the validity of these error estimates?*
	Validation	*Did the simulation results compare favourably to the validation data?* *How close is the validation test to the real-world system?*
	UQ	*What is the uncertainty in the current simulation results?*

- **Required credibility for decision making ?**
- **How to ensure credibility ?**
- **How to measure credibility ?**

Verification, Validation and UQ (VVUQ) are essential credibility elements.
Assessing credibility requires a dedicated procedure.

How to build simulation credibility?



Engineering requirements

Engineering decision making

Simulation requirements

Simulation planning

PIRT

Modeling process

Verification

Validation

Simulation prediction

Credibility assessment

Engineering Assessment

Modeling & Simulation Process

V&V pyramid

Credibility assurance: proactive implementation and monitoring of modeling V&V and UQ (VVUQ) processes, to ensure the required credibility of simulation results.

Requires:
- **VVUQ planning→ V&V pyramid**
- **Application of guidelines on modeling and VVUQ.**
- **Credibility assessment**

V&V frameworks
Best practises

ISO V&V standard definitions

System verification: *”Confirmation, through the provision of objective evidence that specified requirements have been fulfilled.”*
Confirms that the system is designed and built to specifications.

System validation: *”Confirmation, through the provision of objective evidence that the requirements for a specific intended use or application have been fulfilled.”*
Confirms that the system meets the intended purpose and needs of system’s owner and stakeholders

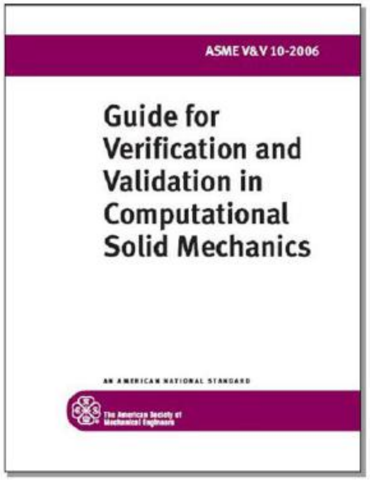
- **Applicable to complex systems / industrial products including hardware and software (ISO/IEC 15288)**
- **Applicable to processes and services (ISO 9000&9001)**

- **Above general definitions require much interpretation when applied to Modeling & Simulation.**

The Genesis of Simulation V&V Frameworks

- First initiatives in the 1970's by the communities of Electrical Engineering, Software Engineering (IEEE), Systems Engineering (ISO), Quality Management (ISO)…
- New initiatives in the 1990's to define simulation specific V&V concepts (DoD, AIAA, ASME…).

- Most popular and mature standards and reference guides for simulation V&V.
  - ASME V&V 10 for Solid Mechanics / FEA (2006)
  - ASME V&V 20 for CFD and Heat Transfer (2009)

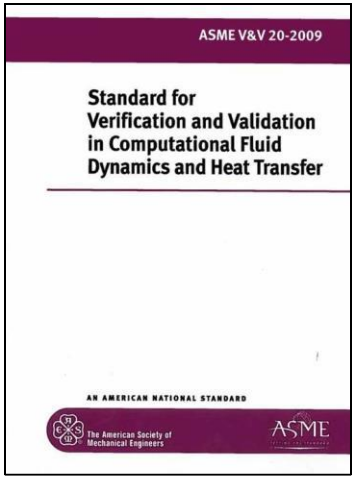


ASME V&V 10-2006

Guide for Verification and Validation in Computational Solid Mechanics

AN AMERICAN NATIONAL STANDARD

The American Society of Mechanical Engineers



ASME V&V 20-2009

Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer

AN AMERICAN NATIONAL STANDARD

The American Society of Mechanical Engineers

ASME

2 decades experience in the Structures, CFD and Thermal domains from pioneering industries.
Recognized benefits for building credibility among technical customers and managerial decision makers.
Limited availability of similar frameworks for Materials Modeling practitioners.

Standard definitions of simulation V&V

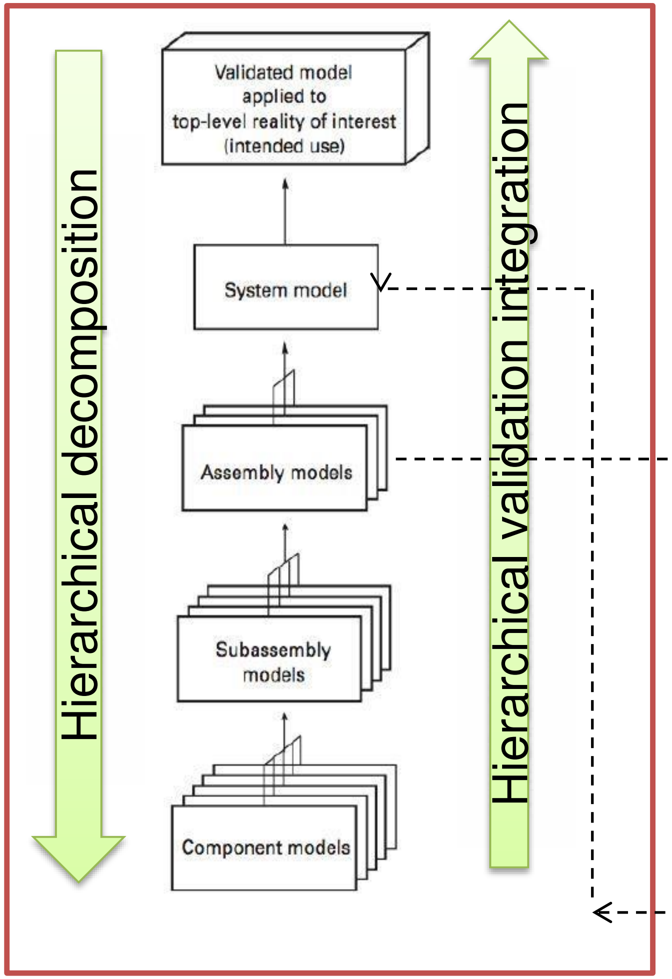
- **Simulation verification:** *"The process of determining that a computational model accurately represents the underlying mathematical model and its solution."*
Assesses code reliability (code verification) and numerical accuracy (solution verification).

- **Simulation validation:** *" The process of determining the degree to which a computational model is an accurate representation of the real world from the perspective of the intended uses of the model."*
Measures simulation accuracy in "representing the real world" by experiments.

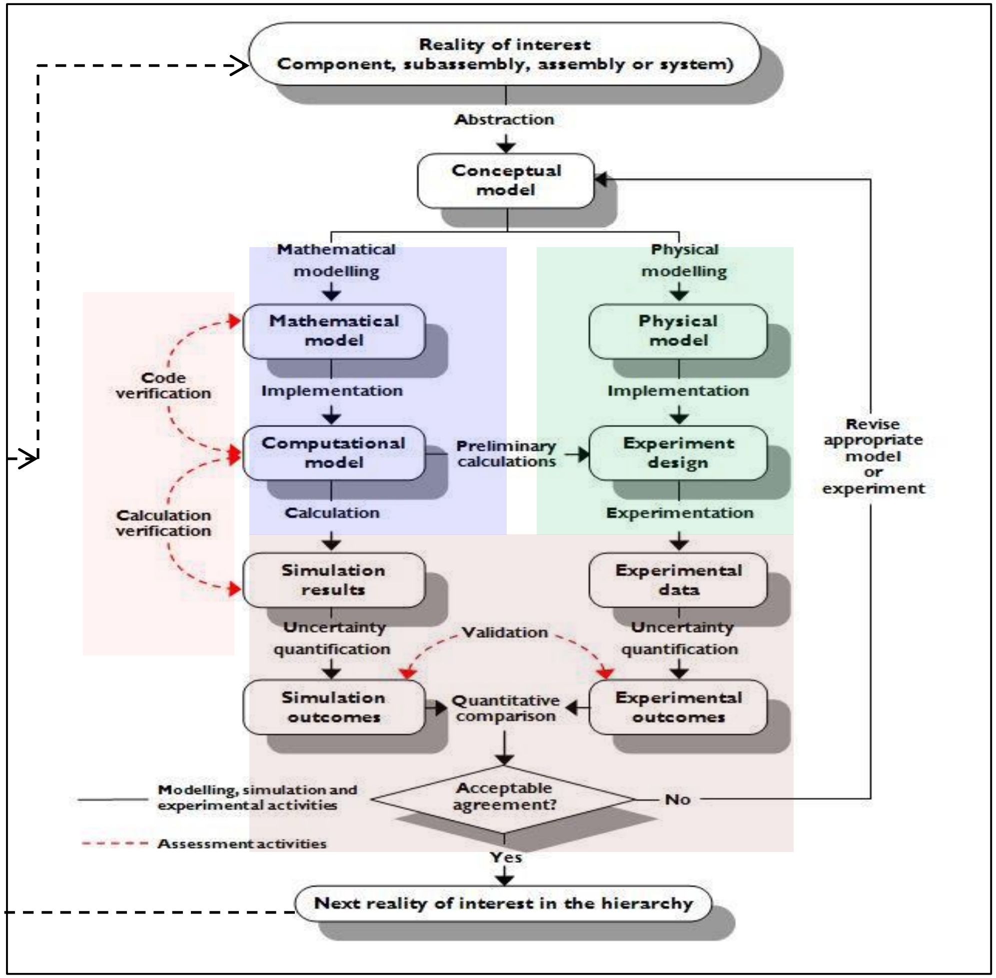
- **Applicable to engineering simulation.**
References: ASME V&V10, ASME V&V20, AIAA CFD Guide...

> *« ASME V&V 10 provides an excellent set of definitions and guidelines applicable to a broad range of computational disciplines and applications. » [Cowles, 2013]*

ASME V&V 10 Flow Chart (2006)

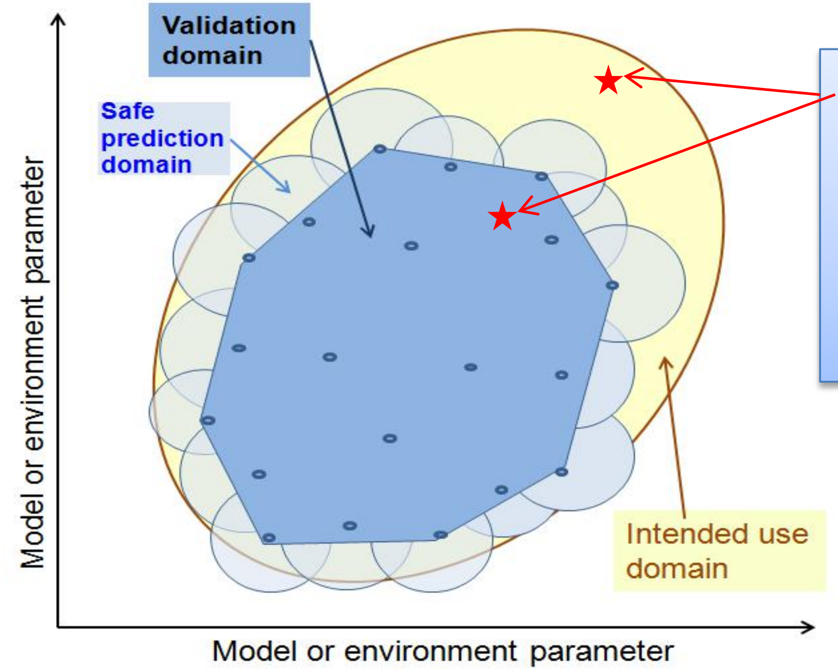


Hierarchical modeling and validation



Validation flow chart for a specific entity in the hierarchy

Validation and predictive capability



Notional concept of validation coverage

- **Predictive capability: ability to predict the required responses and uncertainties,**
  - **for the intended use**
  - **for conditions which are not (or cannot be) physically tested**

Key issues:

- **Experiment representativeness.** Representative experiments often difficult and sometimes impossible.
- **Extent of experiment rationalization.**

Rationalization of validation experiments increase the required predictive capability.

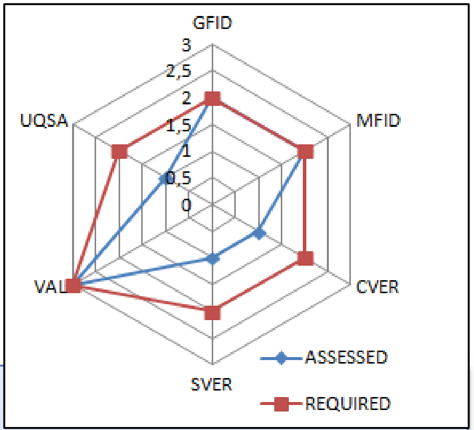
Present validation trends

- Predictive capability assessment, validation coverage analysis
- Consistent validation interpretation from ISO to ASME V&V 10

→Various levels of validation strengths

Credibility Assessment

- **Standard procedure to support decision-making**
  - **For a given application**
  - **From objective evidence**
- **2 decades experience**



Existing procedures

- TRL's (Technology Readiness levels) from NASA (1995), DoD (2005)
- CMM/CMMI (Capability Maturity Model) from Software Engineering Institute since 1987
- **CAS (Credibility Assessment Scale) from NASA-STD-7009 (2008)**
- **PCMM (Predictive Capability Maturity Model) from Sandia Labs (2007)**
- **Specific procedures for Materials Engineering (TML) and Manufacturing**

Recent survey : J.F.Imbert, W.L.Oberkampf « Survey of Maturity Assessment Procedures for Computational Simulation », NWC17 NAFEMS World Conference, Stockholm, June 2017

ICME V&V Guidelines

Developed by:

- **US Air Force Research Lab. (B. Cowles, D. Backman, and R. Dutton)**
- **First published in 2011**
- **Focus on aerospace materials**

**Verification and Validation of ICME
Methods and Models for Aerospace
Applications**

**V&V Guidelines
and
Recommended Best Practice
Revision 1**

Prepared for:

**Dr. R. E. Dutton
USAF AFRL/RXM**

Prepared By:

**B. A. Cowles
Cowles Consulting,
LLC**

**Dr. Dan Backman
Backman Materials
Consulting, LLC**

1 December 2013

Approved for Distribution A by USAF AFMC AFRL/RXR 14 January 2014

DISTRIBUTION STATEMENT A: Approved for public release; distribution is unlimited.

Main features

- **Complies with ASME V&V 10**
- **Facilitates alignment of material TRL's and IPD maturity gates**
- **Provides V&V guidance and checklists to materials practitioners**
- **Recommends V&V planning driven by important phenomena (PIRT)**
- **Includes a maturity assessment procedure →Tool Maturity Level (TML)**
- **Promotes risk assessment practises**

Status:

- **Relatively early in the development and use of the procedure**
- **Limited feedback on benefits within targeted domains**

ICME Tool Maturity Level (TML)

Assessment structure:

- **Five maturity levels are defined**
- **Each maturity level lists requirements for six aspects of maturity and risk**

Assessment of 6 elements

1. Model Rationale, Basis and Definition
2. Complexity and Documentation
3. Supporting Data
4. Model Verification
5. Range of Applicability and Uncertainty Quantification
6. Risk Assessment and Validation

Assessment results in a maturity level

Maturity Levels	Description
1	Analytical process is exploratory in nature.
2	Proven capability for comparative assessment, ranking or trending.
3	Material or process can be developed or assessed with significantly reduced testing.
4	Material or process performance and impact on system or application are understood.
5	All material and process performance and system interaction effects are understood within defined range of application.

Concluding remarks

- EMMC Roadmap is strategic for Europe.
- Modeling & Simulation credibility assurance & VVUQ,
  - Already mature from standard V&V frameworks in pioneering industries,
  - Becomes essential for Materials Modeling.

Recommendations

- Take benefits from existing standards (ASME) and best practices from other engineering domains.
- Establish EMMC V&V Guidelines including a standard credibility assessment procedure
- Develop and deploy a dedicated training programme
- Boost material-specific V&V research,
  - Multiscale materials models: V&V, UQ, calibration
  - V&V data collection and repositories for code verification, validation (e.g. ERCOFTAC)
  - V&V for data-based models…

Thank you for your attention.

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Ich danke ihnen für ihre aufmerksamkeit !

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A selection of references (1/2)

1. EMMC, The EMMC RoadMap 2018 for Materials Modelling and Informatics
2. EMMC, European Materials Modelling Marketplaces: Digitalisation Innovation Hubs for next generation materials development
3. Xuan Liu and Al., Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems, NASA/CR-2018-219771, March 2018
4. Integrated Computational Materials Engineering (ICME): Implementing ICME in the Aerospace, Automotive, and Maritime Industries, The Minerals, Metals & Materials Society, Warrendale, PA 15086, 2013
5. McDowell D.L., Olson G.B. (2008) Concurrent design of hierarchical materials and structures. In: Yip S., de la Rubia T.D. (eds) Scientific Modeling and Simulations. Lecture Notes in Computational Science and Engineering, vol 68. Springer, Dordrecht
6. J.H. Panchal and Al., Key computational modeling issues in Integrated Computational Materials Engineering, Computer-Aided Design, 2012 Elsevier Ltd.
7. David Cebon, Granta Design, Presentation at EMMC International Workshop, Vienna, 5-7 April 2017
8. Hoekstra A, Chopard B, Coveney P., 2014 Multiscale modelling and simulation: a position paper. *Phil. Trans. R. Soc. A* **372**: 20130377.
9. The Composite Materials Handbook CMH-17, http://www.cmh17.org/
10. ERCOFTAC Knowledge Base Wiki https://www.ercoftac.org/products_and_services/wiki/
11. W.L.Oberkampf and C.J. Roy, “Verification and Validation in Scientific Computing”, Cambridge University Press, 2010 (ISBN978-0-521-11360-1)

A selection of references (2/2)

12. ISO 9000:2015 & ISO 9001:2015, Quality Management System
13. ISO/IEC 15288, Systems Engineering – System Life Cycle Processes
14. AIAA, Guide for the Verification and Validation of Computational Fluid Dynamics Simulations. 1998, American Institute of Aeronautics and Astronautics, AIAA-G-077-1998.
15. ASME, “Guide for Verification and Validation in Computational Solid Mechanics”, American Society of Mechanical Engineers, ASME V&V 10-2006.
16. Standard for Verification & Validation in Computational Fluid Dynamics and Heat Transfer, American Society of Mechanics Engineers V&V Standards Committee V&V-20, 2009
17. NASA "Standard for Models and Simulations." National Aeronautics and Space Administration, NASA-STD-7009A (2016), Washington, DC.
18. SEI, (2010). "CMMI for Development, Version 1.3." Software Engineering Institute, CMU/SEI-2010-TR-033, Carnegie Mellon University, MA.
19. W.L.Oberkampf, and Al., “Predictive Capability Maturity Model for Computational Modeling and Simulation,” Sandia National Laboratories, SAND2007-5948.
21. B.Cowles, D. Backman, (2013). "Verification and Validation of ICME Methods and Models for Aerospace Applications - V&V Guidelines and Recommended Best Practice: Revision 1."
22. J.F.Imbert, W.L.Oberkampf ,« Survey of Maturity Assessment Procedures for Computational Simulation », NWC17 NAFEMS World Conference, Stockholm, June 2017
23. J.F.Imbert, On the Credibility Assurance of Engineering Simulation, Keynote Lecture, NAFEMS DACH Conference, Bamberg, May 2018
24. J.F. Imbert, P.Pasquet, NAFEMS Master Class, Simulation V&V in Engineering Simulation, https://www.nafems.org/events/nafems/2019/vandv1/

List of acronyms

CAS Credibility Assessment Scale
CMMI Capability Maturity Model Integration
HPC High Performance Computing
IT Information Technology
ICME Integrated Computational Materials Engineering
M&S Modeling and Simulation
PCA Predictive Capability Assessment
PCMM Predictive Capability Maturity Model
PIRT Phenomena Identification and Ranking Technique
QOI Quantity Of Interest
QMU Quantification of Margins and Uncertainties
SA Sensitivity Analysis
SDM Simulation Data Management
SPDM Simulation Process and Data Management
SW Software
TRL Technology Readiness Levels
UQ Uncertainty Quantification
V&V Verification and Validation
VVUQ Verification, Validation and Uncertainty Quantification