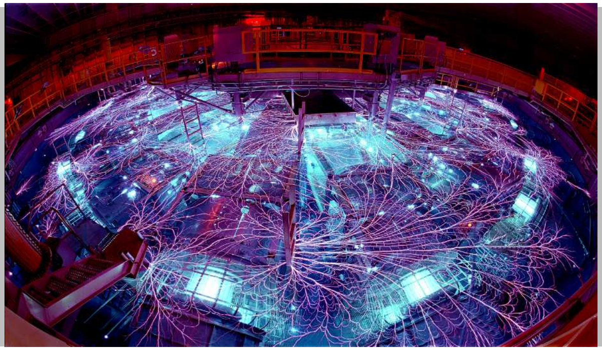
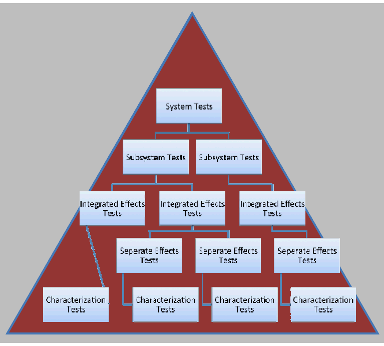
SAND2013-3653C

Exceptional service in the national interest

Sandia National Laboratories





The Validation Hierarchy and Challenges in Rolling Up Validation Results to a Target Application

ASME 2013 V&V Symposium, Las Vegas

Richard Hills

SAND Number: ????????

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

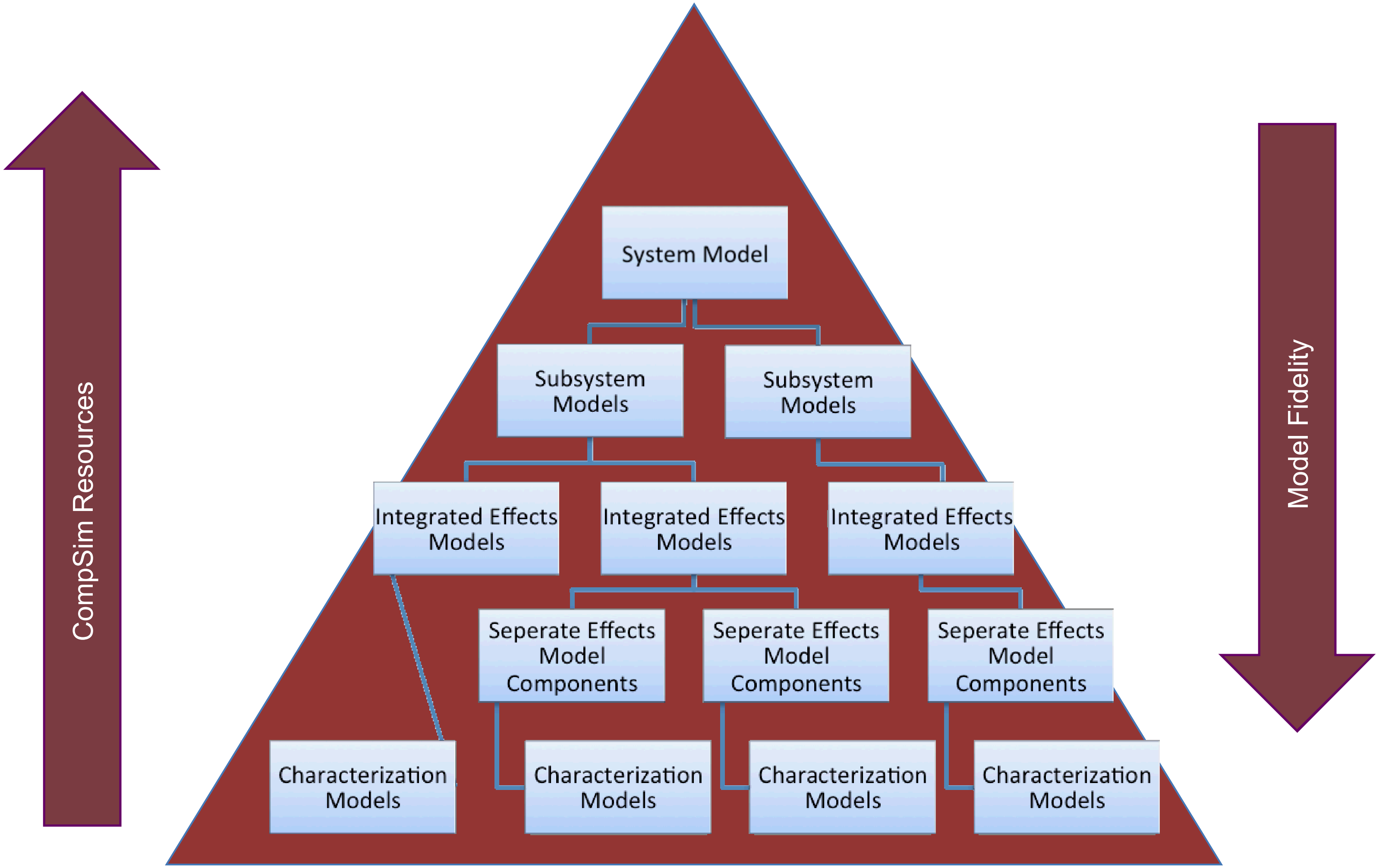
Outline

- Major challenges we face at Sandia National Laboratories (SNL) related to validation results
- The validation and computational hierarchy
- Existing approaches to rolling up validation results to a target application
- Desired features and path forward in developing such methodology

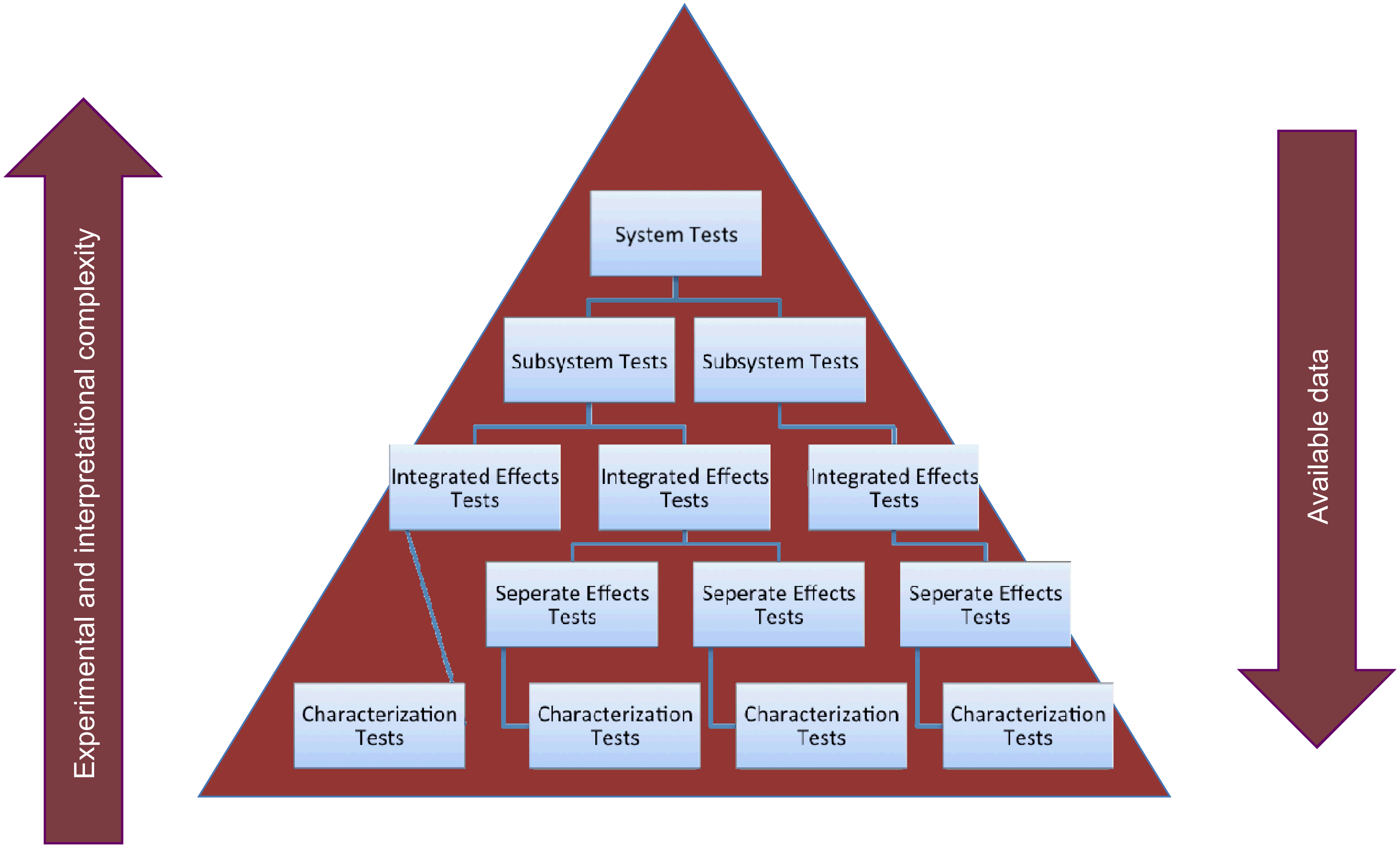
Major Challenges

- Validation experiments are expensive – how can we maximize return?
- CompSim is expensive – how do we optimize the 'error budget'
- Validation hierarchies are designed by humans and rely heavily on judgment
- Validation hierarchies have missing components – sometimes due to expense, sometimes due to inability to reproduce the application conditions
- Uncertainties exist throughout the computation (CompSim), experiments (PhysSim), and the conceptual design of the hierarchy
- Validation hierarchies are heterogeneous – we don't always measure the same quantities at the same conditions as are of interest for the target application
- Model form error is always present, how do we handle this?
- How do observed model form errors and their uncertainty impact the ability to simulate the behavior for the target application?
- Unexpected things happen!

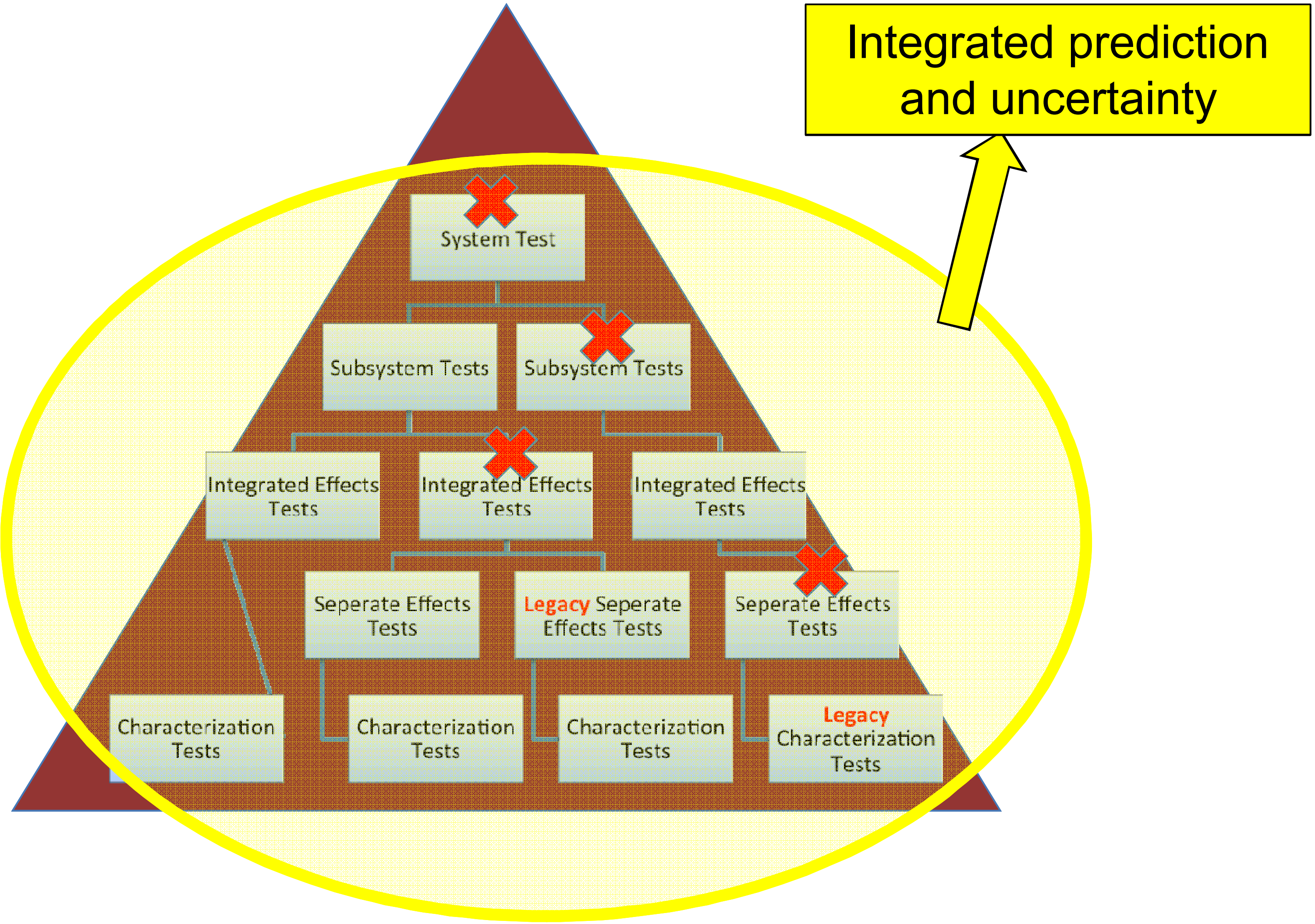
Computational Hierarchy or Pyramid



Validation Hierarchy



Incomplete Validation Hierarchy



An ideal CompSim framework is one that…

Is a team effort between the customers, analyst, experimentalist, and code developers – “no throwing information over the fence”

- Identifies the customer needs for the target application early on
- Identifies the quantities of interest (what are we trying to predict)
- Identifies the important physics that should be addressed by the CompSim
- Identifies the important physics that should be addressed by the validation hierarchy
- Utilizes CompSim models to help design the hierarchy and the individual experiments in the hierarchy, when appropriate

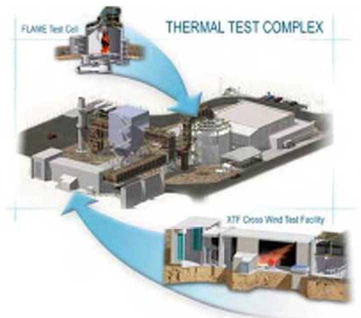
An ideal CompSim framework is one that…

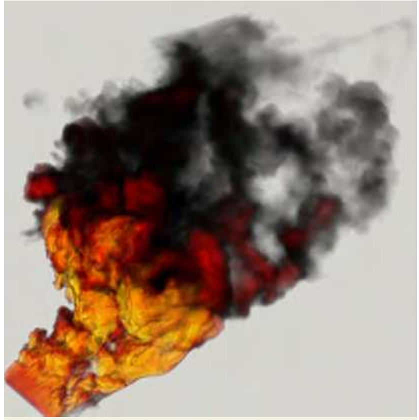
- Quantifies observed differences between prediction and measurements and the uncertainties in these differences - Validation

- Evaluates the impact of these differences and their uncertainties on target applications predictions – UQ

- Evaluates the ‘confidence’ one has in the target application predictions and the quantified uncertainties in these predictions - Judgment

- Is iterative and adaptive - Flexible





Approaches to Roll-Up of Observed Model Form Error

- Calibration or multiple calibrations (Babuška, et al.)
  - Potentially useful if the impact of model form error can be captured by multiple calibrations
- Calibration including model deficit term (Kennedy and O'Hagan)
  - Potentially useful when validation measurement types are the same as the response quantities of interest for the target application (homogeneous hierarchy)
- Bayesian net – evaluates a measure of reliability based on validation results and propagates to target application through common parameters (Mahadevan)
  - Potentially useful if reliability measures defined at the validation level can be related to application conditions through uncertainty in common parameters
- Sampling based Meta-model (Hills) – uses sampling and Partial Least Squares regression to develop a Meta-model to relate validation experimental results to the quantity of interests for the target application
  - Potentially useful for heterogeneous validation hierarchies if the source of model form errors is secondary rather than primary

Best Approach?

- Issue: All approaches utilize the CompSim models for the validation experiments and the target application – if physics is missing, all approaches are approximate at best, misleading at worst

- An open research question: Ideas appreciated

Desirable Features of Methodology

- Provides information to support the design of the validation hierarchy to assess
  - Completeness or coverage of the physics of the target application
  - Impact of lack of completeness on uncertainty in a prediction
  - Importance of specific experiments to the application

- Rolls up the validation results from the hierarchy to the target application to provide
  - Assessments (metrics) that are relevant for the physics and conditions of the application
  - Characterizes the impact of observed validation differences and uncertainties in these differences on an application prediction

- Applies to heterogeneous hierarchies

Path Forward at SNL

- Recognized need to develop and test methodology for roll-up
- Interest by analyst in testing methodology for various applications using available data for their applications
- SNL's approach: Experience, experience, experience on real applications
- Continuing to explore strengths and limitations of existing methodologies
- Continue to be on the lookout for other methodologies that may be applicable

Questions?

Relevant Publications

Sandia National Laboratories

Approaches:

- Babuska, I., F. Nobile, R. Tempone (2008), A Systematic Approach to Model Validation Based on Bayesian Updates and Predicted Related Rejection Criteria, Computer Methods in Applied Mechanics and Engineering 197:2517-2539.
- Kennedy, M.C., O'Hagan, A. (2001), Bayesian Calibration of Computer Models, Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63(3):425-464.
- Mahadevan, S. (2011), Roll-Up of Multi-Level UQ Activities towards System Level QMU, Presented at Sandia National Laboratories, Albuquerque, NM, Oct. 4.
- Hills, R.G., J.R. Hamilton (2009), Validation Experiments to Application: A Model Based Approach, SAND2009-1091 Unlimited Release Printed February 2009
- Hamilton, J. R., R. G. Hills (2010a), Relation of Validation Experiments to Applications, Numerical Heat Transfer, Part B: Fundamentals, 57: 5, pp. 307-332.
- Hamilton, J. R., R.G. Hills (2010b), Relation of Validation Experiments to Applications: A Nonlinear Approach, Numerical Heat Transfer, Part B: Fundamentals, 57: 6, pp. 373-395.