SANDIA REPORT
SAND2017-1753
Unlimited Release
Printed February 2017

Recommend Research Directions for Improving the Validation of Complex Systems Models

Eric Vugrin, Timothy Trucano, Laura Swiler, Patrick Finley, Tatiana Flanagan, Asmeret Naugle, Jeffrey Tsao, Stephen Verzi

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Abstract

Improved validation for models of complex systems has been a primary focus over the past year for the Resilience in Complex Systems Research Challenge. This document describes a set of research directions that are the result of distilling those ideas into three categories of research—epistemic uncertainty, strong tests, and value of information. The content of this document can be used to transmit valuable information to future research activities, update the Resilience in Complex Systems Research Challenge's roadmap, inform the upcoming FY18 Laboratory Directed Research and Development (LDRD) call and research proposals, and facilitate collaborations between Sandia and external organizations. The recommended research directions can provide topics for collaborative research, development of proposals, workshops, and other opportunities.

ACKNOWLEDGMENTS

The authors thank Theresa Brown, William Hart, and Vicente for their thorough and thoughtful reviews. The authors also appreciate the funding and programmatic support provided by Carol Adkins, Peter Davies, Marcey Hoover, William Rhodes III, Steven Kleban, and Rossitza Homan.

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NOMENCLATURE

CS	Complex systems
QOI	Quantity of interest
VVUQ	Verification, Validation, and Uncertainty Quantification
UQ	Uncertainty Qualification
VOI	Value of Information
V&V	Verification and Validation

1. INTRODUCTION

Model[1] development is a multistep process (Figure 1), and model validation is a key step in that process. Model validation addresses the question, “Is the model adequate to use for the intended application?” (Oberkampf and Roy 2010). Validation typically involves a quantitative comparison between experimental data and computational simulation results (Liu et al. 2011). Model validation activities provide model developers and users a better understanding of the model’s strengths, weaknesses, limitations, and appropriate uses. In short, model validation activities are critical for assessing, improving, and providing confidence in models.

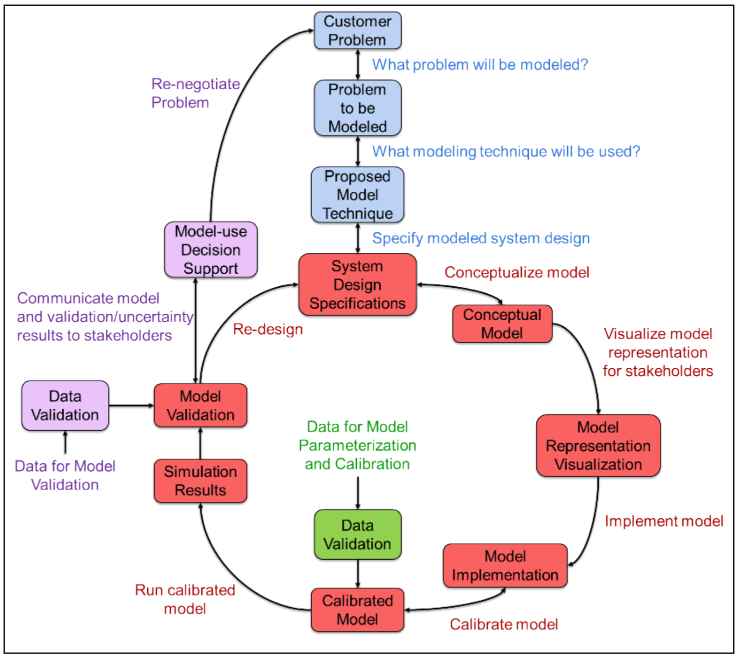

Figure 1. Model Development Process, adapted from Balci (1998).

Three sets of factors typically influence the design and execution of model validation activities:

1. The system being modeled: System attributes and characteristics affect model design and implementation decisions such as which system features to include, which numerical algorithms to select, and other fundamental modeling decisions. Additionally, the system itself affects validation considerations, such as
   - What data is available for testing?
   - Are those data suitable for testing purposes and relevant to the conditions under which the proposed is intended to be used?
   - Can one design and perform experiments to gather additional data? If so, how easily and quickly can we do so?
   - What is the state of knowledge and uncertainty in model parameters and other model features?

[1] For the purposes of this document, we restrict our discussion to computational models, i.e., models that are created to provide numerical quantities of interest and are implemented in some form of software. Hence, in this document, the term “model” is used to refer to computational implementations of physically descriptive mathematical models.

The system itself provides constraints that may limit the validation activities that can be rigorously performed.

2. Intended model uses: model validity is not considered in an absolute sense. Rather, it is considered in the context of the model's intended use. As such, model validation activities are affected by the following:
    - The questions and analyses that one is trying to address through model usage;
    - The requirements that are defined for the model.
    - The specific quantities of interest (QOIs) that the model is used to generate. Selection of the QOIs is an important step for not only giving the model users the information that they require, but the QOIs also guide which model variables will be used in model validation tests and acceptance criteria specification.
    - Additional factors that may be specific to the intended use. For example, acceptance criteria in validation tests for models used to inform high-consequence decisions may permit only small discrepancies between model outputs and experimental data. The need to complete model development and validation activities in a rapid time frame could be another consideration.

    The intended model uses frequently establish the scope on what modeling activities are required.

3. Feasibility constraints: time and resource constraints, information diagnostics limitations, personnel/skill limitations, etc. are all factors that can affect design and implementation of validation activities. Though these factors are not necessarily technical in nature, they can still have significant influence on validation activities.

Improving model validation continues to be an active area of research. The U.S. Department of Energy's Advanced Simulation and Computing (ASC) program (e.g., Goodwin and Juzaitis 2006; Diegert et al. 2007; Higdon et al. 2008), the American Society of Mechanical Engineers 20-2009 Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer (ASME 2009), and the American Institute of Aeronautics and Astronautics' Guide for the Verification and Validation of Computational Fluid Dynamics Simulations (G-077-1998e) (AIAA 1998), and Oberkampf and Roy (2010) are exemplary verification and validation expository efforts that have significantly advanced the state of the art for model validation. Nevertheless, model validation often still presents a challenge to model developers and users, and recent efforts at Sandia National Laboratories (Sandia) have focused on the additional challenges presented when attempting to validate models of complex systems.

Complex systems are emergent, multi-agent systems that operate without central control (Boccara 2004). The following are some of the fundamental attributes of complex systems present significant challenges when attempting to validate models of complex systems:

4. <u>Observation of key system elements</u>: Fundamental system structures of complex systems are frequently unknown or unobserved. In some cases, the mere act of measuring or observing the system will cause the system to fundamentally change (e.g., monitoring security measures may cause adversaries to change approaches). Validation activities not only require some level of observations but also rigorous characterization of those

observations (e.g., what do we really know about the observations and how do we regard them?).

5. Adaptive interactions: Individual system components may be observable, but the interaction mechanisms between the components may be unknown or unmeasurable. So validation activities that focus on individual components may not provide suitable information for validating system-level behaviors.
6. Heterogeneity: Complex systems are often composed of so many different components that it can be difficult and time-consuming to gather necessary validation data on most, if not all, of the components. Decomposition of systems into meaningful, effective subsystems may be difficult and non-unique, presenting additional challenges to data collection.

The intended uses of complex systems models also provide validation challenges. For example, outcomes of interest may be qualitative; models are often built to investigate qualitative repercussions of system structure or assumptions rather than for predictive estimation. Additionally, in most instances, it is simply not possible to run a full-scale, controlled experiment for validation of a complex system application. Modeling the effects of a terrorism event on social networks is one such example.

Sandia has recognized that many of the national security challenges that the Labs address involve complex systems. Consequently, Sandia has initiated the Resilience in Complex Systems Research Challenge (RCS RC; Griffith and Kleban 2015). The goal of the RCS RC is to provide Sandia the capability needed to understand and control the resilience in complex systems important to Sandia's national security missions. The RCS RC has recognized that validation of complex systems models remains a significant challenge to the complex systems community, and at the recommendation of the RCS RC's external advisory board (Hubler et al. 2015), the RCS RC has prioritized improved validation of complex systems as a key research thrust. Towards this goal, Sandia hosted a workshop in Albuquerque, New Mexico June 22–24, 2016, bringing together researchers from the complex systems and validation communities. The purpose of the workshop was to discuss how to advance the state of knowledge and practice of validation for complex systems models. The workshop included two days of extensive presentations, brainstorming, breakout sessions, and discussions. By the end of the workshop, a large amount of ideas and research topics had been put forth and documented (Tsao et al. 2016).

This document describes a set of recommended research directions for validation of complex systems that emerged from the workshop. Following the workshop, a team of Sandians met to discuss and distill the information generated from the workshop into three sets of research directions. The following are the recommended research themes:

- Epistemic uncertainty: All modelers must determine how to handle potential uncertainties within their models. However, some challenges related to addressing epistemic uncertainties are either unique or more prevalent in models of complex systems.
- Strong Tests: Strong tests represent the ideal for validation testing. The development of guidelines for creating stronger validation tests of complex systems models could increase the rigor and formality with which validation activities are performed.
- Value of Information: Modelers of complex systems frequently seem to struggle with information challenges. They either do not have enough, have too much, or do not have the right kind of information. The ability to better understand the tradeoffs between

gathering additional information, the value of the information, and the cost and resources required to do so would help optimize resource use to for all model development stages, including validation.

The remainder of this document is structured as follows. The next section provides a brief literature review of complex systems model validation. The following three sections describe each of the individual research directions in greater detail, and the final section describes opportunities for how this document and the research thrusts can be used.

2. PREVIOUS WORK

Model validation is not a new idea for the complex systems community. Though models of complex systems can take on many forms, much of the validation-related work and discussions have focused on two modeling forms: system dynamics models and individual-based models (e.g., agent-based models). Because the two modeling approaches are rather different, the validation efforts have been unconnected. We describe them briefly below.

2.1. Validation and System Dynamics Models

The system dynamics community in general considers validation to be a process used to build confidence in a model (Forrester and Senge 1980). Since validation must be done in relation to the specific problem of interest, model, and audience, model validity is not an absolute concept. Instead, the system dynamics community frequently considers model validity to be a continuous spectrum in which a model is deemed more valid as more evidence is collected that instills greater confidence (Forrester and Senge 1980; Barlas and Carpenter 1990). This approach does not establish objective, formal validation tests of system dynamics models (Barlas 1996). Nevertheless, Sterman (1984) suggests that formal tests are necessary for instilling confidence, and that model validation can be used to provide confidence that the model has utility as a tool for its intended purpose (Forrester and Senge 1980). Though validation activities have been performed for system dynamics models, validation has admittedly not been a focus of the field, and system dynamics modeling projects often do not attempt validation at all (Barlas 1996; Qudrat-Ullah 2012). Most of the literature on validation in system dynamics was done early in the life of the field, and although much research on validation in system dynamics remains to be done, recent advances are lacking (Groesser 2012).

System dynamics models are often used to identify a system structure that controls the dynamics of interest and not directly used for making predictive estimates about system outputs. Care needs to be taken to ensure how the identified system structures are used and whether that use is valid. This somewhat different use of models likely requires a different approach than validation of a black box model. Rigorous tests have not yet been developed that assess whether a model structure adequately matches the structure of the system it represents (Barlas 1996). Issues with autocorrelation and multicollinearity mean that common statistical tests often do not apply to validation of system dynamics models (Barlas 1996). Structural tests that have been used for system dynamics model validation include expert/literature/personal knowledge assessments, parameter verification, extreme condition tests, boundary adequacy tests (asking whether the model includes everything it should), and dimensional consistency tests (Forrester and Senge 1980), formal reviews, and semantic analysis (Barlas 1996). Roy and Mohapatra (2003) suggest using structural equation modelling for validation of causal structures. Some recent efforts have been made to design data collection opportunities that allow for collecting both structural and behavioral data (Bier and Bernard 2014; Lakkaraju et al. 2014). Qudrat-Ullah (2005) suggests that structural validity should also be applied to individual-based models.

Behavioral validation is another important aspect of system dynamics model validation. Comparisons of model results to data are considered useful but inadequate validation in the system dynamics field because they do not give insight into system structure or causal mechanisms (Barlas 1996). Behavior reproduction tests may look for symptom, frequency, or behavior characteristic generation, or may look to pattern or event prediction (Forrester and Senge 1980). Extreme policies and the sensitivity of modeled behaviors may also be tested (Forrester and Senge 1980). Turing tests have also been suggested for looking at behavior in a structure-oriented manner (Barlas 1996). System dynamics models are most commonly used for policy analysis. Validation options based on policies include tests of system improvement and sensitivity of the model to policies (Forrester and Senge 1980).

2.2 Validation and Individual-Based Models

Distributed, dynamic, individual-based models, such as network and agent-based models, are more commonly starting to be used as an alternative to single-facet, aggregate models. Both individual-based modeling approach and the systems represented in these models affects the manner in which these kinds of models can be validated (Ronald et al. 2010). Disaggregate, individual behaviors, and an evolving network of interactions between individuals and their environment underlie the mechanics of many models of complex systems. As models become more distributed and stochastic, individual-driven tools, such as agent-based models and networks, offer the possibility of modeling a wider class of phenomena than is possible with analytic tools alone. (Crooks et al. 2008).

A few important issues can affect validation activities for individual-based models, including solutions by simulation, excessive detail, and unknown processes. Individual-based models are solved by simulations, and are meant to represent phenomena that generally lack an analytical solution (Windrum et al. 2007; Ormerod and Rosewell 2009). A simulation result is not necessarily meant to exactly match a specific set of data, which can make it difficult to demonstrate that the model is valid for an intended use. Additionally, as individual-based models move towards more detail, the validation challenges can increase (Gilbert 2004; Batty et al. 2006, Crooks et al. 2008). Further, validation of these models may involve an assessment of the extent to which the model is a good representation of an (unknown) process that generates a set of observed data (Windrum et al. 2007).

Several proposed approaches exist to address the validation of individual-based models. Gilbert (2004) notes the importance of validating individual-based models at different levels—at the individual level, and at the aggregate level. However, performing the validation may be difficult due to lack of data that represents these abstract behavioral concepts and emerging aggregate patterns formed from individual behaviors. Windrum et al. (2007) and Ormerod and Rosewell (2009) suggest two approaches to deal with validation in agent based models. First, a clear definition of the question, or “what is being explained” and “what is not being explained”, needs to be specified. Secondly, model simplicity should be considered. Windrum et al. (2007) and Ormerod and Rosewell (2009) assert that a model with complicated agents requires additional justification for their validation, and should not be accepted until it is shown that a simpler model will not explain the phenomenon.

Developers of individual-based models have followed a diversity of approaches to conduct verification and validation of models, each of which deserves closer consideration. For example, two authors used replication and experimental techniques. Bert et al. (2014) used model comparisons, and Sornette et al. (2007) used iterative trust building. These approaches have unresolved issues. Repeatability of validation experiments can be hampered by difficulties in controlling all variables, making it difficult to ensure comparability (Crooks et al. 2008). Similarly, docking (testing different models on a fixed dataset) may present difficulties as the models' design and calibration includes idiosyncratic decisions made by the modelers, making comparisons impossible (Axtell et al. 1996; Crooks et al. 2008). It is worth mentioning that Bert et. al (2014) included a mixture of supporting techniques, such as empirical, component-based validation, and consultation with subject matter experts.

An application of a model can have a certain degree of validity, encapsulated in several measures of fit (Law and Kelton 1991). In this respect, authors have also sought to create metrics that better measure the difference of model output to the real world data it seeks to represent (e.g., information-theoretic metrics by Ronald et al. 2010). For complex systems models, these metrics may need to be different from traditional measures of goodness of fit to real-world data. Regardless of this effort, there is still debate on which best statistics to use for model calibration (Crooks et al. 2008).

The problems and issues facing validation of complex systems models provide many open questions and a large opportunity for future research. There is evidence that the field of individual-based modeling is thriving with powerful and productive methods that need to be formalized and validated. Windrum et al. (2007) and Ormerod and Rosewell (2009) pose the following questions for thought:

- Should empirical validation be the primary/unique basis for rejecting or accepting a model?
- How should one use available data?
- Which classes of empirical objects do we really want to replicate and test?

The relationship between calibration and validation in individual-based models needs to be further explored as well. Further directions may include methodological protocols for both the modeling, and the analysis of individual-based models (Windrum et al. 2007; Ormerod and Rosewell 2009). Further, a shift in expectations is likely needed both by end-users and modelers regarding validation (Ronald et al. 2010). This shift could include steering towards making models to help answer questions and to develop associated theory and techniques rather than making models meant to be a facsimile of the real world.

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3. EPISTEMIC UNCERTAINTY AND COMPLEX SYSTEMS MODELS

Every model developer must reconcile how to address sources of uncertainty within his/her model, but complex systems present some unique challenges for addressing those uncertainties. Uncertainties in computational simulation are often categorized into aleatory or epistemic uncertainty. Aleatory uncertainty refers to inherent variable or randomness in a process which is irreducible, while epistemic uncertainty is lack of knowledge uncertainty due to incomplete information or incomplete knowledge (Oberkampf and Roy 2010, Helton 2009). In many situations epistemic uncertainty dominates, but it is often more difficult to characterize and parameterize than aleatory uncertainty. Characterizing and managing epistemic uncertainty appears to be a significant challenge when developing and using models of complex systems. Two sources of epistemic uncertainty stand out in particular—model form error and scaling uncertainty.

3.1 Model Form Error

Multiple factors can contribute to epistemic uncertainty, but model form error seems to be especially relevant for models of complex systems. Consider the example of creating a model to determine which military strategies are most effective for defeating terrorism networks such as Al Qaeda. Decades worth of data from military engagements with nation-states exists. If one was to model the conflict between the US military and Al Qaeda as a conflict between two nation-states, the model would likely predict that the superior efficiency of the US military should result in a rapid defeat of the Al Qaeda network (McChrystal et al. 2015). This conclusion could be confirmed by historical data that indicates in most military conflicts, the more resource rich and efficient combatant prevails rapidly. However, the conflict between Al Qaeda and the U.S. military did not play out as expected, given the resource differentials. So what could cause such a significant discrepancy between the hypothetical model and the actual conflict?

Most model development efforts assume that the difference between simulation estimates and observational data is a random error quantity that is equal to the difference of the simulation error and the measurement error. This random error term is assumed to be Gaussian with mean equal to zero. The simulation error is often assumed to be comprised of errors in input parameters and numerical approximation schemes, and if these errors could be reduced completely to zero, the only difference between simulation estimates and observation data would be due to measurement error.

This assumption is frequently invalid when working with models of complex systems because the model itself can be a significant source of uncertainty. In the example above, the assumption that Al Qaeda would behave and act in the same manner as a nation-state is fundamentally incorrect (McChrystal et al. 2015). Relying on historical observations of military, nation-state conflicts is not suitable because Al Qaeda operated in a fundamentally different manner than had previously been observed. In this example, the model itself is a significant source of error and uncertainty.

This uncertainty, termed model form error, often arises when working with models of complex systems. One approach to understanding if a significant model form error exists is to formulate a model discrepancy term. Instead of assuming that the difference between observational data and simulation estimates is equal to an entirely random error term, model form prediction error or model discrepancy is defined to be the following:

Model Discrepancy = Observation – Simulation – random error

Model discrepancy is not assumed to be entirely random or represented with a Gaussian distribution; rather, it represents systematic errors that result from representing the system with a specific model formulation. Note that this formulation is only able to state something about the differences between the prediction of the model and the observations. That is, the discrepancy or model form error is in "response" or prediction space. The QoIs being compared are output responses, and the discrepancies quantified by validation are in these units, not in units of the internal structures, quantities, and parameters of the model. Once validation quantifies the direction and magnitude of QoI prediction errors, the project may turn to considering model-form shortcomings and structural issues that could explain the errors, but this is a different activity than model validation. That is, the estimation of a model discrepancy term does not say where or how the model form is incorrect, it only helps us understand that it is incorrect. We have written the discrepancy term very abstractly above, but it may be a function that is parameterized by various model parameters or model scenarios, which can help indicate where the model may be improved or re-considered in some situations.

Model form error is not unique to models of complex systems, but it does seem to arise frequently when working with models of complex systems, and it may be more profound. For example, developers sometimes do not know the underlying phenomena that lead to behavior of the overall complex system. Developers may create a model or series of models attempting to determine these phenomena through simulation experimentation. However, the developers may not have a good understanding of which models are fundamentally more appropriate. This limited understanding frequently seen in models of complex systems contributes to model form error.

Additionally, accurate estimation of model form error requires observational data. This may or may not exist. In the example above, Al Qaeda represented a fundamentally different network, and previous, historical observational data of nation-state conflicts is not valid. Similarly, when trying to model responses to potential policy options that have never previously been put forth, it is not clear whether historical data from implementation of previous, different policies are suitable for identifying model form errors. The challenge associated with gathering necessary observational data is a fundamental challenge for accurate estimation of model form error.

Estimation of model form error is a subject matter *and* statistical challenge, even for models of systems that are not considered to be complex. Kennedy and O'Hagan (2001), Arendt et al. (2012), Brynjarsdóttir and O'Hagan (2014), and Wallen and Brake (2014) are examples of recent research efforts that are working to improve model form error estimation.

3.2 Scaling Error

Scaling error is another source of uncertainty that can affect models of complex systems. Complex systems often consist of large numbers of interacting subcomponents. Representing each individual element in a model may not be computationally tractable, so model developers may actually simulate a smaller number of components in their models and then assume the results hold to scale for the actual system. For example, Chicago, Illinois, has a population of approximately three million people. If one tried to develop an agent-based model of disease spread in the population of Chicago, it is unlikely a model with only three agents (scaling factor of 1: 1,000,000) could provide reasonable estimates, and it may be computational intractable to have a model consisting of three million agents (scaling factor of 1:1). However, it is less clear what intermediate scaling factors between 1:1 and 1: 1,000,000 provide reasonable estimates while minimizing the computational burden. Further, since complex systems exhibit non-linear scaling of behavior from individual to ensemble, it is unknown whether the aggregate behavior of a few will be representative of the aggregate behavior of many. The way a particular system model result “scales” with size, or number of components will be highly dependent on the nature of the system, the modeling approach, and the intended use of the model, but, in general, formal guidance on how to choose such a scaling factor and how to calculate the resulting error that comes from choosing that factor does not exist.

3.3 Research Directions for Epistemic Uncertainty and Complex Systems Models

We propose the following research areas as opportunities for better characterizing uncertainty and errors in models of complex systems:

- Model Form Error:
    - What does “model form error” really mean for complex systems model where theory and “ground truth” may be contingent?
    - Recognizing that estimation of model discrepancy is not solely a statistical challenge, what advances can be made with respect to statistical elements, and how far can we rely on statistics to address this issue?
    - When the required observational data is available, how can we leverage ongoing research into estimation of model discrepancy in hierarchical model validation to quantify model form error in models of complex systems?
    - When the required observational data is not available, can we leverage surrogate data and models instead to estimate model discrepancy? And, can we adequately estimate the additional error introduced with the surrogates?
    - When neither the required observational nor surrogate data are available, can we develop informative bounding estimates of model form error, based upon our knowledge of the other sources of error (e.g., measurement error, parameter error, numerical approximation error, etc.)?
- Scaling uncertainty: Can we develop formal guidance and methods for how to scale models of complex systems in a way that balances error reduction with computational efficiency?
- Epistemic uncertainty in general:
    - How can we better communicate with project sponsors about the various sources of epistemic uncertainty and the potential effects those sources may have on modeling results and intended uses of the model? How is risk associated with model form error best managed?

- Can we characterize the uncertainty related to the outcome or consequence of a decision that model results support? Would doing so decrease consequence uncertainties and therefore decision-making uncertainties and enable better characterization of these uncertainties, relative to characterizing uncertainties in the phenomena prediction model itself and its results? Would doing so present a greater set of challenges, and what would those additional challenges be?

Making progress on these research directions would provide a number of benefits to the complex systems modeling community. First and foremost, progress would enable a better understanding of epistemic uncertainties inherent to models of complex systems. This understanding will help model developers and users better determine appropriate (and inappropriate) uses of the model, how to interpret simulation results, and identification of opportunities for improving the model and reducing uncertainties (when appropriate and if possible). More generally, progress will facilitate honest and clear communications about uncertainties in the model and how those uncertainties should be considered when making decisions informed by simulation results.

4. STRONG TESTS

4.1 Constructs Aiding Strong Test Development

Design and execution of validation tests is an important part of validation activities, and "strong tests" represent the ideal for validation tests. Strong tests have the following characteristics:

- The tests are explicitly defined. That is, the tests are written, precise, list the relevant input parameters and code settings, and list the relevant QOIs. The tests are written in sufficient enough detail to ensure reproducibility.
- The tests list explicit evaluation criteria that indicate how to compare QOIs with predicted results. The evaluation criteria can be specified either in terms of acceptance criteria (What result is required for the model to pass?) or failure criteria (What outcomes will result in a failure and, thus, indicate the model is not acceptable for the intended purpose?)
- The tests provide descriptions of the appropriateness of the test. These explanations would describe "Why the test is appropriate and provides useful information."

Development of strong tests can be a challenge for model developers and users, so a number of constructs have been developed for modeling efforts related to high-consequence application areas. One such construct is validation test development guidelines for models supporting nuclear reactor safety, nuclear weapons testing, and other high consequence applications. For example, Trucano et al. (2002) describe "What is a validation test for the ASC program?", and Oberkampf and Trucano (2008) provide guidelines for validation tests and benchmarks for these application areas. Oberkampf and Trucano (2008) provide six guidelines for validation test development. Among other relevant topics, these guidelines address who should be involved in the testing, identify which features of the system ought to be included in tests, suggest various testing measurements, and identify the types of error that the tests should be designed to estimate and analyze. Oberkampf and Trucano (2008) also provide recommendations for information that should be included in benchmark tests, including conceptual descriptions, mathematical descriptions, accuracy assessments, code comparison instructions, and other topics. Not surprisingly, these types of information are consistent with what is needed to develop a strong test.

A hierarchy of validation tests is another construct developed for models supporting high-consequence applications. The base of the hierarchy, shown in Figure 2, consists of many "separate effects" tests that evaluate individual components of the models. The next higher level in the hierarchy includes integral effect tests that include multiple components and subsystems. As one proceeds up in the hierarchy, fewer integral effects tests are performed, but the tests are evaluating increasingly integrated components and subsystems. The peak of the hierarchy includes full system level tests that are intended to provide total system validation.

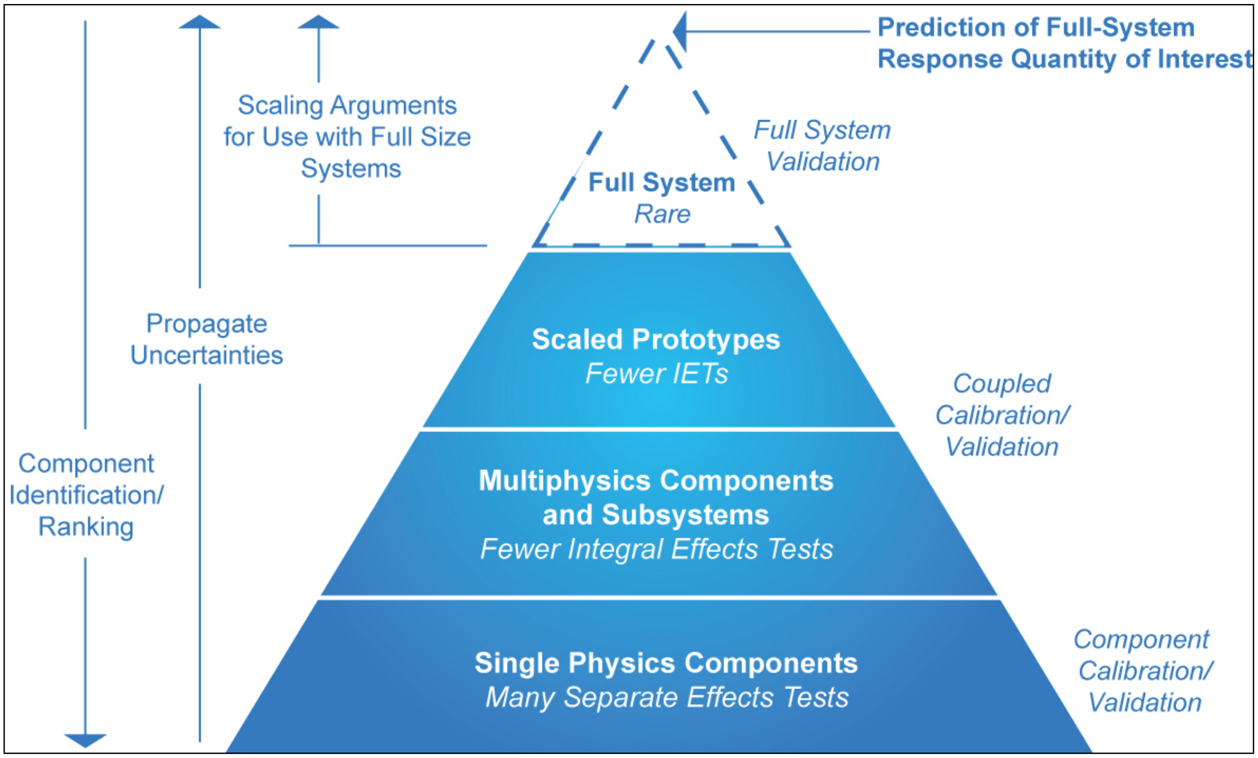

Figure 2. Validation Test Hierarchy (Wiler 2016).

The hierarchy concept can be helpful for thinking about test design, but it is also very useful for understanding the information that a specific test or category of tests would provide, if performed. The hierarchy can also help one understand what additional testing would be required as one attempts to move towards total system validation.

The constructs mentioned above have been developed primarily for physics-based models related to high-consequence applications. The development of comparable constructs specific to models of complex systems would lead to stronger validation tests of these models.

4.2 Research Directions for Strong Tests

We propose the following research areas as opportunities for better characterizing uncertainty and errors in models of complex systems:

- Can we develop validation test and benchmark guidelines that are comparable to those of Oberkampf and Trucano (2008) but are specific for models of complex systems?
    - Can we define what a validation experiment is for a model of complex systems and how that experiment would differ from validation experiments defined for the ASC program and other physics-based applications?
    - If we could characterize the complexity of a system with a limited number of parameters, how might the validation experiments change as we “increase the complexity related parameters?”
    - Oberkampf and Trucano’s (2008) guidelines are fairly general, but can we identify the implications of trying to apply them to models of complex systems?
    - Can we develop rigorous validation tests that incorporate subject matter expert opinion, qualitative information, metadata, and other information that are not

    - commonly used in current validation tests but seem to be more easily acquired than field or experimental data for models of complex systems?
    - If so, how do we develop suitable pass/fail criteria?
    - Under what conditions is it possible to develop suitable benchmarks that will remain valid for a long time (10+ years)? This question seems particularly valid for models of complex systems in which the systems seem to change, adapt, and evolve at time scales much shorter than our knowledge of physical systems changes.
- Can we develop a validation test hierarchy that is specific to models of complex systems?
    - Can we use the concept of a validation hierarchy that includes validation at a component and subsystem level to provide meaningful information? This is particularly at issue for complex systems that are considered to be irreducible, i.e., the behavior of the overall system cannot be accurately represented merely by replicating the behavior of individual components.
    - If so, to what extent can we decompose the system into individual subsystems and components for testing and still get meaningful information?
    - What guidelines and recommendations can be developed to determine an appropriate level of decomposition?

Progress towards these research directions would provide several benefits to the complex systems community. The overall benefit would be better-designed validation tests and benchmarks. Guidance to test developers would enhance transparency and reproducibility of tests. Increased standardization of testing approaches would be another benefit. Additionally, modelers of complex systems would be able to better communicate with stakeholders about validation testing. The modelers would be able to show where a proposed testing regime would reside on the hierarchy and the benefits and limitations of the testing regime.

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5. VALUE OF INFORMATION

5.1 Information Acquisition and Usage for Model Development

Data and information are essential to all model development activities. Data and information are used to inform conceptual model formulation, parameter development and calibration, boundary conditions, and validation testing. Field data, experimental results, subject matter elicitations, surrogates, metadata, and qualitative information can all be useful at various stages in the model development process. However, not all types and sources of information are equally useful. Data quality can vary from one source to another, and it may be difficult to determine how to use or weight information that appears to conflict (or is inconsistent with) other sources of information. Some information sources may be easy to harvest but provide only limited benefit to the modeling effort. Others may provide significant benefits but require significant time, effort, and cost to acquire. Evaluating the costs and benefits of data and information acquisition is something that every model developer must go through.

Modelers of complex systems seem to face even greater challenges when searching for data and information:

- Complex systems can be composed of so many different components that it can be time- or cost-prohibitive to characterize every component. (e.g., see Gabert 2016).
- Conducting a controlled field experiment to collect data may not be possible (e.g., modeling human behaviors in response to a hurricane event).
- Measuring model components may be difficult, if not impossible (e.g., social and cultural attributes in the Dynamic Multi-Scale Assessment Tool for Integrated Cognitive-behavioral Actions (DYMATICA) projects (Bernard et al. 2016)).
- Observation and interaction with the system may fundamentally change the system and its behaviors (e.g., cyber and physical security systems).
- Measurement of individual component features may be relatively easy but not representative of the overall system behavior (e.g., foraging by a single ant contrasted with aggregate foraging behavior of ant colonies).
- Stakeholders for models of complex systems may want model results within short periods of time (e.g., incident response (DHS 2016)).
- When systems are constantly changing, validity of data may have a short shelf-life (e.g., social networks in high schools).

Consequently, “We can’t get any data” is too often a common refrain for complex systems modelers. In some cases, this statement may be true, but more often, the correct statement is “Quality information collection is difficult, time-intensive, and expensive.” Given the many benefits that quality information can provide models, complex systems modelers could benefit from better understanding how to evaluate the tradeoffs between the effort required to gather additional information and the benefits the additional information would provide.

“Value of information” (VOI) is a related concept that has recently emerged in the medical literature and is being used with increasing frequency. The principal current research area for VOI is analysis of what medical research should be funded, focusing on what the additional anticipated information from a proposed study will provide in terms of measurable patient or organizational outcome.[2] VOI is becoming prevalent in the medical decision-making literature (e.g., see Strong et al. 2014; Jalal et al. 2015;), but the underlying, classical operations formulations are less reported upon since available parameters from medical studies often do not align well with these formulations. Even though the VOI concept may not be fully developed, its further maturation, especially with regards to models of complex systems, would benefit validation activities. Efforts that could be built upon include Clemen and Winkler (1985), Brand and Small (1995), Nosy et al. (2011), Singh et al. (2008), Fischoff (2013), Lefgran (2014), Manski (2013), Barnes et al. (2016), Purcell and Roozbeh (2016), Pedrycz and Bargiela (2012), Heckerman et al. (1993), and Wang and Watada (2010).

5.2 Research Directions for Value of Information

We propose a research direction that focuses on the research and development of formal methods for evaluating the value of information for models of complex systems. Formal VOI methods for models of complex systems would likely need to include the following:

- Categorization and identification of potential information sources
- Specification of activities required to acquire these information sources
- Methods and metrics for quantifying resources, costs and other "effort" factors related to performing these activities
- Specification and categorization of how the acquired information could be used in the model development process (e.g., calibration, boundary condition specification, validation testing, etc.)
- Methods and metrics for quantifying the benefits of using the additional information in the specified manner
- Methods for analyzing and optimizing the cost-benefit tradeoffs
- Applications and demonstrations of the proposed methods and metrics

Research activities should be focused on both the individual research items and overarching processes for integrating the individual pieces. Additionally, specific attention ought to be paid to the relative merits of proxy or "analogue" data. These data may be more easily available; however, determining the benefits that proxy data, relative to data for the specific phenomenon being modeled, needs to be rigorously evaluated.

Maturation and formalization of VOI concepts for models of complex systems would provide multiple benefits. This research would provide a better understanding of the tradeoffs between the costs and benefits of gathering additional information for model development activities. This work would also provide increased understanding of the limits and diminishing returns that would eventually come with information gathering activities. This understanding will help model developers and users understand "what is needed" and "what is good enough."

Additionally, this research could help focus information-gathering activities. By understanding which information sources will provide the greatest return, modelers can scope their information-gathering activities to be more efficient. Better information also ought to lead to better experimental design.

[2] The April and July 2016 issues of the journal *Medical Decision Making* highlight current practices and applications of VOI in medical decision making.

Ultimately, this research will help facilitate communication about models, information, and validation between model developers and users. Sponsors can more fully understand the cost of model development and validation, and all stakeholders can have more realistic expectations about model limitations and confidence in model results.

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6. CONCLUSIONS

Improved validation for models of complex systems has been a primary focus over the past year for the Resilience in Complex Systems Research Challenge. Sandia hosted a workshop focused on this topic in June 2016, and the workshop generated a plethora of research ideas and discussion. This document describes a set of research directions that are the result of distilling those ideas into three categories of research. The recommended research direction themes are epistemic uncertainty, strong tests, and value of information.

The content of this document can be used to inform future research activities in a number of ways. First, the recommended research actions lend themselves to some potential actions that could be taken in the near term. These potential actions include the following:

- Draft a white paper that is a complex systems-specific version of the Oberkampf and Trucano (2008) paper. This paper could describe the implications of applying their validation test and benchmark guidelines for models of complex systems. Application of the guidelines to a specific model will provide insights in the context of a real, tangible example.
- For a selected project that is currently developing a model of a complex system, bring together the project team with staff from the Research Challenge to jointly develop and execute a set of validation tests using the above white paper.
- For a selected model of complex systems, map out how one would go about doing a VOI assessment for a set of validation tests. This activity could include identifying potential experiments and data sources, the resources needed to gather the related data, assessing the benefits of going through the process, and formulation for evaluating the tradeoffs between the options.

These and many other potential actions could be performed.

Second, this document can be used to inform the Resilience in Complex Systems Research Challenge's roadmap. The Research Challenge is in the process of updating its roadmap, and these research directions can be used to identify and prioritize specific research activities for advancing the research challenge.

Third, these research directions can be used to inform the upcoming FY18 Laboratory Directed Research and Development (LDRD) call and research proposals. The LDRD program is Sandia's principal source of discretionary research and development funding, and it gives Sandia the flexibility to invest in long-term, high-risk, and potentially high-payoff R&D that builds and stretches the Labs' science and technology capabilities. Successful research into better validation for models of complex systems would be a long-term, high-payoff result for Sandia. The Research Challenge leadership ought to engage with Sandia's Program Management Unit (PMU) leads that are developing the LDRD in order to describe the benefits to the PMUs and to have elements of the recommended research directions incorporated into the LDRD call. Additionally, any Grand Challenge LDRD Proposals that the Research Challenge endorses should include elements of the recommended research directions.

Finally, the recommended research directions can be used to facilitate collaborations between Sandia and external organizations. The recommended research directions can provide topics for collaborative research, development of proposals, workshops, and other opportunities. Potential collaborators could be modelers needing assistance with validation, validation experts seeking opportunities to apply new/experimental validation approaches to real models, staff from Sandia's Academic Alliance partners and other universities, and other interested individuals.

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