Session B1

V&V (esp. validation) for M&S in Computational Science and Engineering Applications

Session B1 leaders:

Co-Chairs: **Unmeel Mehta** (NASA/Ames) and **Hans Mair** (IDA)
Session Recorder: **Len Schwer (Schwer** Engineering & Consulting)

B1 Materials in Foundations '02 proceedings:

Paper

Verification, Validation, and Predictive Capability in Computational Engineering and Physics (74 pp)

William L. Oberkampf (Sandia National Laboratories)
Timothy G. Trucano (Sandia National Laboratories)
Charles Hirsch (Vrije Universiteit Brussel -- Brussels, Belgium)

Slides (may contain back-up materials and notes)

Verification, Validation, and Predictive Capability in Computational Engineering and Physics (36 slides) [B1B – only in pdf format]

William L. Oberkampf (Sandia National Laboratories)
Timothy G. Trucano (Sandia National Laboratories)
Charles Hirsch (Vrije Universiteit Brussel -- Brussels, Belgium)

Supplemental Presentations

There were two supplemental, alternative view, presentations that are documented by the viewfoils used in presentations by **Hugh Coleman** and **Unmeel Mehta**. The slides of these presentations follow the discussion below.

Participants in this session are listed at the end of the Discussion Synopsis.

Discussion Synopsis (to provide perspective on papers & briefings identified above).

Discussion Issues

There were four distinct topics covered in the discussion portion of the session:

1. Definition of Verification
2. Uncertainty Quantification
3. Validation Metrics
4. Predictability

Verification Definition

Do the words correctness and accuracy mean the same thing in your definition of verification? They are closely related, but they are not the same. We to use the word "accuracy," because we can only evaluate accuracy. Correctness implies that the code is correct.

Uncertainty Quantification

How do you calculate uncertainties in simulation (referring to viewfoils presented by Coleman – these are at the end of the discussion section)? We do not have good ways to estimate. Separate uncertainty into numerical error and model uncertainty and experimental side bias and random uncertainty. Use of Richardson Extrapolation on unstructured grids is more difficult than on structured grids. Thus numerical errors are difficult to quantify.

Of the two ways to account for model bias uncertainty: 1) correct for statistically, or 2) via improved physics, which is preferred? Eliminate bias error as much as possible via model improvement as much as affordable, for example, by including omitted physics. If you are close to the validation database, i.e. know a lot about the problem, you can easily correct the bias error. Increase in risk occurs as your predictions move away from the validation database.

Is there a way to correct for bias error in experiments? For known bias errors, account for them and eliminate the error. For unknown bias error you can move the experiment to another facility, or make independent measurements of the same quantity. For certain correlated bias errors, one can eliminate these using statistical methods combined with symmetry techniques. You can also use an analytical model of the measurement to check the bias.

Validation Metrics

Do you consider validation metrics associated with various system responses to be separate from prediction uncertainty quantification, i.e. associated with characteristics of the system? This list of metrics includes parametric metrics that described model parameters. Figure 12 (Oberkampf, et al paper presented immediately below) shows increasing validation metric complexity. There is clearly a hierarch of system response metrics that should be used. The key point is the customer requirements must provide guidance to the modeler as to that metrics are importance and what level of accuracy is required. Can historical data uncertainty quantification metrics be propagated through a new model and thus help lend confidence to the model predictions? This can be done provided the model and prediction spaces are close.

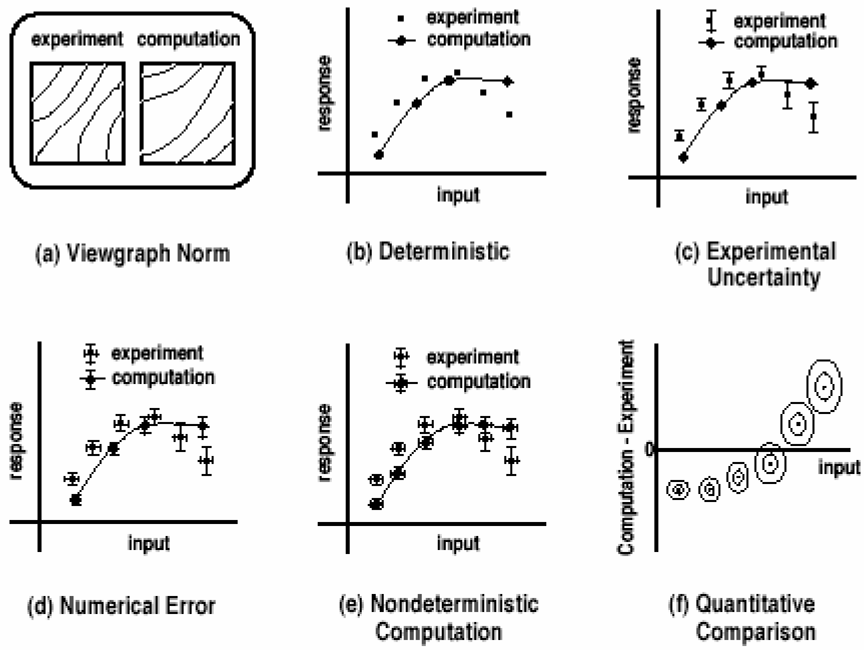


Figure 12
Increasing Quality of Validation Metrics
(adapted from Ref. [185])

Predictability

How do you quantify uncertainty in model predictions? Can only quantify the error in the model space, but currently there is no good way to project what the error will be in the predictions space. The extrapolation to the predictions space is mostly one of extrapolating the physics, but this must be done using statistical techniques. Another approach is to use Alternative Plausible models of the physical Processes – i.e. multiple models to make the predictions, where each model has a different physics basis. The hope is that if these models provide similar predictions there is some confidence the prediction is correct, but of course all the models could have the same flaw of lack of correct physics needed to make the sought after prediction. In ship model example, Coleman presented, there is a rich history of extrapolating from small tank models to full-size ships, so confidence in predictions is increased. This is similar to Bayesian updating where the small tank results are your prior data. This is also a case where the prediction space is close to the model space.

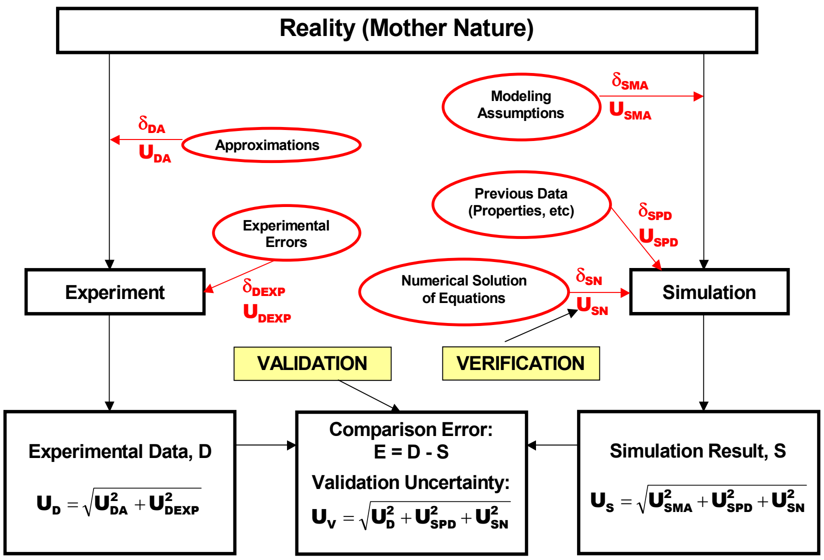
Confidence in the prediction is a function of the confidence demonstrated in the complete system, as well as subsystem models. This is particularly important when the complete system cannot be experimentally tested.

Can sensitivity analysis be used to guide confidence in predictions? Yes, sensitivity analysis is useful in adding to prediction confidence to prioritize the many parameters in a model.

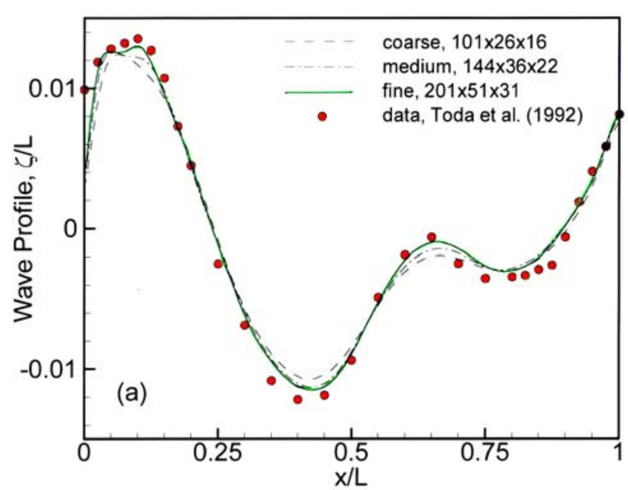
Referring to validation metric Figure 12 (shown above), is the lower right (most complex) validation metric an indication of confidence in the prediction? No. These validation metrics apply only to the validation tests and their associated models. But as has been mentioned before, the issue of predictive capability is related to the "closeness" relationship of the validation domain to the prediction space.

Coleman presentation (4 slides):

Schematic of Verification and Validation of a Simulation

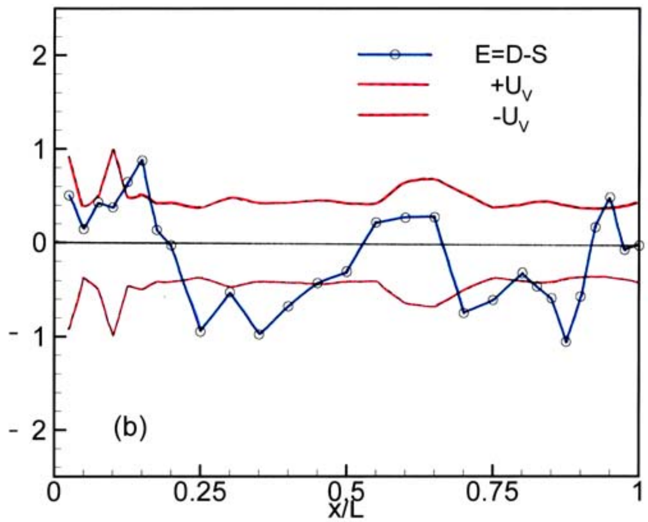


Ship Wave Profile Validation
Traditional Comparison



Ship Wave Profile Validation

Coleman-Stern Comparison

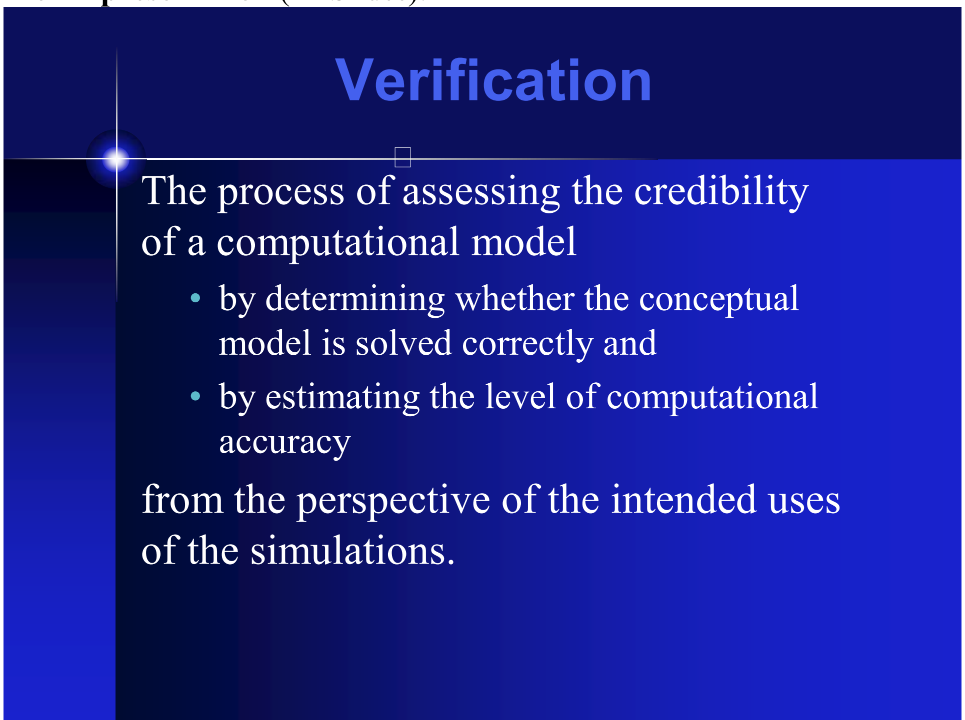


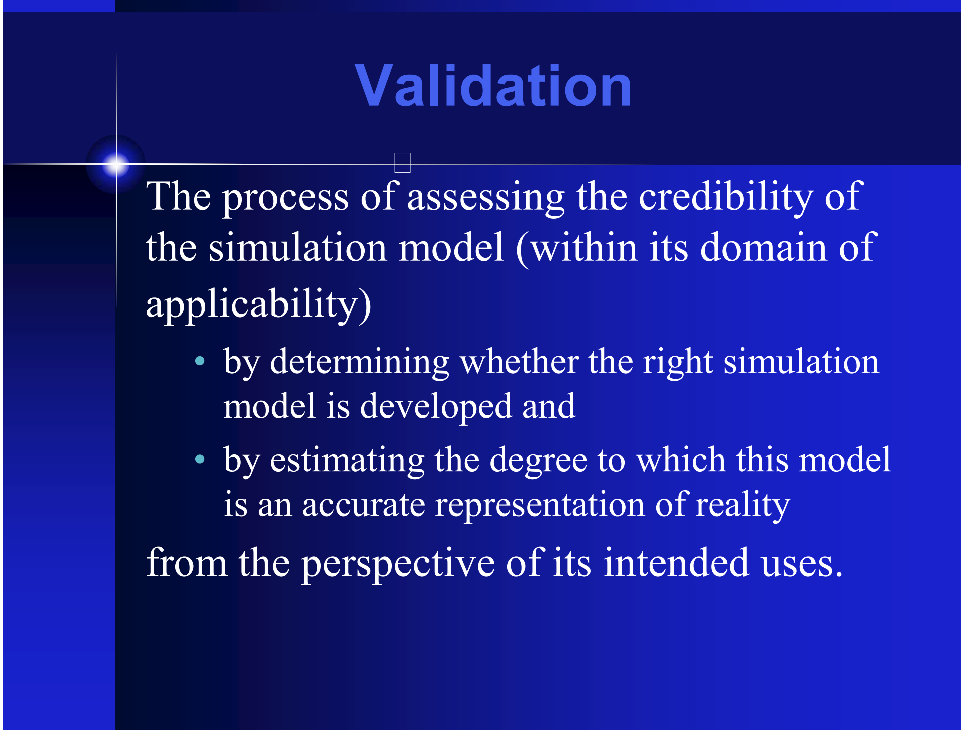
→ suppose U_{reqd} = 0.2? = 2.0?

Some Selected References

- Coleman, H.W. and Stern, F., "Uncertainties in CFD Code Validation," ASME J. Fluids Eng., Vol. 119, pp. 795-803, Dec. 1997. (See also Roache, P. J, "Discussion" and Coleman and Stern, "Authors' Closure," ASME J. Fluids Eng., Vol. 120, pp. 635-636, Sept. 1998.)
- Roache, P. J., Verification and Validation in Computational Science and Engineering, Hermosa, 1998. (www.hermosa-pub.com)
- Guide for the Verification and Validation of Computational Fluid Dynamics Solutions, AIAA Guide G-077-1998, 1998. (www.aiaa.org)
- Coleman, H. W., Stern, F., Di Mascio, A., and Campana, E. "The Problem With Oscillatory Behavior in Grid Convergence Studies," *J. Fluids Engineering*, Vol. 123, No. 2, p438-439, June 2001.
- Stern, F., Wilson, R. V., Coleman, H.W., and Paterson, E. G., "Comprehensive Approach to Verification and Validation of CFD Simulations—Part 1: Methodology and Procedures," ASME J. Fluids Eng., Vol. 123, pp. 793-802, Dec. 2001.

Mehta presentation (12 Slides):





DMSO's Definitions for V&V

- Definitions are developed principally for operations research problems.
- Philosophy
  - Verification deals with the implementation (code/system).
  - Validation deals with the representations embedded for simulation.
- Practice
  - Verification checks "Did I build the code right?" given the specification.
  - Validation checks for the credibility of simulation in terms of numerical accuracy *and* phenomenological accuracy for the intended use.

"What we observe is not nature itself, but nature exposed to our method of questioning."

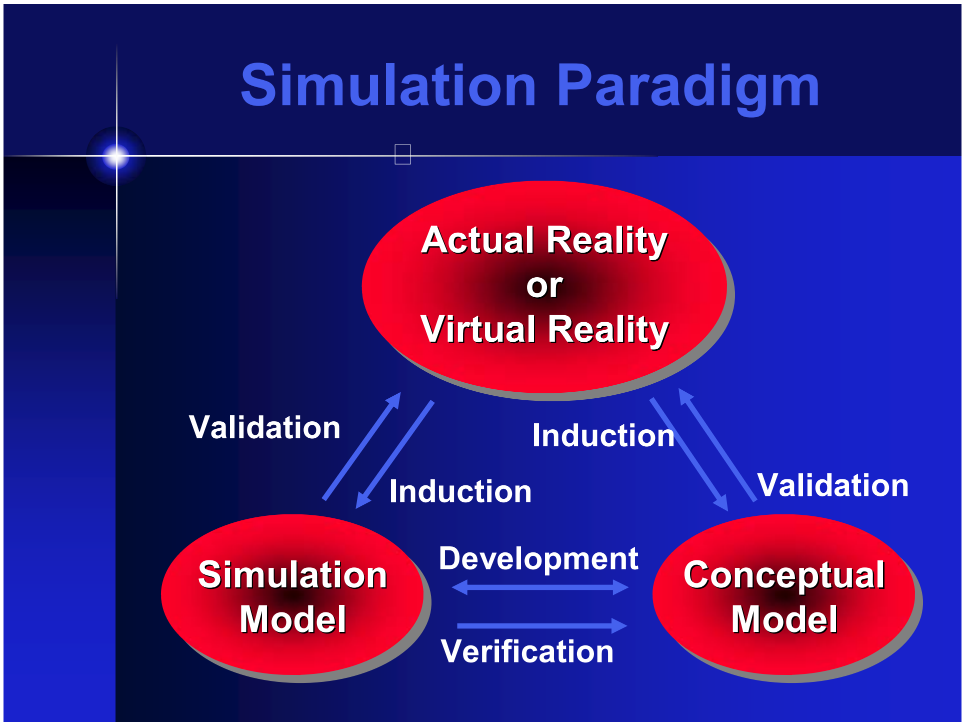
— Werner Karl Heisenberg

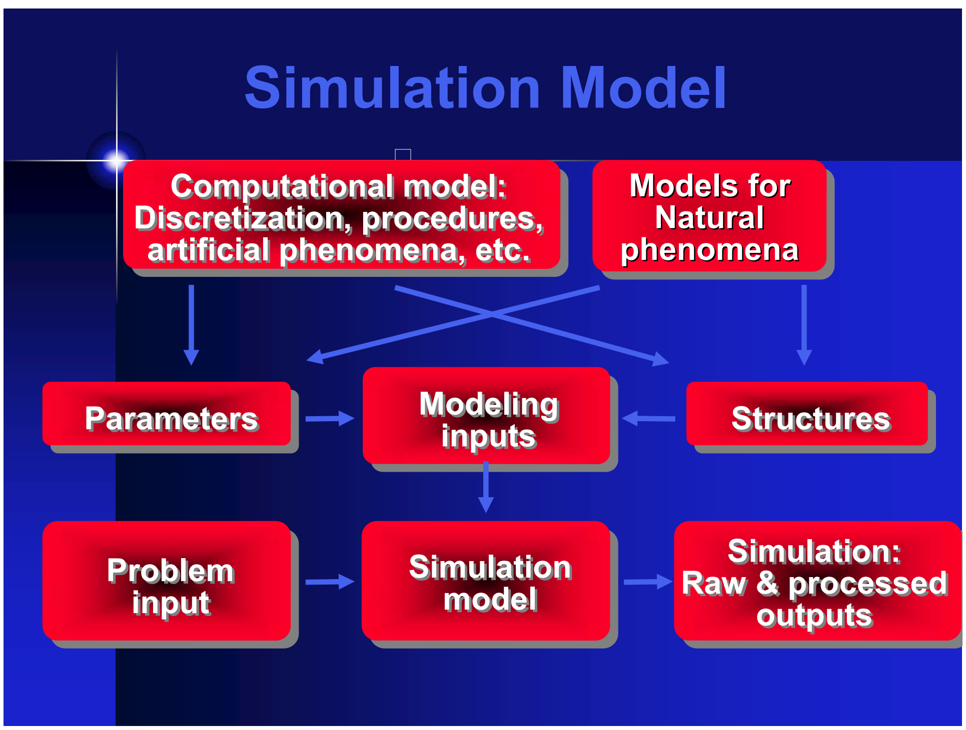
Error and Uncertainty in Mathematics

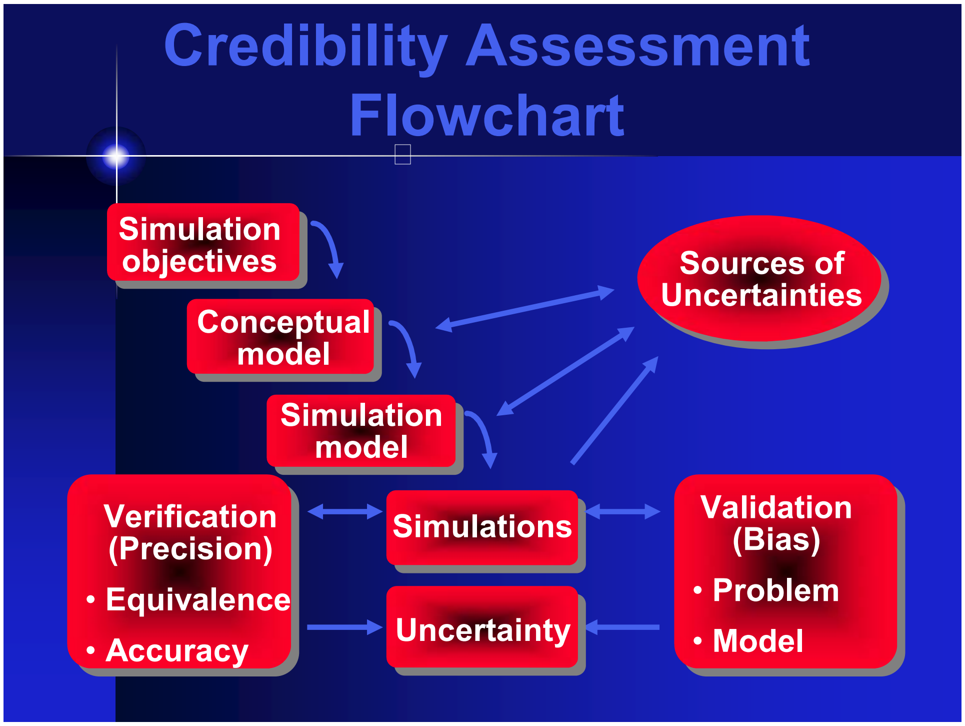
- Error: "The difference between a computed or measured value and a true or theoretically correct value." (*The American Heritage Dictionary of the English Language*, 3rd Ed., 1992.)
- Uncertainty: "The estimated amount or percentage by which an observed or calculated value may differ from the true value." (*The American Heritage Dictionary of the English Language*, 3rd Ed., 1992.)
- "Uncertainty may range from a falling short of certainty to almost complete lack of definite knowledge especially about an outcome or result." (*Webster's Ninth New Collegiate Dictionary*, 1990.)

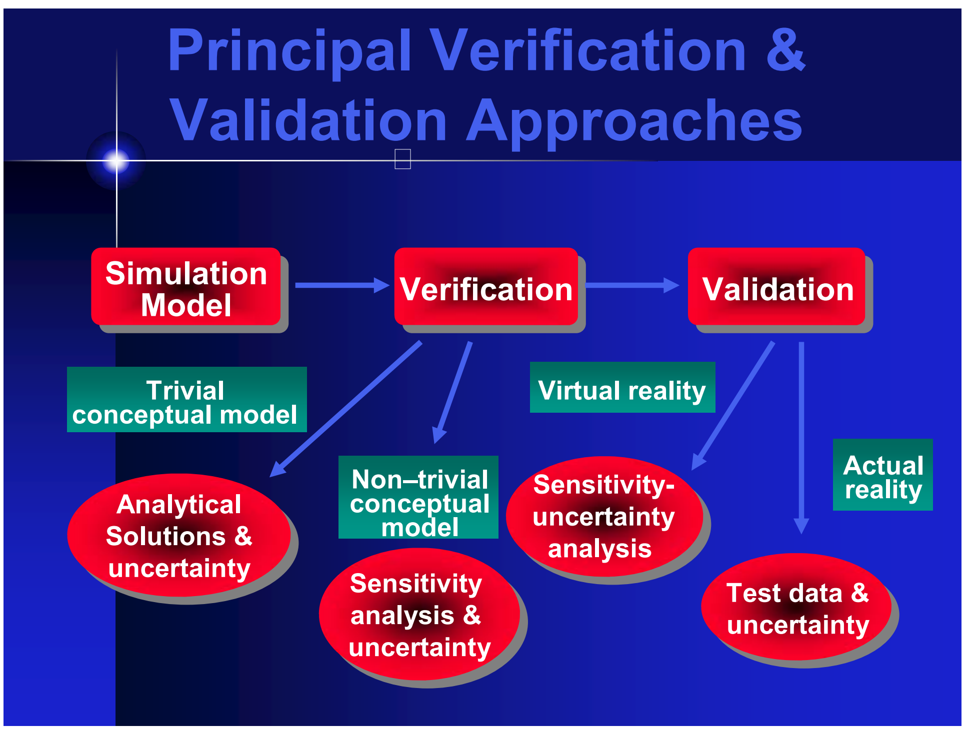
Uncertainty Exist

- We do not have sufficient understanding of nature.
- We do not have sufficient computational capability.
- We cannot measure initial conditions with sufficient accuracy.
- Models and simulations are inherently uncertain.


Simulation Paradigm
Actual Reality
or
Virtual Reality
Validation
Induction
Induction
Validation
Simulation
Model
Development
Verification
Conceptual
Model


Simulation Model
Computational model:
Discretization, procedures,
artificial phenomena, etc.
Models for
Natural
phenomena
Parameters
Modeling
inputs
Structures
Problem
input
Simulation
model
Simulation:
Raw & processed
outputs


Credibility Assessment Flowchart
Simulation objectives
Conceptual model
Simulation model
Sources of Uncertainties
Verification (Precision)
• Equivalence
• Accuracy
Simulations
Uncertainty
Validation (Bias)
• Problem
• Model


Principal Verification & Validation Approaches
Simulation Model
Verification
Validation
Trivial conceptual model
Virtual reality
Actual reality
Analytical Solutions & uncertainty
Non–trivial conceptual model
Sensitivity-uncertainty analysis
Sensitivity analysis & uncertainty
Test data & uncertainty

Observations

- What matters is uncertainty (precision and bias), not veracity or validity, because the best measure of numerical or physical accuracy is uncertainty.
- The sensitivity-uncertainty analysis is the key for achieving credible simulated virtual reality.
- The management of uncertainty is a critical and principal activity for fully achieving the promise of modeling and simulation technology.

Uncertainty Evaluation

- Type A uncertainty evaluation is done by the statistical analysis of a series of simulations.
- Type B uncertainty evaluation is conducted by means other than the statistical analysis of a series of simulations.
- Systematic (or random) uncertainty may be obtained by either a Type A or Type B evaluation.

B1 Session Participants (39)

First Name	Last Name	Organization
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Timothy	Hasselman	ACTA, Inc.
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Wu	Li	NASA Langley
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Jian	Tu	General Motors
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