Verification and Validation of ICME Models

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1/14/14

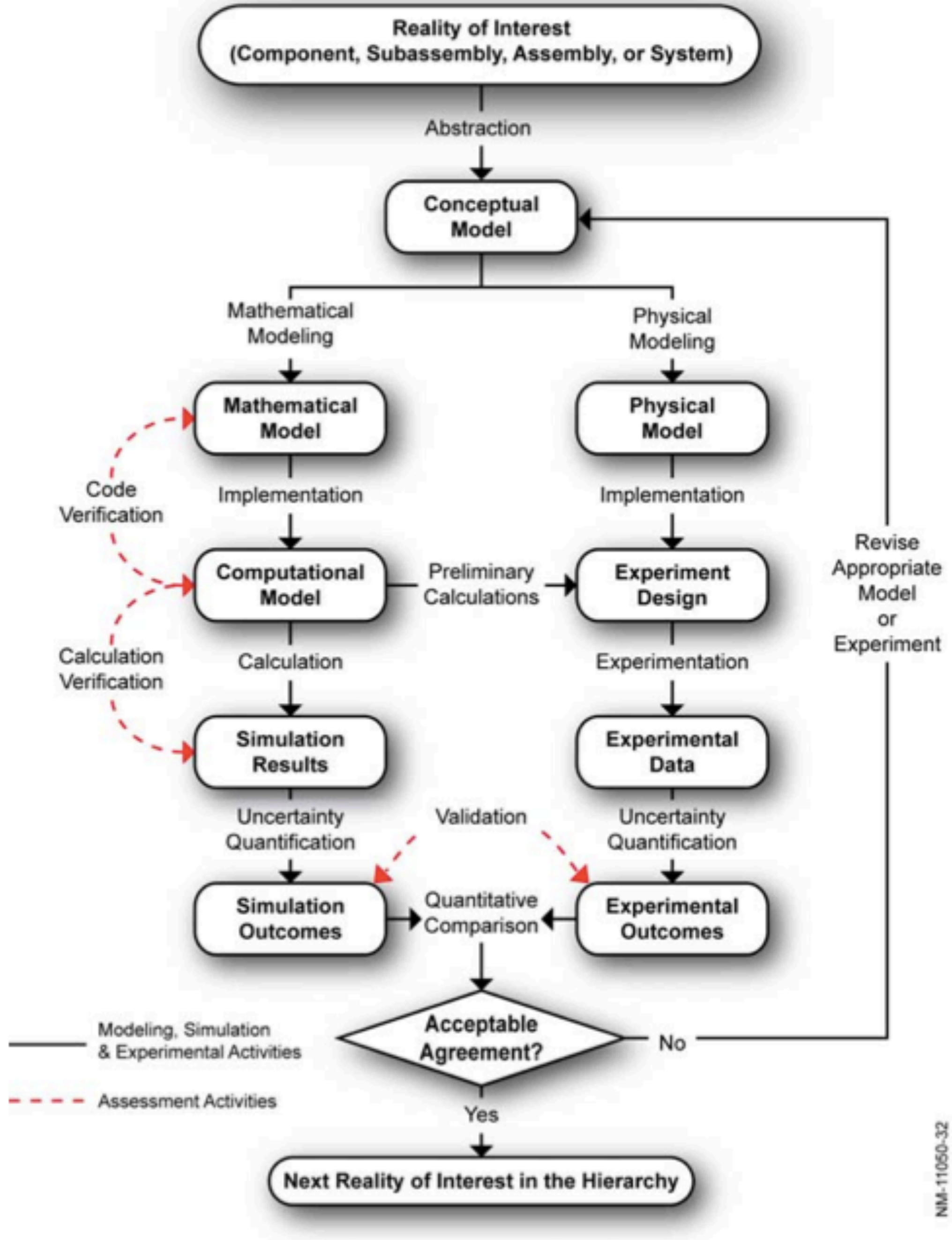


Figure 2 Verification & Validation activities and outcomes. (*Guide Figure*)

Goals for this course:

- Establish Standards based Basic Vocabulary
  - "V&V activities promote team-wide communication"
- Present consensus best practices for V&V to the team in the form of lecture, discussion, and demonstration using a contextualized model.
- Introduce Standards and Tools
- Identify areas where ICME projects will encounter different challenges than have been addressed in current standards
- Contextualized Example to Illustrate core concepts of V&V and initiate discussion
- Provide References
- Feedback for improving

What we will not cover

- Prescriptive step-by-step approach
  - No one-size-fits-all solution exists
- In depth description of statistical theory
  - Proper application of statistical theory to actual engineering problems can be subtle and often counterintuitive
- Computational Tool Recommendations
  - Many excellent choices
  - User preference

Agenda

Start	Duration	End	Topic	Instructor
2:00	0:30	2:30	Model V&V Introduction	Benedict
			Background and motivation	
			ASME Standard	
			ICME checklists and model maturity	
2:30	0:10	2:40	Case Study and business case	Benedict
2:40	0:20	3:00	V&V Plan/Process	Benedict
			Verification	
			Validation metrics	
			Case study example	
3:00	0:30	3:30	Methods	Riha
			UQ	
			Case study examples	
			Calibration	
			Case study examples	
3:30	0:30	4:00	Case Study V&V Summary	Riha
			Documentation and Tracking	

Webinars

4 Follow up webinars are planed that go into the topics presented in greater detail:

1. ICME focused V&V introduction
2. V&V plan and process with examples
3. Methods: UQ and Calibration
4. End to End Case Study V&V summary

with detailed review of the ICME checklists and TRL

Acknowledgments:

This course and the material contained within is the product of a large number of contributors that we would like to thank, including but not limited to:

- Southwest Research Institute
- ASME V&V 10 committee
- Metals Affordability Initiative GE-12 Team
- Dan Backman and Brad Cowles
- AFRL/RX ICME IPT and Rollie Dutton

Integrated Computational Materials Science & Engineering

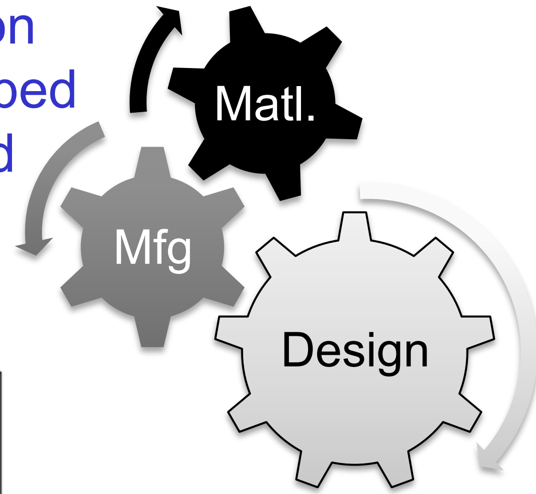
- Vision

  Drive aerospace systems design by coupling computation and experiment to predict and deliver optimized materials and manufacturing solutions.

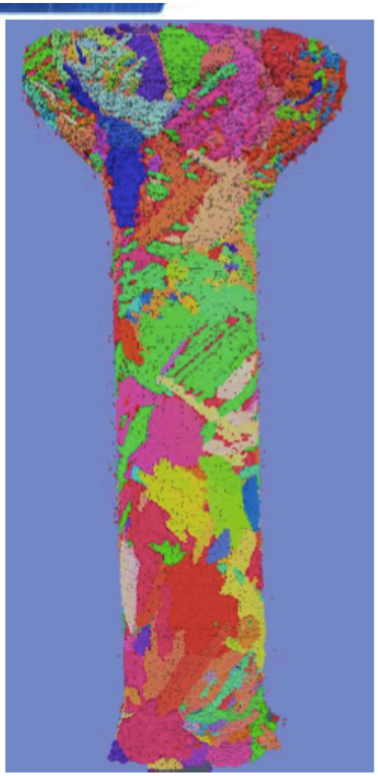
- Key elements of ICME:
  - *Quantitative & predictive*
  - *Computation and Experiment*
  - *Addresses complete materials life cycle*
  - *Integrated with system design framework*

The challenge ICME addresses

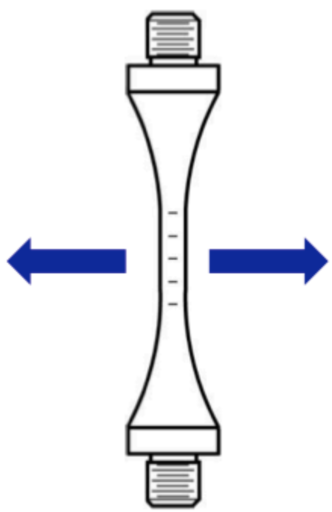
- Materials are currently defined by static specs based on lengthy empirical testing. They are traditionally developed outside of the product design loop, limiting choices and opportunities



What a tensile test looks like:



To a Materials Engineer



MIL-HBK-5H

Table 5.4.1.0(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

Specification	AMS 4911 and MIL-T-9046, Comp. AB-1					MIL-T-9046, Comp. AB-1			
Form	Sheet		Plate			Sheet, strip, and plate			
Condition	Annealed					Solution treated and aged			
Thickness, in.	≤ 0.1875		0.1875-2.000		2.001-4.000	≤ 0.1875	0.1875-0.750	0.751-1.000	1.001-2.000
Basis	A	B	A	B	S	S	S	S	S
Mechanical Properties:									
F_{tu}, ksi:									
L	134	139	130^a	135	130	160	160	150	145
LT	134	139	130^a	138	130	160	160	150	145
F_{ty}, ksi:									
L	126	131	120	125	120	145	145	140	135
LT	126	131	120^a	131	120	145	145	140	135
F_{cy}, ksi:									
L	133	138	124	129	124	154	150	145	...
LT	135	141	130	142	130	162	...	...	...
F_{su}, ksi	87	90	79	84	79	100	93	87	...
F_{bru}, ksi:									
(e/D = 1.5)	213^b	221^b	206^b	214^b	206^b	236	248	233	...
(e/D = 2.0)	272^b	283^b	260^b	276^b	260^b	286	308	289	...
F_{bry}, ksi:									
(e/D = 1.5)	171^b	178^b	164^b	179^b	164^b	210	210	203	...
(e/D = 2.0)	208^b	217^b	194^b	212^b	194^b	232	243	235	...
e, percent (S-basis):									
L	8^c	...	10	...	10	5^d	8	6	6
LT	8^c	...	10	...	10	5^d	8	6	6
E, 10^3 ksi	16.0								
E_c, 10^3 ksi	16.4								
G, 10^3 ksi	6.2								
μ	0.31								
Physical Properties:									
ω, lb/in.^{3}	0.160								
C, K, and α	See Figure 4.5.1.0								

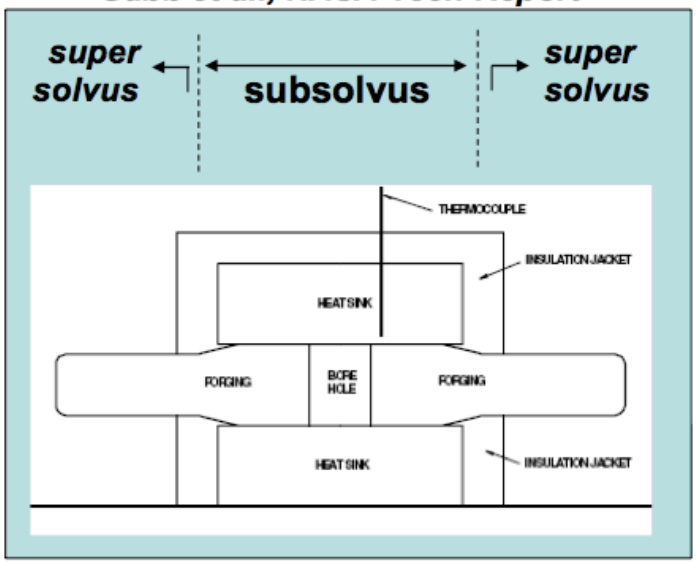
a The rounded T_{99} values are higher than specification values as follows: F_{tu}(L) = 131 ksi, F_{tu}(LT) = 132 ksi, and F_{ty}(LT) = 123 ksi.
b Bearing values are "dry pin" values per Section 1.4.7.1.
c 8%—0.025 to 0.062 in. and 10%—0.063 in. and above.
d 5%—0.050 in. and above; 4%—0.033 to 0.049 in. and 3%—0.032 in. and below.

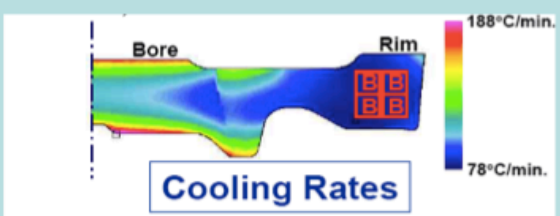
To a Mechanical Engineer

Case Study: Ni superalloy Yield strength model

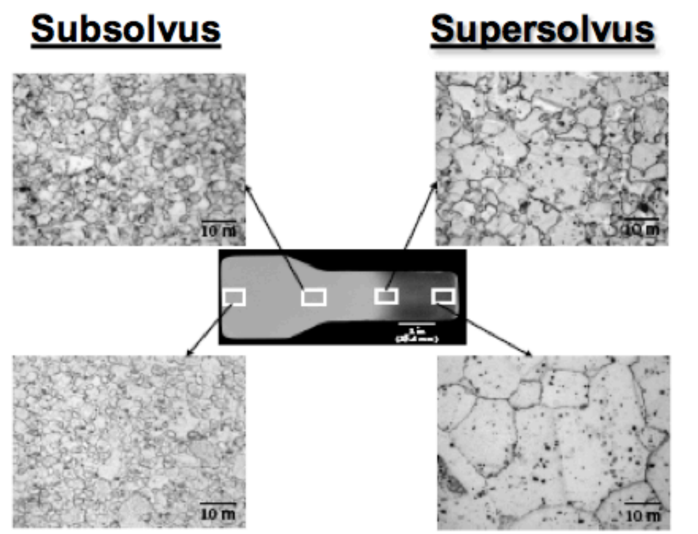
Dual Microstructure Disks

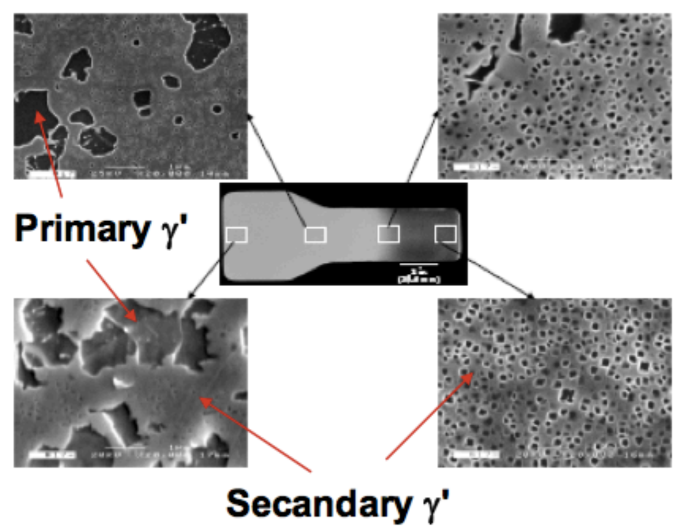
Gabb et al., NASA Tech Report



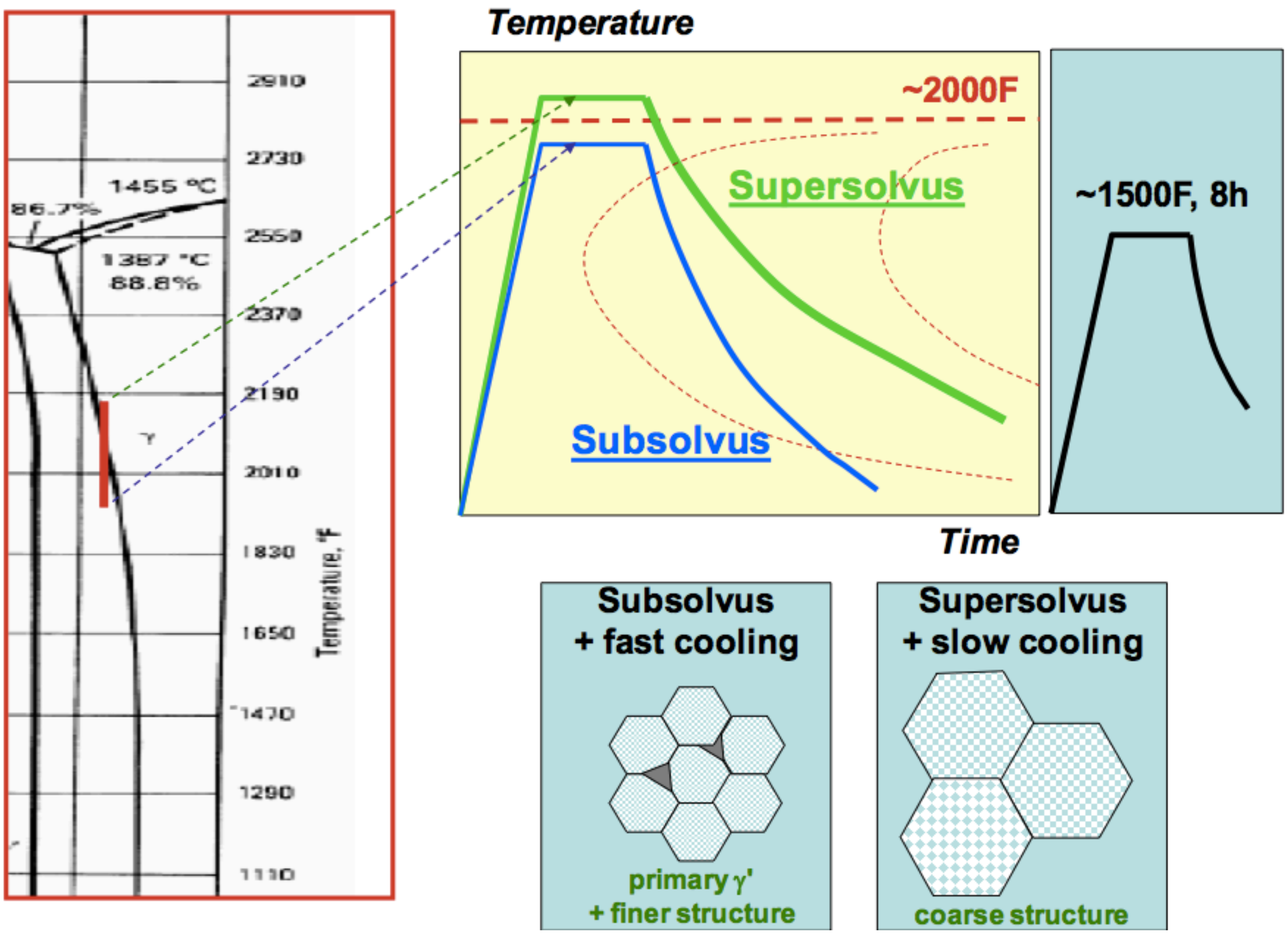


140 F/min to 338 F/min



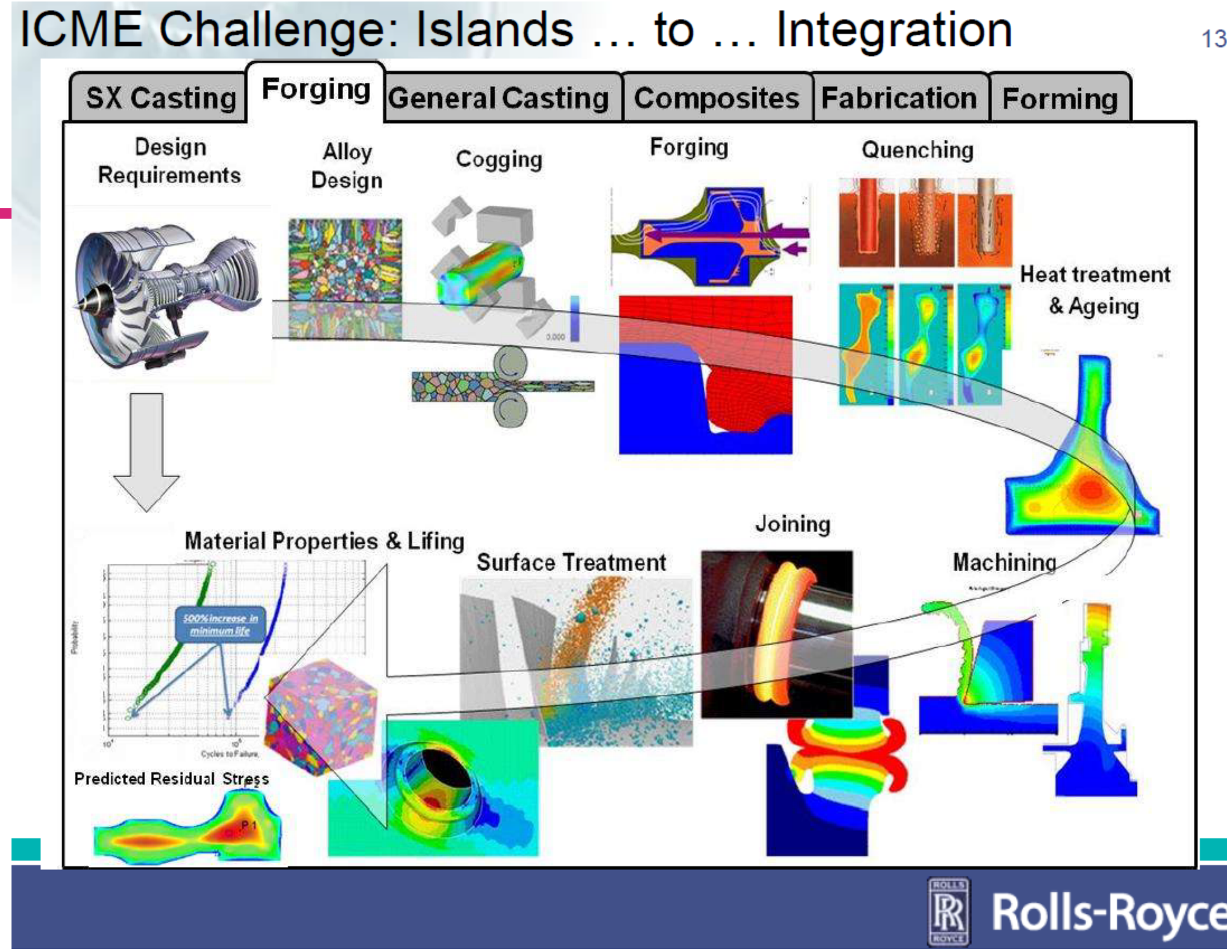


Microstructure control through H.T. of disk superalloys



ICME Goal:

ICMSE must deliver solutions we can **trust** and use

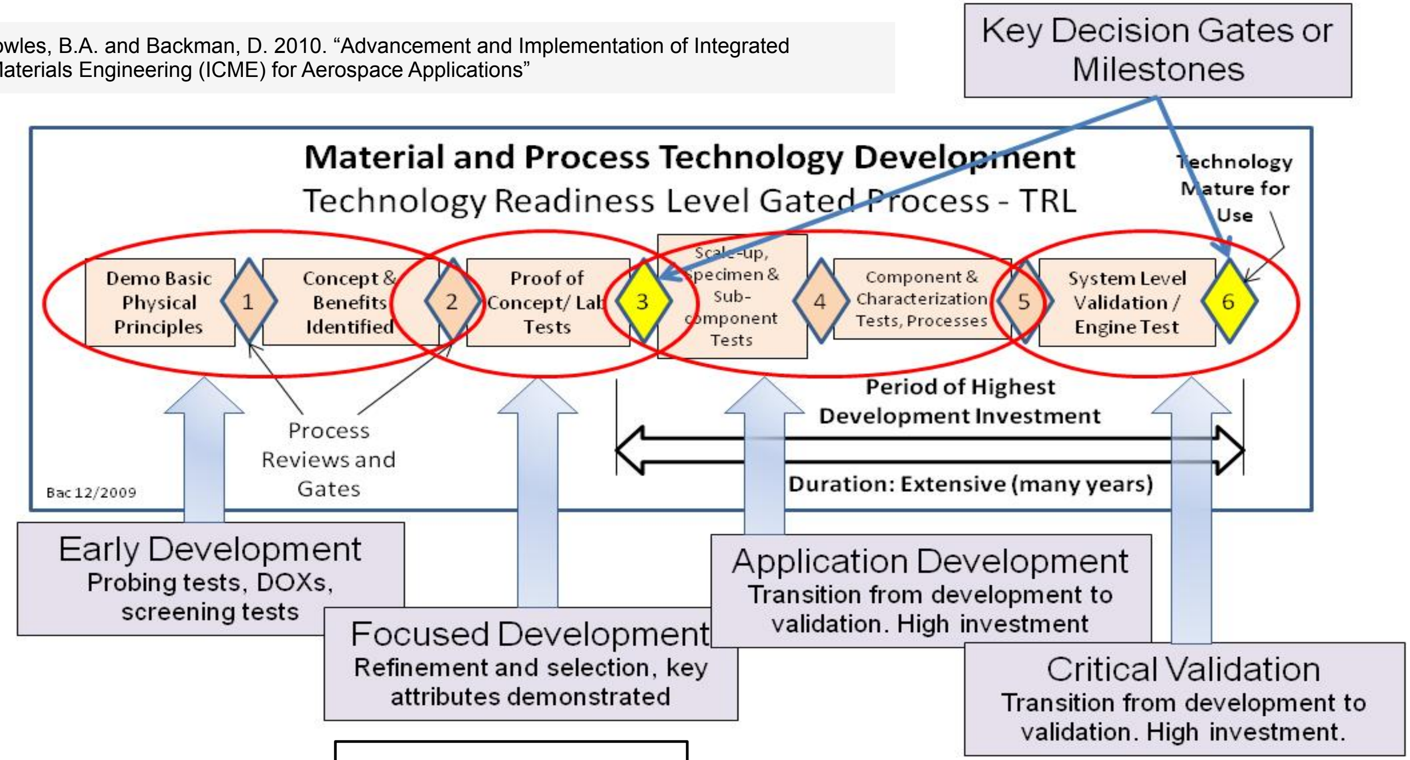


How much confidence do we need to build in these models to use them?:

- Researcher: “Will other people believe the results?”
- Engineer: “Do I believe the results enough to modify the process?”
- Engineering Project Manager: “Am I willing to bet my project (my career, my company) on these results?”
- Decision maker on high-consequence systems: “ Am I willing to bet the lives of the flight crew/public safety/national security on these results?”

Validation requirements, and investment, increase with TRL...

Adapted from Cowles, B.A. and Backman, D. 2010. "Advancement and Implementation of Integrated Computational Materials Engineering (ICME) for Aerospace Applications"



ICME

Early Development: Trending, DOX reduction, feasibility assessments. **Validation & Maturity:** Low to Moderate

Focused Development: Key attribute assessments, down-selection decisions **Validation & Maturity:** Moderate,+

Application, Characterization, Validation: Quantitative, precise, statistical assessments **Validation & Maturity:** High

Implementation: Process limits, production implementation **Validation & Maturity:** High

ICME Maturity Requirements Increase as TRL Process Progresses

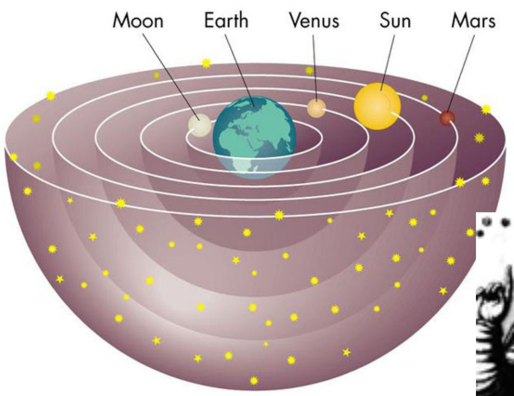
Truth vs. Accuracy

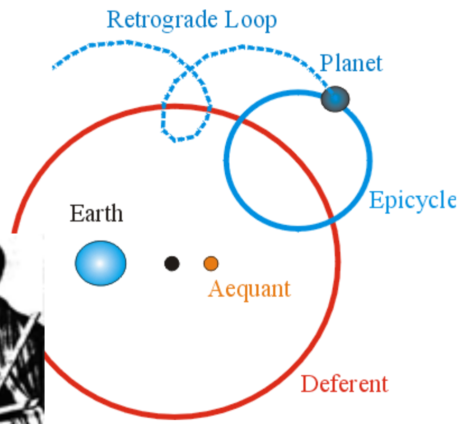
“Essentially, all models are wrong, but some are useful.”

•*Empirical Model-Building and Response Surfaces* (1987), George Box and Norman R. Draper, p. 424, ISBN 0471810339

Modelers and Physicists tend to focus on whether a model is right or wrong

Engineers often ask a more useful question: How accurate is the model?





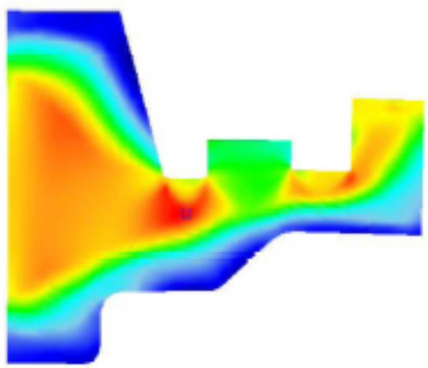
The Universe of Aristotle

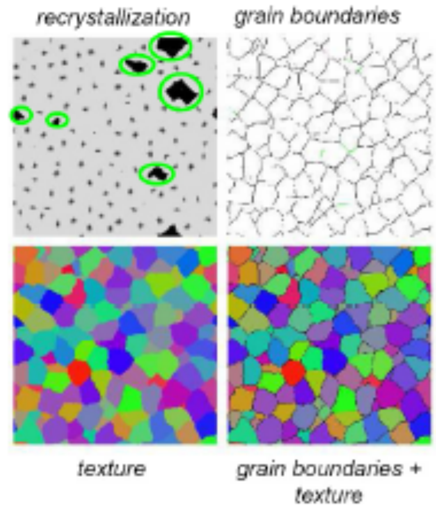
Ptolemaic Model
Rome 100 AD

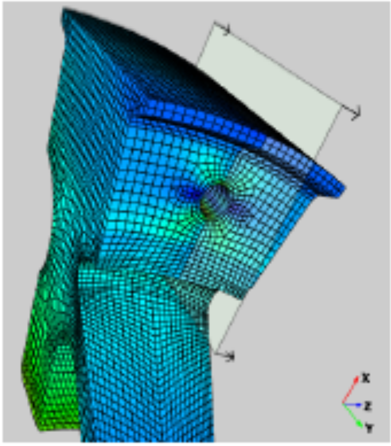
Modern Planetariums

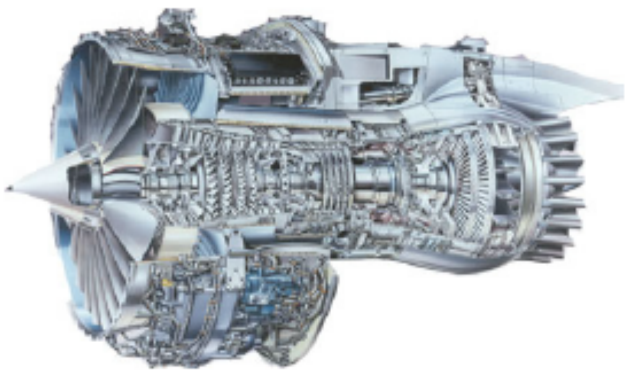
Fidelity:

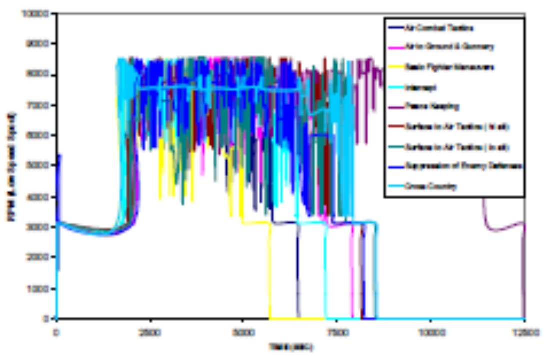
Current models contain an unprecedented level of detail

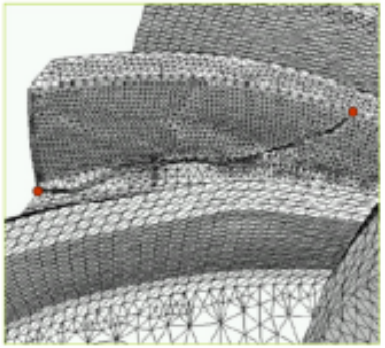












But How Credible Are These Models for Decision Making?

Error And Uncertainty

Error: Difference between simulations results and true value

- Limited Physics Fidelity (incompressible fluid, negligible air resistance, …)
- Numeric solution method
- Spatial or temporal discretization
- Finite precision arithmetic

Uncertainty: When a true value is not known or defined it is a measure of possible states or values

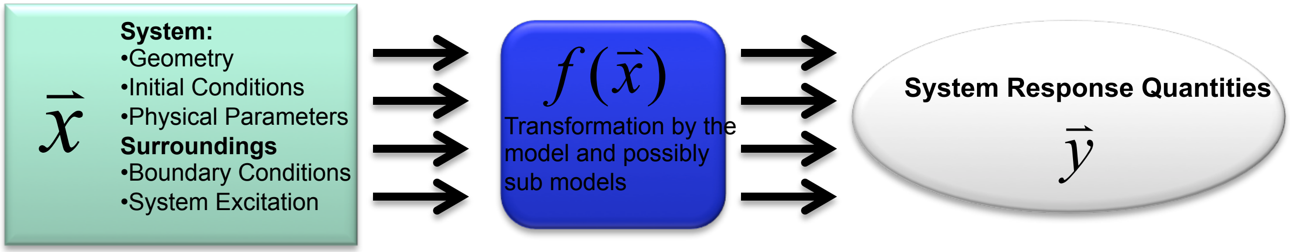
Two broad categories of uncertainty:

- **Epistemic**: lack of knowledge (property of the observer)
- **Aleatory**: inherent randomness (property of the system)

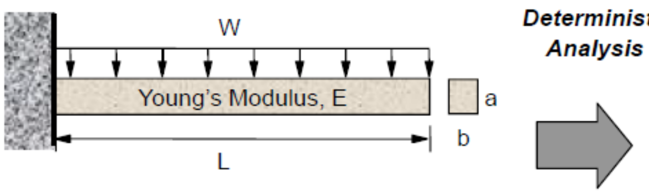
Sources of Simulation Uncertainty:
Input Uncertainty
Model Form Uncertainty
Numerical Error
iterative error
discretization error

John R. Taylor, *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements, 2d Edition, University Science Books, 1997*

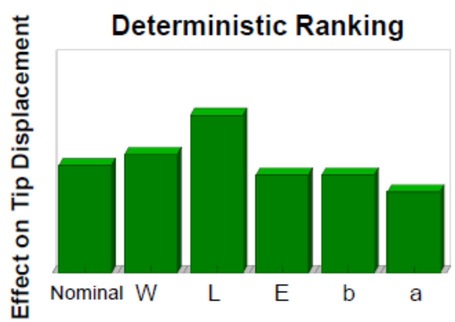
Deterministic vs. Stochastic

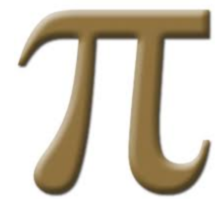


Structural Model with Deterministic Parameters



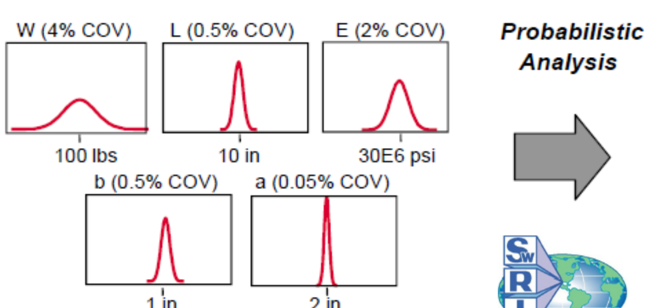
W=100 lbs, L=10 in, E=30E6 psi, b=1 in, a=2 in

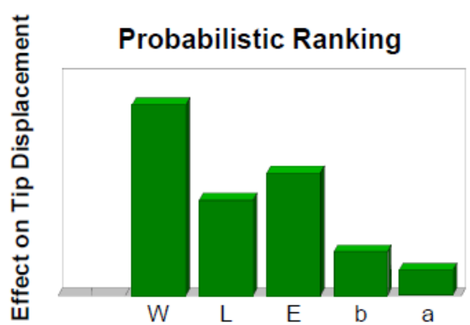


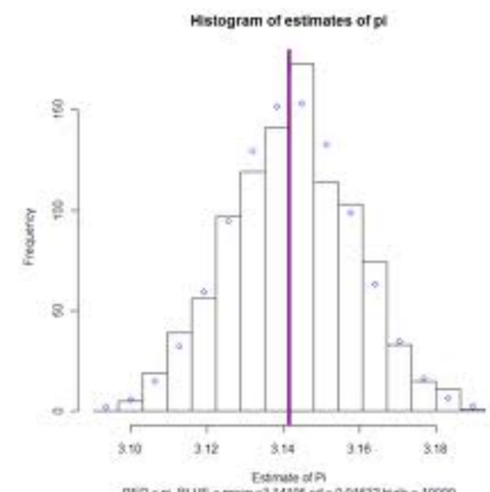


Vs.

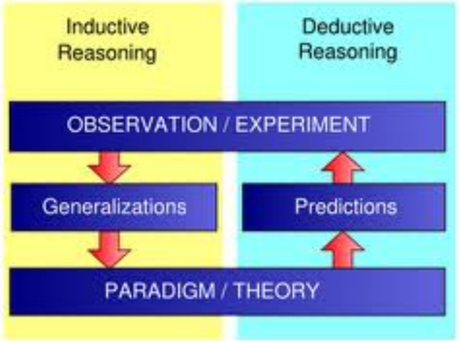
Structural Model with Uncertain Parameters







How is Credibility built in Modeling and Simulation?



- Verification
  - Credibility from understanding the mathematics
  - Are the equations being solved correctly?
  - Compare computed results to known solutions

  } **Mathematical Evidence**

- Validation
  - Credibility from understanding the physics
  - Are the correct equations being solved?
  - Compare computed results to experimental data

  } **Experimental Evidence**

- Uncertainty Analysis
  - Credibility from understanding the uncertainties
  - How accurate is the model prediction?
  - Quantify uncertainty & variability from all sources

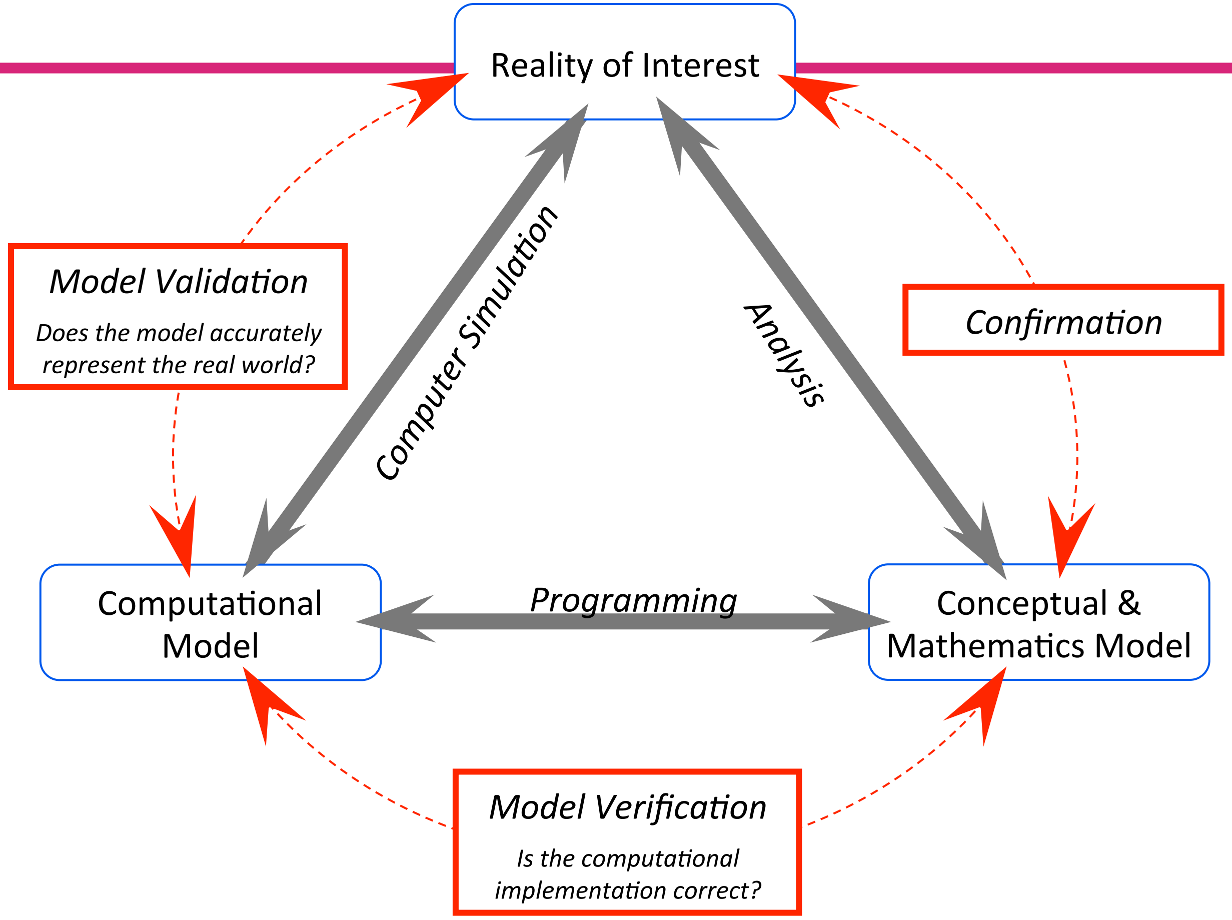
  } **Statistical Evidence**

- Verification: Process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model
  - Math issue: "Solving the equations right"

- Validation: Process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
  - Physics issue: "Solving the right equations"

Verification must precede validation; and when used, calibration must precede validation and use different data .

Verification and Validation Standards



Extracted From: B. Thacker (SWRI), AIAA Structures Technical Committee, 09-06-02; proceeded by (1) AIAA V&V Guide 1998 and (2) S. Schlesinger, "Terminology for Model Credibility", *Simulation*, Vol.32, No. 3, 1979 pp.103-104

- The process of building credibility remained largely ad hoc until American Institute of Aeronautics and Astronautics (AIAA), "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations", AIAA G-077-1998.
- Heavily influenced "Guide for Verification and Validation in Computational Solid Mechanics", ASME V&V 10-2006. This is often recommended as an excellent starting point for further investigations into the practice of V&V.

ASME V&V History and Structure

- In 1999 an ad hoc verification & validation specialty committee was formed under the auspices of the United States Association for Computational Mechanics (USACM)
- In 2001 the American Society of Mechanical Engineers (ASME) approved the committee's charter:
  - To develop standards for assessing the correctness and credibility of modeling and simulation in computational solid mechanics.
- Committee was assigned the title and designation of the ASME Committee for Verification & Validation in Computational Solid Mechanics (PTC 60).
- With the addition of other V&V committees, an overarching committee (V&V Standards Committee) was formed and PTC 60 was changed to V&V 10

Current Structure:

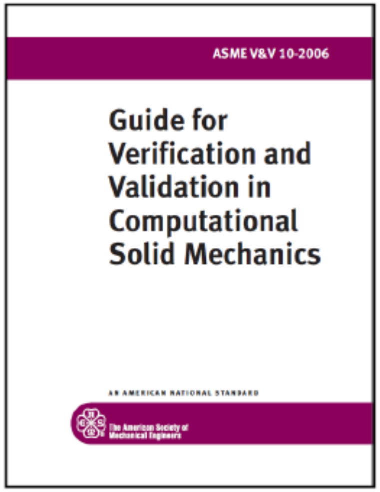
V&V Standards Committee in Computational Modeling and Simulation

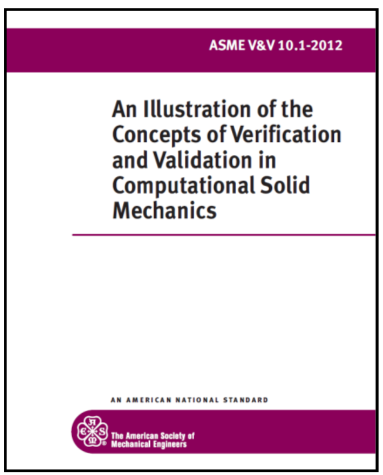
- V&V 10 - Verification and Validation in Computational Solid Mechanics
- V&V 20 - Verification and Validation in Computational Fluid Dynamics and Heat Transfer
- V&V 30 - Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior
- V&V 40 - Verification and Validation in Computational Modeling of Medical Devices

Current and Near Term Efforts for ASME V&V 10:

- V&V 10-2006 - Guide for Verification and Validation in Computational Solid Mechanics – Published 2006 (revision soon)
- Draft V&V 10.1 - An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics – Published 2012
- Draft V&V 10.2 - Role of Uncertainty Quantification in Verification and Validation of Computational Solid Mechanics Models – Rough draft
- Draft V&V 10.3 - Role of Validation Metrics in Verification and Validation of Computational Solid Mechanics Models – Outline
- Draft V&V 10.X – Value of V&V for Decision Making – Not started
- Several others identified…

ASME Verification & Validation Process Chart





Simple Models

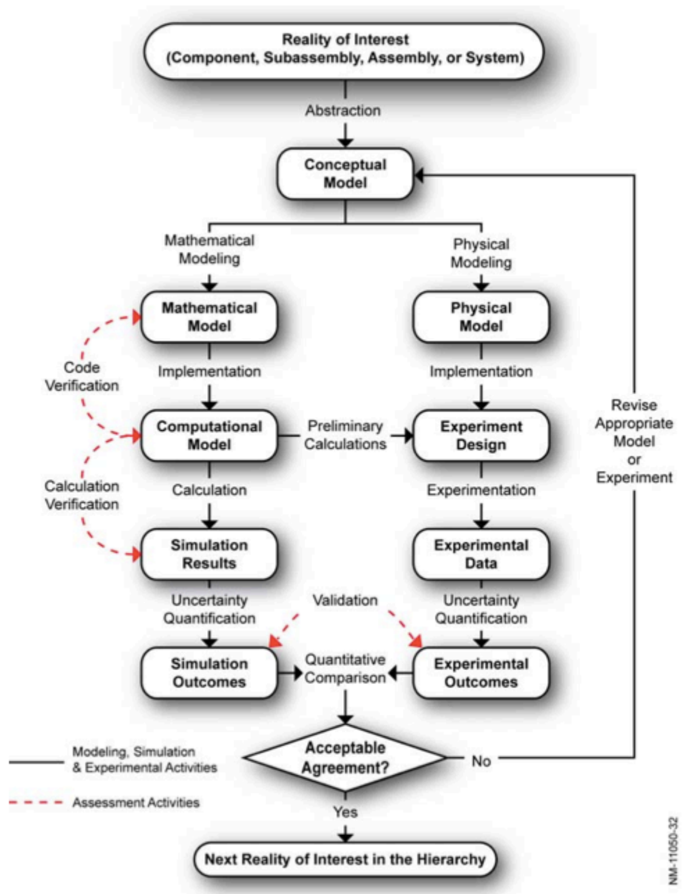
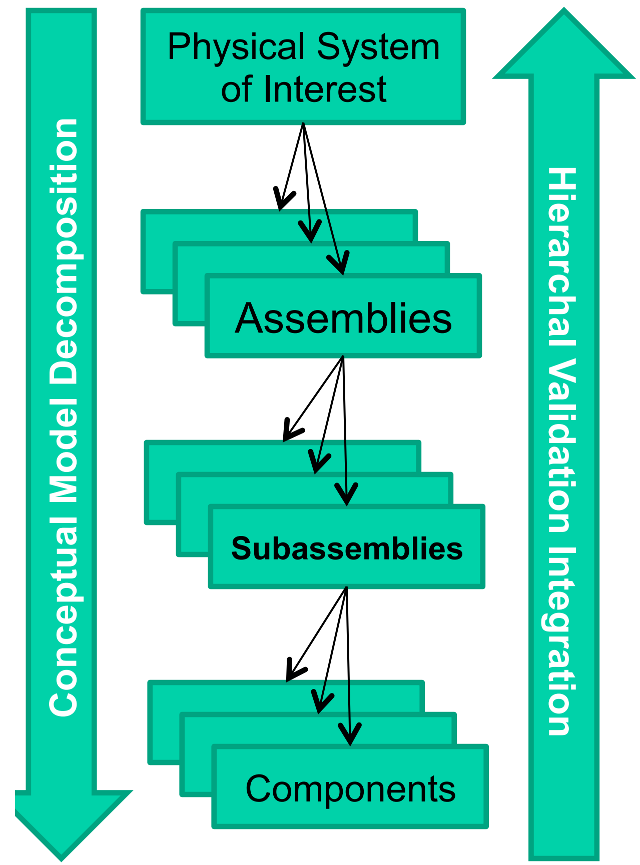
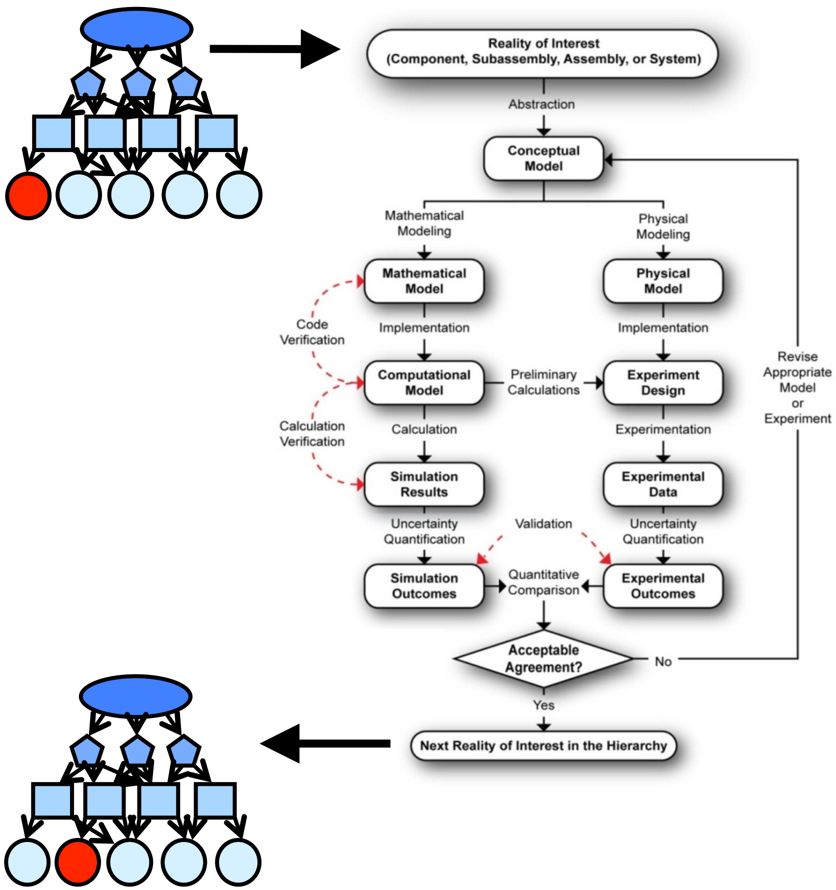


Figure 2 Verification & Validation activities and outcomes. (*Guide Figure*)

Complex Models

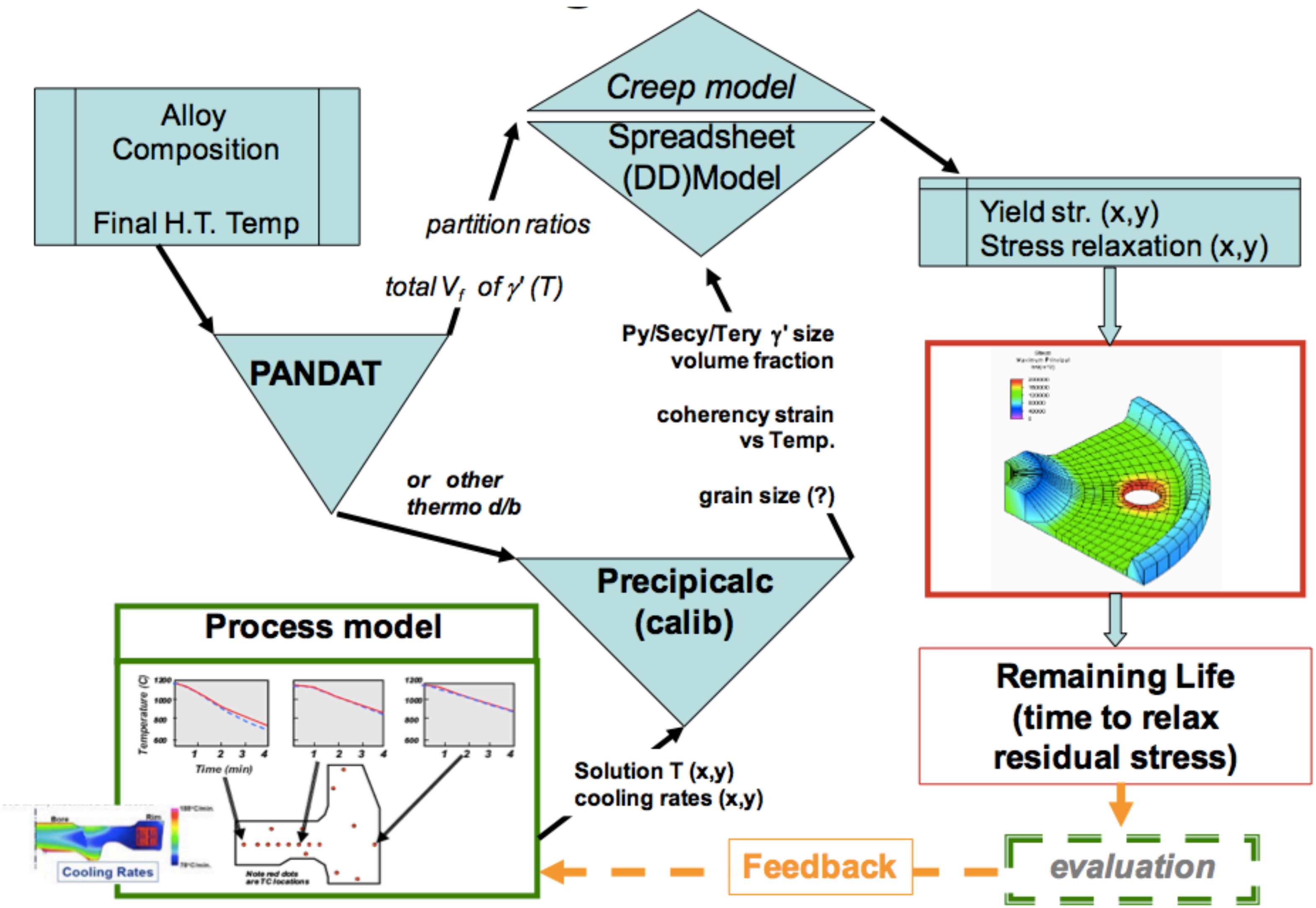


Validation Hierarchy



- Validation hierarchy
  - Breaks the problem into smaller parts
  - Validation process employed for every element in the hierarchy (ideally)
  - Allows the model to be challenged (and proven) step by step
  - Dramatically increases likelihood of right answer for the right reason
- Customer establishes intended use and top-level validation requirement
- Validation team constructs hierarchy, establishes sub-level metrics and validation requirements
- In general, validation requirements will be increasingly more stringent in lower levels
  - Full system sensitivity analysis can provide guidance

Case Study: Model Hierarchy



Summary: V&V Process

- Design and develop the modeling and V&V plan
- Design and develop models
- Verify the model implementation
- Perform UQ and sensitivity studies to understand uncertainties
- Design validation/calibration experiments
- Perform experiments
- Assess accuracy (validation)
- Revise model/experiment
- Document the model, process, and accuracy assessments