Simulation Foundations, Methods and Applications

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Research Challenges in Modeling and Simulation for Engineering Complex Systems

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Preface

A two-day workshop was held on January 13–14, 2016, at the National Science Foundation in Arlington, Virginia, with the goal of defining directions for future research in modeling and simulation and its role in engineering complex systems. The workshop was sponsored by the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the Air Force Office of Scientific Research (AFOSR), and the National Modeling and Simulation Coalition (NMSC) in conjunction with its parent organization the National Training and Simulation Association (NTSA). This book documents the findings emanating from this workshop.

The goal of the workshop was to identify and build consensus around critical research challenges in modeling and simulation related to the design of complex engineered systems—challenges whose solution will significantly impact and accelerate the solution of major problems facing society today. Although modeling and simulation has been an active area of study for some time, new developments such as the need to model systems of unprecedented scale and complexity, the well-documented deluge in data, and revolutionary changes in underlying computing platforms are creating major new opportunities and challenges in the modeling and simulation (M&S) field. The workshop focused on four main technical themes: (1) conceptual models, (2) computational issues, (3) model uncertainty, and (4) reuse of models and simulations.

The workshop resulted in large part from an initiative led by the research and development committee of the National Modeling and Simulation Coalition (NMSC) aimed toward defining a common research agenda for the M&S research community. Recognizing that the modeling and simulation community is fragmented and scattered across many different disciplines, communities, and constituencies, there is a need to gather individuals from different communities to articulate important research problems in M&S. Presentations and panel sessions at several modeling and simulation conferences were held leading up to and following the January workshop to raise awareness of this activity.

Detailed planning began in September 2015 with the formation of the workshop steering committee consisting of Richard Fujimoto (chair, Georgia Tech, and then

NMSC Policy Committee chair), Steven Cornford (NASA Jet Propulsion Laboratory), Christiaan Paredis (National Science Foundation), and Philomena Zimmerman (Office of the Secretary of Defense). An open call was developed and disseminated that requested nominations of individuals, including self-nominations, to participate in the workshop. A total of 102 nominations were received. The steering committee reviewed these nominations, and several rounds of invitations were made until the workshop capacity was reached. Selection of participants focused on goals such as ensuring balance across the four technical theme areas, broad representation from different research communities, inclusion of senior, distinguished researchers in the field, and ensuring inclusion of individuals from underrepresented groups.

A total of 65 individuals attended the workshop. Four working groups were formed, each representing one of the technical theme areas. Participants were initially assigned to one of the working groups; however, attendees were free to participate in a group different from that which the individual was assigned (and some did so), and some chose to participate in multiple groups throughout the course of the two-day workshop. Three individuals within each group agreed to organize and facilitate discussions for that group and help organize the workshop findings.

Each group was charged with identifying the four or five most important research challenges in the specified technical area that, if solved, would have the greatest impact. It was anticipated that within each of these main challenges, there would be some number of key subchallenges that would need to be addressed to attack the research challenge.

Prior to the workshop, several read-ahead documents concerning research challenges in M&S were distributed to the participants. These read-ahead materials included the following:

- National Science Foundation Blue Ribbon Panel, “Simulation-Based Engineering Science,” May 2006.
- National Research Council of the National Academies, “Assessing the Reliability of Complex Models, Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification,” 2012.
- A. Tolk, C.D. Combs, R.M. Fujimoto, C.M. Macal, B.L. Nelson, P. Zimmerman, “Do We Need a National Research Agenda for Modeling and Simulation?” *Winter Simulation Conference,* December 2015.
- J.T. Oden, I. Babuska, D. Faghihi, “Predictive Computational Science: Computer Predictions in the Presence of Uncertainty,” Encyclopedia of Computational Mechanics, Wiley and Sons, to appear, 2017.
- K. Farrell, J.T. Oden, D. Faghihi, “A Bayesian Framework for Adaptive Selection, Calibration and Validation of Coarse-Grained Models of Atomistic Systems,” Journal of Computational Physics, 295 (2015) pp 189–208.
- Air Force Office of Scientific Research and National Science Foundation, “Report of the August 2010 Multi-Agency Workshop on Infosymbiotics/DDDAS: The Power of Dynamic Data Driven Application Systems” August 2010.

In addition, workshop attendees were invited to submit brief position statements of M&S research challenge problems or areas that should be considered for discussion at the workshop. Each proposal was assigned to one of the four technical theme areas and distributed to attendees prior to the meeting.

The workshop program included five application-focused presentations on the first day that described important areas where technical advances in M&S were needed within the context of these domains: sustainable urban growth (John Crittenden), healthcare (Donald Combs), manufacturing (Michael Yukish), aerospace (Steven Jenkins), and defense (Edward Kraft). These presentations, the read-ahead materials, and research challenge proposals submitted by workshop participants were the main inputs used in the workshop.

The remainder of the workshop focused on breakout groups and cross-group discussions with the goal to build consensus around key research challenges that could form the basis for a common research agenda. The first day focused on collecting and consolidating views concerning important research challenges. The second day included brief presentations and discussions reporting progress of the four groups, and further discussion to refine and articulate recommendations concerning research challenges in each of the four technical areas.

This document describes the main findings produced by the workshop. We would like to thank the many individuals and organizations who helped to make this workshop possible. First, we thank the workshop sponsors, especially NSF (Diwakar Gupta) and NASA (John Evans) who provided the principal funding for the workshop. NMSC/NTSA (RADM James Robb) sponsored a reception held at the end of the first day of the workshop, and AFOSR (Frederica Darema) participated in events leading up to the workshop and provided valuable guidance as the workshop was being developed. The five plenary speakers (John Crittenden, Donald Combs, Michael Yukish, Steven Jenkins, and Edward Kraft) provided outstanding, thought-provoking presentations regarding the impact of M&S in their respective application areas. Administrative support for the workshop was provided by Holly Rush and Tracy Scott, and Philip Pecher helped with the development of the final report and Alex Crookshanks help with the graphics used in some of the figures.

Finally, we especially thank the many participants who devoted their time and effort to participate and help develop this workshop report. We thank the group leads for carefully managing the discussions of their groups as well as efforts to organize and, in many cases, write much of the text that is presented here.

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Executive Summary

Engineered systems are achieving unprecedented levels of scale and complexity in the midst of a rapidly changing world with many uncertainties. Cities face enormous challenges resulting from aging infrastructure, increased urbanization, and revolutionary technological changes such as smart electric power grids, photovoltaics and citizen generation of electricity, electrification of the vehicle fleet, autonomous vehicles, and widespread deployment of drones, to mention a few. Forces such as climate change threaten to dramatically impact future developments. The healthcare delivery system faces growing demands for service from an aging population while the system adapts to an explosion in patient medical data, changing payment models, and continued advances in medical technologies. Advances in manufacturing offer the potential for dramatic increases in competitiveness and economic growth, but require rapid increases in automation and fast, seamless integration while new technologies such as additive manufacturing and new approaches to materials design come online. Advanced space missions call for stringent requirements for robustness and flexibility in the face of harsh environments and operation over extreme distances in the presence of environmental surprises, possible technology failures, and heavily constrained budgets. Similarly, defense acquisitions face challenges from asymmetric threats, changing missions, globalization of technology and siloed decision-making processes in the face of declining budgets, a shrinking defense industrial base, and congressional and service imperatives, mandates, and regulations.

In these and many other areas of critical societal importance, modeling and simulation (M&S) plays a key role that is essential to successfully navigate through these challenges and uncertainties. Consideration of alternative futures is inherent in decision making associated with complex socio-technical systems. Empirical investigations of yet-to-exist futures are impossible to realize; however, they can be explored computationally through M&S. Advances in M&S are critical to addressing the many “What if?” questions associated with these and other examples. Advanced modeling techniques, integrated with current and advancing computing power, visualization technologies, and big data sets enable simulations to inform decisions on policies, investments, and operational improvements.

Although systems arising in the aforementioned applications are very different, they have at least one aspect in common. They are composed of many interacting components, subsystems, and people. Systems such as these that consist of many interacting elements are commonly referred to as *complex systems*. For example, a city can be viewed as a set of infrastructures such as water, energy, transportation, and buildings combined with the social, economic, and decision-making processes that drive its growth and behavior over time. Interactions among the parts of a complex system may give rise to unexpected, emergent phenomena or behaviors that can have desirable consequences, such as the creation of ethnic neighborhoods, or undesirable ones such as urban sprawl. M&S provides critical tools and technologies to understand, predict, and evaluate the behavior of complex systems, as well as the means to develop and evaluate approaches to steer the system toward more desirable states.

Computer-based models and simulations have been in use as long as there have been computers. The value of M&S technologies throughout history is without question. However, the development and use of reliable computer models and simulations is today time-consuming and expensive and can sometimes produce unreliable results. These issues become even more critical as engineered systems increase in complexity and scale and must be deployed in uncertain environments. Advances in M&S technologies *now* are essential to enable the creation of more effective, robust, and less costly engineered complex systems that are critical to modern societies.

Here, we identify key research challenges that must be addressed to enable M&S to remain an effective means to meet the challenges of creating and managing the complex systems that increasingly pervade our society. Key findings of identified challenges fall into four areas:

- *Conceptual modeling*. Understanding and developing complex systems require the collaboration of individuals with widely different expertise. The models through which these individuals communicate and collaborate are commonly referred to as *conceptual models*. Once defined, conceptual models can be converted to computer models and software to represent the system and its behavior. Advances in conceptual modeling are essential to enable effective collaboration and cost-effective, error-free translation of the model into a suitable computer representation.
- *Computational challenges*. Computing and communications technologies have advanced rapidly in the last decade. M&S has not yet fully realized the potential and opportunities afforded by technologies such as mobile and ubiquitous computing, big data, the Internet of Things, cloud computing, and modern supercomputer architectures. This has kept M&S from achieving its fullest potential in modeling complex systems, or being widely deployed in new contexts such as online management of operational systems. Research advances are needed to enable M&S technologies to address issues such as the complexity and scale of the systems that need to be modeled today.

- *Uncertainty*. Models and simulations are necessarily approximate representations of real-world systems. There are always uncertainties inherent in the data used to create the model, as well as the behaviors and processes defined within the model itself. It is critical to understand and manage these uncertainties in any decision-making process involving the use of M&S. New approaches are required to gain better fundamental understandings of uncertainty and to realize practical methods to manage them.
- *Reuse of models and simulations*. It is often the case that models and simulations of subsystems such as the components making up a vehicle are created in isolation and must later be integrated with other models to create a model of the overall system. However, the reuse of existing models and simulations can be costly and time-consuming and can yield uncertain results. Advances are needed to enable cost-effective reuse of models and simulations and to ensure that integrated models produce reliable results.

Findings concerning important research challenges identified in the workshop in each of these areas are discussed in the following and elaborated upon in the subsequent chapters that follow.

A. Conceptual Modeling: Enabling Effective Collaboration to Model Complex Systems

Conceptual modeling is recognized as crucial to formulation and simulation of large and complex problems, but is not well-defined or well-understood, making it an important topic for focused research. Conceptual models are early-stage artifacts that integrate and provide requirements for a variety of more specialized models, where the term "early" applies to every stage of system development. This leads to multiple conceptual models: of reality, problem formulation, analysis, and model synthesis. Developing an engineering discipline of conceptual modeling will require much better understanding of how to make conceptual models and their relationships explicit, the processes of conceptual modeling, as well as architectures and services for building conceptual models.

Finding A.1. Conceptual models must be interpreted the same way by everyone involved, including those building computational tools for these models.

Conceptual models today are most often expressed using some combination of sketches, flowcharts, data, and perhaps pseudo-code. Lack of general agreement on how to interpret these artifacts (i.e., ambiguity) limits the computational assistance that can be provided to engineers. More explicit and formal conceptual modeling languages are needed to support engineering domain integration and analysis tool construction, while retaining accessibility for domain experts via domain-specific modeling languages. Formal conceptual modeling applies not only to the system of interest, but also to the analysis of that system. Several structures have been studied as simulation formalisms; however, there is little consensus on the best approach. Achieving an engineering discipline for M&S will require a more complete set of formalisms spanning from rigorous discrete event, continuous, and stochastic system specification to higher level, perhaps domain-specific, simulation languages.

Finding A.2. Processes for conceptual modeling must meet resource constraints and produce high quality models.

M&S facilities are themselves complex systems, typically requiring multiple steps and decisions to move from problem to solution (*life cycle engineering*). Regardless of complexity, the underlying principle for any type of life cycle engineering is to ensure that unspent resources (e.g., money, time) are commensurate with the remaining work. Reducing uncertainty about work remaining and the rate of resource consumption requires determining the purpose and scope of the system, the kind of system modeling needed (continuous/discrete, deterministic/stochastic, etc.), appropriate modeling formalisms, algorithms, data for calibrating and validating models, and other models for cross-validation. Currently, answering these questions is hampered by a lack of formalized engineering domain knowledge to constrain life cycle decisions and processes. In addition, workflows are central to any approach for making life cycle processes explicit and manageable, but evaluation of these workflows is hampered by the lack of metrics to assess their quality and to assess the quality of the resulting models.

Reducing model defects introduced during the modeling process helps avoid difficult and high-cost amendments of the model as it nears completion. During model development, program leadership must determine what knowledge is to be acquired at each point in the life cycle to maximize value to program stakeholders. Further research is needed on how to set knowledge goals at particular milestones in a system development life cycle. In particular, which knowledge elements are associated with which aspects of the system of interest and its environment? How does one determine the value of acquiring particular kinds of knowledge at particular times in the development life cycle? A complementary approach is to develop a method of measuring the degree of formality and optimization (*maturity*) of M&S processes. No such standardized and systematic assessment methodology is available for M&S processes, but the capability maturity model (CMM) and CMM Integration (CMMI) approach have been applied to many areas, after originating in the software engineering community. Achieving a capability maturity model for M&S processes requires research in a number of areas, including quantitative analysis of the complexity and uncertainties in modeling processes, optimization, risk analysis and control of modeling processes, and quantitative measures of process quality and cost.

Regarding conceptual model validation, the challenge is to find universally applicable concepts, with a theory that is satisfying to all the stakeholders and technology that is germane to a broad set of problems. For example, how does a conceptual model that is suitable for a specific use inform the development of other simulation process artifacts? How do the various stakeholders in the simulation activity use the conceptual model, valid or otherwise? Following the best practice to consider validation early in the development process, advances in theory involving validation of conceptual models will support the rigorous use of conceptual models throughout the simulation life cycle.

Finding A.3. *Architectures and services for conceptual modeling must enable integration of multiple engineering disciplines and development stages.*

Reliable modeling on a large scale for complex systems requires an architecture that enables models to be composed across disciplines. Arriving at such a model architecture requires developing mechanisms for efficient interaction among many sets of laws, determining the level of detail needed to observe emerging behaviors among these laws when integrated, and identifying design patterns appropriate to various communities of interest. The architecture must be supported by services that enable sharing of model elements at all levels, and extension of the architecture as needed. Implementing the architecture and services requires development of integration platforms for modeling, simulation, and execution. One of the major challenges to model integration is the semantic heterogeneity of constituent systems. Simulation integration (co-simulation) has several well-established architectures and standards, but there are many open research issues related to scaling, composition, the large range of required time resolutions, hardware-in-the-loop simulators, and increasing automation in simulation integration. Execution integration is needed as distributed co-simulations are shifting toward cloud-based deployment, a Web-based simulation-as-a-service model, and increased automation in dynamic provisioning of resources.

Reliable model integration depends on sufficient formality in the languages being used. In particular, formalizing mappings between the conceptual models of a system and its analysis models is critical to building reliable bridges between them. Combined with formal conceptual models of both system and analysis, a basis is provided for automating much of analysis model creation through model-to-model transformation. Perhaps the most fundamental challenge in achieving this for conceptual modeling is understanding the trade-offs in recording analysis knowledge in the system model, analysis model, or the mappings between them.

B. Computation: Exploiting Advances in Computing in Modeling Complex Systems

Computing has undergone dramatic advances in recent years. The days are long gone when computers were out of sight of most people, confined to mainframes locked away in machine rooms that could only be operated by highly trained specialists. Today, computers more powerful than yesterday's supercomputers are routinely owned and used by average citizens in the form of smartphones, tablets, laptops, and personal computers. They are key enablers in our everyday lives. Other major technological developments such as big data, cloud computing, the Internet of Things, and novel high-performance computing architectures continue to dramatically change the computing landscape.

Finding B.1. New computing platforms ranging from mobile computers to emerging supercomputer architectures require new modeling and simulation research to maximally exploit their capabilities.

The vast majority of M&S work completed today is performed on traditional computing platforms such as desktop computers or back-end servers. Two major trends in computing concern advances in mobile computing, on the one hand, and the shift to massive parallelism in high-performance computers on the other. As discussed momentarily, exploitation of mobile computing platforms moves models and simulations into new realms where the models interact with the real world. Maximal exploitation of M&S in this new environment, often in conjunction with cloud computing approaches, is not well-understood.

At the same time, modern supercomputer architectures have changed dramatically in the last decade. The so-called power wall has resulted in the performance of single processor computers to stagnate. Improved computer performance over the last decade has arisen from parallel processing, i.e., utilizing many computers concurrently to complete a computation. By analogy, to reduce the time to mow a large lawn, one can utilize many lawn mowers operating concurrently on different sections of the lawn. In much the same way, parallel computers utilize many processors to complete a simulation computation. Modern supercomputers contain hundreds of thousands to millions of processors, resulting in *massively parallel* supercomputers. Further, these architectures are often *heterogeneous*, meaning there are different types of processors included in the machine that have different, specialized capabilities. Effective exploitation of these platforms by M&S programs as well as new, experimental computing approaches is still in its infancy.

Finding B.2. Models and simulations embedded in the real world to monitor and steer systems toward more desirable end states is an emerging area of study with potential for enormous impact.

We are entering an age of "smart systems" that are able to assess their current surroundings and provide useful recommendations to users, or automatically effect changes to improve systems on the fly while the system is operating. For example, smart manufacturing systems can automatically adapt supply chains as circumstances evolve, or smart transportation systems can automatically adapt as congestion develops to reduce traveler delays. Models and simulations driven by online data provide a predictive capability to anticipate system changes and can provide indispensable aids to manage these emerging complex systems. However, key foundational and systems research questions must be addressed to realize this capability. Further, key questions concerning privacy, security, and trust must be addressed to mitigate or avoid unintended, undesirable side effects resulting from the widespread deployment of such systems.

Finding B.3. New means to unify and integrate the increasing "plethora of models" that now exists are needed to effectively model complex systems.