Research Challenges in Modeling & 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 & Simulation Coalition (NMSC) in conjunction with its parent organization the National Training & Simulation Association (NTSA). This report 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 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 modeling and simulation (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. Toward this end, several events were held leading up to the January workshop. These included:

- Winter Simulation Conference: plenary talk conference presentation (December 9, 2014, Savannah, Georgia).
- NMSC national meeting: panel session (February 26, 2015, Arlington, Virginia).
- Modsim World Conference: panel session (April 2, 2015, Virginia Beach Virginia).
- SIMULTECH Conference: plenary talk conference presentation (July 22, 2015, Colmar, France).
- Simulation Interoperability Workshop: plenary talk conference presentation (August 31, 2015, Orlando, Florida).
- Winter Simulation Conference: panel session (December 7, 2015, Orange County, California).

After funding commitments for the workshop were obtained, 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 took into account issues such as areas of technical interest in order to ensure balance across the four technical theme areas as well as other issues such as expertise, representation from different communities, seniority, and diversity considerations.

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 report. The workshop participants, their initial assignments to groups, and the group leads are included as an appendix to this report.

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 sub-challenges 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:

- 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 workshop. The submitted position statements are included in this report as an appendix.

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 break-out 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. At the time of this writing, several follow up events related to the workshop have taken place, or are under development:

- 2016 M&S Congressional Caucus Leadership Summit (Black Swans: Supporting National Priorities with Modeling and Simulation) and NMSC National Meeting, March 9-10, 2016, Chesapeake, Virginia.
- 2016 ACM SIGSIM Conference on Principles of Advanced Discrete Simulation (panel session), May 15, 2016, Banff, Alberta Canada.
- 2016 Interservice/Industry Training, Simulation and Education Conference (I/ITSEC) (panel session), November 29, 2016, Orlando, Florida.

We would like to thank the many individuals and organizations who helped to make this workshop possible. First, we thank the workshop sponsors, and 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 formed. 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.

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 case write much of the text in this report. The following individuals contributed to the writing of this report:

Introduction and Concluding Remarks: Richard Fujimoto and Margaret Loper

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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 to 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 the collection of infrastructures such as water, energy, and transportation along 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 in cities, or undesirable ones such as stock market crashes or 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, 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.

The workshop on *Research Challenges in Modeling and Simulation for Engineered Complex Systems* identified 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 the workshop identified challenges in four areas:

- *Conceptual modeling*. Understanding and developing complex systems requires the collaboration of individuals with widely different expertise. The models that form the language 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, reuse of existing models and simulations can be costly and time consuming, and can yield uncertain results. Advances are need 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 the formulation and simulation of large and complex problems, but is not yet well-defined or understood, making it an important topic for focused research. The workshop concluded that conceptual models are early stage artifacts that integrate and provide requirements for a variety of more specialized models, and that the term "early" applies to every stage of system development, leading 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 relationship 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 integration across engineering domains and construction of analysis tools, while retaining accessibility for domain experts, leading to 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 up 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 (*lifecycle engineering*). Regardless of complexity, the underlying principle for any type of lifecycle engineering is to ensure that unspent resources (e.g., money, time) are commensurate with work remaining. 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 lifecycle decisions and processes. In addition, workflows are central to any approach for making lifecycle processes explicit and manageable, but evaluation of these workflows is hampered by the lack of metrics for their quality and for 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 lifecycle to maximize value to program stakeholders. Further research is needed on how to set knowledge goals at particular milestones in a system development lifecycle. 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 lifecycle? 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 (CMMI 2016). 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 lifecycle.

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 between many sets of laws, determining the level of detail needed to observe emerging behaviors between 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, large range of required time resolution, 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, developing simulation-as-a-service use model via web interfaces and increasing automation in dynamic provisioning of resources as required.

Reliable model integration depends on sufficient formality in the languages used. In particular, formalizing mappings between 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 tradeoffs in recording analysis knowledge in the system model, analysis model, or 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 smart phones, 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.

As discussed earlier, complex systems contain many interacting components. Different components often require different types of simulations. For example, some subsystems may be best represented by equation-based, physical system simulations, while others are abstracted to only capture "interesting" events, jumping in time from one event to the next. Simulator platforms, frameworks, tool chains, and standards are needed to allow these simulations to seamlessly interoperate with each other. The simulations may be operating on vastly different time and spatial scales creating mismatches at boundaries where they must interact. Further, many executions of the simulation will usually be required to explore different designs or to assess uncertainties. Many problems call for thousands of runs to be completed. New approaches are needed to complete these runs in a timely fashion.

Finding B.4. Modeling and simulation is synergistic with "big data," and offers the ability to advance predictive capabilities well beyond that which can be accomplished by machine learning technologies alone.

"Big data" analysis techniques such as machine learning algorithms provide powerful predictive capabilities, but are limited because they lack specifications of system behavior. Simulation models provide such specifications, offering the possibility to augment the capability of pure data analysis methods, e.g., to answer "What if?" questions or to be used in non-recurring situations where sufficient data does not exist. There are clear synergies between M&S methods and machine learning algorithms to realize much more effective models that can be used to greatly improve decision making. However, important questions such as effective model and data representation and approaches to create effective integrated models and systems must be addressed to realize this potential.

C. Uncertainty: Understanding and Managing Unknowns in Modeling Complex Systems

All models have inherent uncertainties which limit them from fully explaining past events and predicting future events. Understanding this uncertainty and its implications is essential for M&S activities.

Finding C.1. There is a need to unify uncertainty-related efforts in M&S under a consistent theoretical and philosophical foundation.

Multiple communities have addressed issues related to uncertainty in models using different mathematical formulations; however, there is a lack of a rigorous theoretical and philosophical foundation. The lack of such a foundation has resulted in ad-hoc approaches for dealing with uncertainty, e.g., use of ad-hoc measures of model validity, and the artificial distinction between aleatory and epistemic uncertainty. Unification of efforts under a consistent framework is essential for further progress. It is recognized that probability theory is the only theory of uncertainty consistent with the established normative tenets of epistemology. There is agreement that Bayesian probability theory is the consistent foundation for uncertainty in M&S.

Finding C.2. Advancements in theory and methods are needed both for decision making in the M&S process and for M&S to support decision making.

M&S are purpose-driven activities which must be considered in the eventual context of use. The specific context defines the role and scope of the model in the decision-making process, and the resources available. From this perspective, M&S activities support decision making. Further, modelers are also decision makers who decide how much effort and resources to expend based on the potential impact on the decision. While decision theory provides the necessary foundation for making M&S decisions, there are unique challenges associated with M&S decisions in an organizational context. Examples of challenges include consistently deducing preferences for individual uncertainty management decisions from overall organizational goals, and the complexity of sequential decisions in M&S.

Finding C.3. Advancements are needed to understand and address aggregation issues in M&S.

M&S of complex systems involves aggregation of information from multiple sources. Techniques such as multi-physics, multi-disciplinary, multi-fidelity, and multi-scale modeling integrate models typically developed by different modelers. Aggregation of information and integration of models is associated with a number of challenges such as seamlessly integrating models across different levels and ensuring consistency in modeling assumptions. Even if consistency across different models is achieved, the fundamental nature of aggregation can also result in erroneous results due to the path dependency problem. There is a need to address the challenges associated with aggregation of physics-related and preference-related information in modeling complex systems.

Finding C.4. While there has been significant progress on understanding humans as decision makers, the utilization of this knowledge in M&S activities has been limited.

Humans are integral parts of socio-technical systems. Accurately modeling human behavior is essential for simulating overall system behavior. Further, the developers and users of models are human decision makers. Therefore, the effectiveness of the model development and usage process is highly dependent on the behavior of the human decision makers. Better understanding of biases that exist in human decisions can help towards better designed control strategies for socio-technical systems, better M&S processes, more efficient allocation of organizational resources, and better model-driven decision making. Addressing human aspects in M&S would require collaboration between domain-specific modeling researchers and researchers in social, behavioral, and psychological sciences.

Another key challenge in M&S is communication of model predictions and associated uncertainty among stakeholders. There is a need for techniques for consistently communicating the underlying assumptions and modelers' beliefs along with their potential impact on the predicted quantities of interest. There is a need for bringing uncertainty at the core of educational curricula. A modern curriculum on probability in engineering and science is needed to equip students with the foundation to reason about uncertainty. Finally, while "big data" has been used to inform the models of the simulated system, the use of "big data" has introduced new challenges associated with incomplete or noisy samples, high dimensionality, "overfitting", and the difficulties in characterizing uncertainty in extrapolative settings and rare events. New research approaches that incorporate rigorous mathematical, statistical, scientific, and engineering principles are therefore needed.

D. Reuse of Models and Simulations: Reducing the Cost of Modeling Complex Systems

As discussed earlier, the ability to reuse models and simulations can substantially reduce the cost of creating new models. This topic overlaps with some of the challenges discussed earlier. For example, the challenges of conceptual modeling and computational challenges play pivotal roles in reuse processes as well. However, the facets highlighted in those areas focused on identifying reusable solutions, selecting the best reusable solution under the given conceptual and technical constraints, and the integration of the identified solution into the appropriate solution framework, all while taking organizational and social aspects into account. The following three challenges were identified to categorize solution contributions: (1) the theory of reuse, (2) the practice of reuse, and (3) social, behavioral, and cultural aspects of reuse.

Finding D.1 Advancements in the theory of reuse are needed to provide a firm theoretical foundation for producing robust and reliable reuse practices.

A firm theoretical foundation is needed for producing robust and reliable reuse practices. While heuristics and best practices can guide the practitioners successfully, it is the theory behind these approaches that ensures their applicability. While good heuristics and practices have worked well elsewhere, and have led to good results, only a theoretic framework can provide formal proofs of general validity. In support of these tasks, key questions are related to composability, the use of metadata to enable reuse, and opportunities for reuse automation.

Finding D.2 Guides of good practices on reuse of simulation solutions, data, and knowledge discovery can in particular support the workforce.

Although work in recent years contributed to solving various challenges to the day-to-day practice of reuse in modeling, good practices are still needed to support the simulation workforce. To this end, the workshop addressed the reuse of M&S, the reuse of data, and the reuse of knowledge management. M&S research addresses primarily issues confronting the reuse of representations of models and their implementation in simulation languages and frameworks. Research on data reuse focuses on input needs and output possibilities of simulation systems, as well as the necessary metadata approaches. Finally, knowledge management research is coping with general challenges applicable to all these topics.

Finding D.3 Research on social, behavioral, and cultural aspects of reuse shows that they may stimulate or impede reuse at least as much as technical constraints.

Several recent studies show that often intangible human and organizational factors hinder the reuse of models, simulations, and data, even when all conceptual and technical aspects can be solved. Key research questions have the objective to identify and teach the skills necessary for a model or simulation producer to increase the ease of reuse by others if the producer chooses to, and can afford to do so. Programmatic issues, questions on risk and liability, and general social and behavioral aspects must be better understood and disseminated to contribute to reuse practices.

In summary, solutions to the research challenges described across the four technical areas discussed in the workshop will greatly expand our abilities to design and manage complex engineered systems. Advances in M&S will have broad impacts across many of the most important and challenging problems facing society today. The world is rapidly becoming more and more interconnected and interdependent, resulting in consequences that are increasingly more difficult to anticipate or plan for. While M&S has served us well in the past and is a critical tool widely used today, new advances are essential for the technology to keep pace with a rapidly changing world, and create new capabilities never even considered in the past.

1 Introduction

Computer-based models and simulations are vital technologies needed in advanced economies to guide the design of complex systems. M&S technologies are essential to address the critical challenges facing society today such as the creation of smart, sustainable cities, development of advanced aircraft and manufacturing systems, and creating more secure and resilient societies and effective health care systems, to mention a few.

However, the development and use of reliable computer models and simulations is today time consuming and expensive, and results produced by the models may not be sufficiently reliable for their intended purpose. M&S faces unprecedented new challenges. Engineered systems are continually increasing in complexity and scale. Advances in M&S are essential to keep up with this growing complexity and to maximize the effectiveness of new and emerging computational technologies to engineer the increasingly complex systems that are needed in the future.

1.1 Why Now?

Computer-based models and simulations have been in use as long as there have been digital computers. For example, one application of the ENIAC, the first electronic digital computer, was to compute trajectories of artillery shells to create firing tables used in World War II. There is no question that computer simulations have had major impacts on society in the past, and will continue to do so in the future. The importance of M&S was recognized in the United States House of Representatives that declared it a critical technology of national importance (U.S. House of Representatives 2007).

New developments in M&S technologies are of critical importance now. M&S applications are rapidly increasing in scale and complexity as systems become more complex and interconnected. For example, consider the use of M&S to inform policy makers to steer urban growth toward more sustainable trajectories. It is widely recognized that one must view cities as a whole, and consider interdependencies among critical infrastructures such as transportation, water, and energy, as well as interactions with social processes and policy. Each of these systems and infrastructures is a large, complex adaptive system in its own right. Creating simulation models able to capture the behaviors and interactions among these infrastructures and social-economic processes is even more challenging. Advances in modeling and simulation technologies are needed.

While the emerging demands of new applications built using M&S present one set of challenges, the underlying computing platforms and technologies exploited by M&S have undergone dramatic changes in the last decade, also highlighting the timeliness of this initiative. These advances create new opportunities, and challenges, for modeling and simulation to achieve even greater levels of impact. Trends such as the Internet-of-Things and “Big Data” have strong implications concerning the future of modeling and simulation. Online decision-making is an area of increasing importance with the emergence of mobile computing and growth in technologies such as sensor networks. Modeling and simulation is complementary to the exploitation of data analytics. While models derived purely from data analytics offer much benefit, they do not include behavioral descriptions of the system under investigation that are necessary for prediction of dynamic system behaviors that are necessary for what-if experimentation, or analysis of situations where sufficient data, or the right data are not available, e.g., due to privacy or other concerns. At the same time, power and energy consumption has become an important consideration in computing, both for mobile computing platforms and computing in data centers. Massively parallel multiprocessor systems containing over a million cores, GPUs, and cloud computing have emerged in importance in the last decade, motivating research to effectively exploit these platforms. Cloud computing offers much broader exploitation of M&S technologies by making high performance computing capabilities much more broadly accessible, and embedding simulations into operational environments presents new opportunities and challenges.

1.2 Modeling and Simulation

There are several definitions of models, simulations and the M&S discipline. The U.S. Department of Defense (DoD) defines these terms as follows in their online glossary (MSCO 2013):

- *Model:* a physical, mathematical, or otherwise logical representation of a system, entity, phenomenon, or process.
- *Simulation:* a method for implementing a model and behaviors in executable software.
- *Modeling and Simulation (M&S):* the discipline that comprises the development and/or use of models and simulations.

Here, we are specifically concerned with computer models where the representation is stored and manipulated on an electronic computer. A simulation captures salient aspects of the dynamic behavior of the modeled system over time. Typically, a simulation model captures the state of the system being modeled at one instant in time through a set of values assigned to variables and data structures in the computer program, commonly referred to as state variables. For example, a simulation of vehicle transportation system might define state variables for each vehicle in the system indicating its current location, direction of travel, speed, acceleration, etc. A set of procedures or programs transform these state variables to represent the state of the system from one time instant to the next. In this way the simulation constructs a trajectory or sample path of the state of the system over the period of time that is of interest.

We note that modeling and simulation are closely related, but distinct areas. *Modeling* is primarily concerned with the representation of the system under investigation. Models always involve a simplified representation of the system. Therefore, a key question concerns what is included, and by implication, what is left out of the model. *Simulation* is concerned with transforming the model to mimic the behavior of the system over time. Key questions include the algorithms, procedures, and software that are required to perform this transformation. In some cases, creation of the model is of primary concern, and simulation may be secondary or not required at all. For example, when creating the design of an automobile that is to be handed over to a factory that is responsible for manufacturing, the dynamics of the vehicle as it is travelling on the roadway are not important. Here, we are concerned with both modeling and simulation aspects of complex engineered systems.

The modeling and simulation discipline covers many aspects. The elements that are most relevant to this report are perhaps best described within the context of the life cycle of an M&S project or study. The process depicted in Figure 1.1 captures the basic elements of this life cycle (Loper 2015). The life cycle begins by defining the purpose and scope of the study. Specific questions concerning the actual or envisioned system under investigation are defined. The purpose and scope forms the basis of the *conceptual model* that characterizes the system under investigation. Elaborated upon below, the conceptual model includes descriptions of the abstractions used to describe the system; key assumptions used by the model are defined explicitly or (more often) implicitly in the conceptual model as well as key inputs and outputs. Data used to characterize the system and information concerning important processes are collected, analyzed, and incorporated

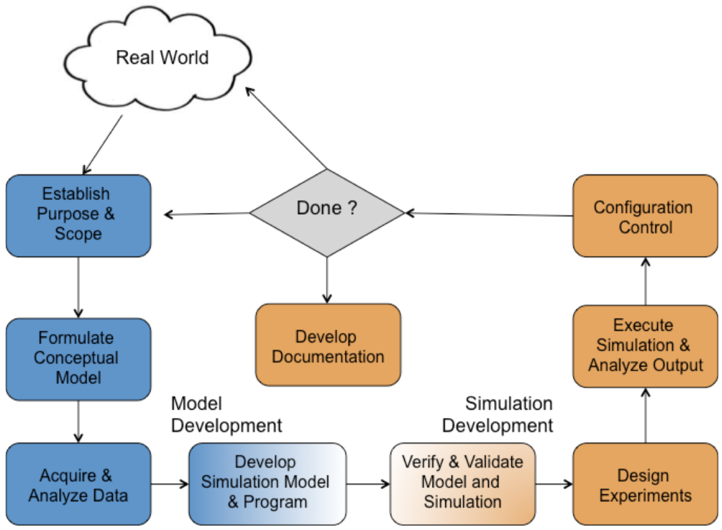


Figure 1.1: M&S Lifecycle Process

into the model. The conceptual model is then converted into a simulation model and computer program. Verification is concerned with ensuring that the simulation program is an acceptable representation of the conceptual model. Verification is to a large extent a software development activity. Validation is concerned with ensuring the simulation program is an acceptable representation of the system under investigation for the questions posed in the study. This is often accomplished by comparing results produced by the simulation program with data measured from the system under investigation or, in the absence of an implemented system that can be measured, other models of the system. Once the simulation model has been validated to an acceptable degree of certainty, it is applied to answer the questions posed in the first step of the life cycle. The model will be executed many times, e.g., using different random number streams for stochastic simulation models, or to explore various parameter settings; the experiment design defines the simulation runs that are to be completed. Output analysis concerns characterization and quantification of model results, e.g., to determine confidence intervals and variance of output values. Simulation models often must be modified and evolve during the life cycle, e.g., to improve the validity of its results or to incorporate new capabilities or to answer new questions not recognized in the initial design. Configuration control refers to the processes necessary to manage these changes. Finally, once the necessary results have been produced, they must be documented and presented to the individuals or decision-makers to illustrate key behaviors and outcomes predicted by the simulation model.

The boxes in blue in Figure 1.1 represent model development activities and the orange boxes represent simulation development activities. These boxes do not represent an absolute separation between modeling and simulation – the "develop simulation model & program" box bridges between the modeling and simulation activities, and the "verify & validate model and simulation" box represents activities that are performed throughout the entire lifecycle.

Here we focus on four key aspects of the life cycle, discussed next:

- Development of the conceptual model.
- Computational issues concerning the execution of simulation models.
- Understanding and managing uncertainty that is inherent in models.
- Reuse of models and simulations to accelerate the simulation model development process.

Conceptual Model

A model is a simplification and approximation of reality, and the art of modeling involves choosing which essential factors must be included, and which factors may be ignored or safely excluded from the model. This is accomplished through the process of simplification and abstraction. Simplification is an analytical technique in which unimportant details are removed in an effort to define simpler relationships. Abstraction is an analytical technique that establishes the essential features of a real system and represents them in a different form. The resultant model should demonstrate the qualities and behaviors of a real world system that impact the questions that the modeler is trying to answer. The process of simplification and abstraction is part of developing the conceptual model. A simulation conceptual model is a living document that grows from an informal description to a formal description and serves to communicate between the diverse groups participating in the model's development. It describes what is to be represented, the assumptions limiting those representations, and other capabilities (e.g., data) needed to satisfy the user's requirements. An informal conceptual model may be written using natural language and contain assumptions about what one is or is not representing in the model. A formal conceptual model is an unambiguous description of model structure. It should consist of mathematical and logical relationships describing the components and the structure of the system. It is used as an aid to detect omissions and inconsistencies and resolve ambiguities inherent in informal models, and is used by software developers to develop code for the computational model.

Simulation Development and Reuse

Once the conceptual model has been created, the next step is to create the simulation by coding the conceptual model into a computer recognizable form that can calculate the impact of uncertain inputs on decisions and outcomes that are important relative to the purpose and scope of the study. Translating the model into computer code and then into an executable involves selecting the most appropriate simulation methodology and an appropriate computer implementation. Methodologies appropriate for modeling complex systems include: discrete event simulation, discrete event system specification (DEVS), petri nets, agent-based modeling and simulation, system dynamics, surrogate models, artificial neural networks, Bayesian belief networks, Markov models, game theory, network models (graph theory), and enterprise architecture frameworks, among others (Kinder 2015).

The development of new simulation programs can be greatly accelerated by reusing existing simulations rather than developing everything "from scratch" for each new model. At its most basic level, common components of the program such as key data structures and libraries for random number generation can be readily reused rather than redeveloped. A much more ambitious goal is to reuse entire model components or entire simulations. Many large, complex systems may be viewed as collections of subsystems, each of which may be a complex system in its own right, that interact with each other in some fashion. A simulation model of such "systems-of-systems" may be derived by integrating existing simulation models of the subsystems. The end goal is to create simulations that may be easily composed with other simulations, much like composing mathematical functions to create more complex functions.

Simulation Model Execution

A single execution of the simulation model is commonly referred to as a trial. A simulation study will typically require many hundreds or thousands of trials. Each trial is an experiment, or instance, where we supply numerical values for input variables, evaluate the model to compute numerical values for outcomes of interest, and collect these values for later analysis. Exhaustive exploration of all input parameters, e.g., to identify an optimal solution is usually impractical due to the large number of runs that would be required. Further, for stochastic models where random numbers are used to characterize uncertain variables, the output of a simulation run produces a single sample. Hence, simulation often relies on random sampling of values for the uncertain variables. To obtain more accurate results the number of trials may be increased, so there is a tradeoff between accuracy of the results, and the time taken to run the simulation.

The platform on which the simulation executes is an important consideration in executing the simulation model. For large models parallel processing techniques utilizing parallel and distributed computing platforms may be used to accelerate model execution. In other contexts, the simulation may be used to control an operational system. In this case, data from the system is collected and fed directly into the simulation model. The simulation may then analyze alternate options and produce recommended courses of action that are then deployed in the operational system. This feedback loop may be automated, or may include human decision makers. This paradigm of utilizing online data to drive simulation computations and to use these results to optimize the system or adapt the measurement process is referred to as dynamic data driven application systems (DDDAS).

Uncertainty and Risk

A simulation model is always an approximate representation of reality. As such, there are always uncertainties concerning the relationship between the model and the actual system. Uncertainty can enter mathematical models and experimental measurements in various contexts. For example, parameter uncertainty comes from the model parameters that are inputs to the mathematical model, but whose exact values are unknown and cannot be controlled in physical experiments, or whose values cannot be exactly inferred by statistical methods. Parametric variability comes from the variability of input variables of the model. Structural uncertainty, aka model inadequacy, model bias, or model discrepancy, comes from the lack of knowledge of the underlying true physics. Algorithmic uncertainty, aka numerical uncertainty, comes from numerical errors and numerical approximations per implementation of the computer model. Interpolation uncertainty comes from a lack of available data collected from computer model simulations and/or experimental measurements. For other input settings that don't have simulation data or experimental measurements, one must interpolate or extrapolate in order to predict the corresponding responses.

A quantitative risk model calculates the impact of the uncertain parameters and the decisions we make on outcomes that we care about. Such a model can help decision makers understand the impact of uncertainty and the consequences of different decisions. The process of risk analysis includes identifying and quantifying uncertainties, estimating their impact on outcomes that we care about, building a risk analysis model that expresses these elements in quantitative form, exploring the model through simulation, and making risk management decisions that can help us avoid, mitigate, or otherwise deal with risk.

1.3 Preliminary Questions

Prior to the workshop five topic areas were identified to generate challenges for modeling and simulation research:

1. Selected applications that would benefit from advances in modeling and simulation
2. Conceptual modeling

3. Computational methods: algorithms for simulation and other types of inference
4. Uncertainty in modeling and simulation
5. Reuse of models and simulations

Important application areas and questions posed prior to the workshop are discussed next.

Applications

Engineered systems continue to grow in complexity and scale. Existing modeling and simulation capabilities have not kept pace with the need to design and manage new emerging systems. Although the workshop was focused on modeling and simulation per se, distinct from the domain in which the technology is applied, the requirements of modeling and simulation technologies are ultimately derived from the application. In this context the workshop explored new emerging developments in specific applications of societal importance in order to assess the needs and impacts that advances in modeling and simulation will have within those domains.

Specific application domains targeted by the workshop included:

- Aerospace
- Healthcare and medicine
- Manufacturing
- Security and defense
- Sustainability, urban growth and infrastructures

Conceptual Modeling

Although one of the first steps in the development of a model is the development of a conceptual model, such conceptual models have traditionally been informal, document-based. As the complexity of simulation models increases and the number of domain experts contributing to a single model grows, there is an increasing need to create formal, descriptive models of the system under investigation and its environment. This is particularly important for the engineering of complex systems where multiple system alternatives are explored, compared and gradually refined over time. The descriptive model of each system alternative – describing the system of interest, the environment and interactions between them – can serve as a conceptual model for a corresponding analysis or simulation model. Formal modeling of these descriptive, conceptual models poses significant research challenges:

- How can models expressed by different experts in different modeling languages be combined in a consistent fashion?
- What level of formality is suitable for efficient and effective communication?
- What characteristics should a modeling environment have to support conceptual modeling in an organizational context – a distributed cognitive system?
- What transformations of conceptual models to other representations are possible, and useful? What are the major impediments to realizing such transformations?

Computational Methods

The main reason for modeling is to extend human cognition. By expressing our knowledge in a mathematical formalism, the rules of mathematical inference implemented in computer algorithms can be used to draw systematic conclusion that are well beyond the natural cognitive ability of humans. For instance, simulation allows us to project how the state of a system will change over time for complex systems with millions of state variables and relationships. Advancing the algorithms for such inference so that ever larger models can be processed more quickly is likely to remain a crucial capability for engineering and science. Besides simulation, there is an increasing role for model checking, especially for engineered systems that are affected by high-impact low-probability events.

This leads to the following questions for discussion:

- What are current trends in computing affecting modeling and simulation and how can they best be exploited?
- How will these trends change the nature of simulation and reasoning algorithms?
- What are the major gaps in computational methods for modeling and simulation, and what are the most important research problems?
- How can one best exploit the vast amounts of data now becoming available to synergistically advance M&S for engineering complex systems?

Model Uncertainty

The goal of modeling and simulation often is to make predictions, either to support decisions in an engineering, business or policy-making context, or to gain understanding and test hypotheses in a scientific context. It is impossible to prove a model is correct – the predictions are always uncertain. Yet, many models and simulations have been proven to be useful, and their results are routinely used for many purposes. To further improve the usefulness of models, it is important that we develop a rigorous theoretical foundation for characterizing the accuracy of the predictions. Within the modeling and simulation community, there is still a lack of agreement on how best to characterize this uncertainty. A variety of frameworks have been proposed around concepts of validation and verification, and a variety of uncertainty representations have been proposed.

This leads to the following questions for discussion:

- What is the most appropriate approach to consistently represent and reason about uncertainty in complex systems consistently?
- What is the best approach to characterizing the uncertainty associated with a simulation model in order to enable and facilitate reuse?
- How should one aggregate knowledge, expertise, and beliefs of multiple experts across different domains?
- What is the best approach to take advantage of the large and diverse datasets for characterizing uncertainty and for improving model accuracy?
- What are the most promising approaches to accelerate the validation of models for specific application contexts?

Model Reuse

Although modeling has become indispensable in engineering and science, the cost of creating a good model can be considerable. This raises the question of how these costs can be reduced. One approach is to encode domain knowledge into modular, reusable libraries of models that can then be specialized and composed into larger composable models. Such a modular approach allows the cost of model development, testing, and verification to be amortized over many (re)uses. However, reuse also introduces new challenges:

- How can a model user be confident that a planned re-use of the model is within the range of uses intended by the model creator?
- How can one characterize the uncertainty of a model that is reused (possibly with some adaptations to a new context)?
- How can one characterize the uncertainty of simulation models obtained through the composition of multiple models?
- How can one accelerate the process of adapting and reusing models for different purposes? What are the fundamental limitations of technologies for model reuse?

The chapters that follow discuss each of these topics. Chapter 2 reports on the five targeted application areas. Chapter 3 reports on discussions and research challenges concerning conceptual models. Chapter 4 describes computational challenges in M&S. Chapter 5 discusses uncertainty and associated research challenges. Finally, Chapter 6 characterizes and presents research challenges concerning the reuse of models and simulations and Chapter 7 presents concluding remarks.

2 Applications

Modeling and simulation provide a powerful means to understand problems, gain insights into key tradeoffs, and inform decisions at all echelons of the domain. Applications of modeling and simulation should be driven by the nature of the problems of interest and the appropriateness of the model or simulation for the problem and domain in which it is being considered or applied.

This chapter begins by reviewing the five keynote presentations from the workshop to understand the nature of the problems addressed rather than the approaches to modeling and simulation employed in these instances. This leads to consideration of crosscutting challenges associated with these examples. This chapter concludes with a discussion of specific modeling and simulation challenges identified.

2.1 Five Examples

The workshop provided examples of five problems where modeling and simulation can provide the means to understand problems, gain insights into key tradeoffs, and inform decisions.

- Urban Infrastructure (Crittenden)
- Healthcare Delivery (Combs)
- Automated Vehicle Manufacturing (Yukish)
- Deep Space Missions (Jenkins)
- Acquisitions Enterprise (Kraft)

Table 2.1 compares these five examples in terms of the nature of the problem addressed rather than the specific modeling and simulation employed. The five examples are contrasted in terms of top-down forces, bottom-up forces, human phenomena, and the difficulty of the problem.

Top-Down Forces

The top-down forces affecting Urban Infrastructure include the consequences of climate change, forced migration, and macroeconomic trends. In contrast, Healthcare Delivery is being affected by increased demand for services from an aging population, increased prevalence of chronic disease, and changing payment models. Many of these forces are exogenous to the urban and healthcare enterprises.

Automated vehicle manufacturing is being affected by demands from the Department of Defense for rapid design, development, manufacturing, deployment, and sustainment. This occurs in the broader context of the Acquisitions Enterprise, which is being affected by Congressional and military services' imperatives, mandates, and regulations, as well as budget pressures. These forces are endogenous to the defense enterprise, but exogenous to particular programs.

The top-down forces affecting Deep Space Missions include mission requirements for robustness and flexibility, as well as the magnitude and timing of budgets. These requirements are seen as exogenous to the extent that they are taken as non-negotiable. There could be, of course, tradeoffs between requirements and budgets.

Bottom-Up Forces

Bottom-up forces tend to come from within the enterprise and hence can be seen as endogenous to the system. Such forces are often more amenable to prediction, control, and perhaps design.

Thus, they are more likely to be explicitly represented in models and simulations rather than seen as being external to the phenomena being modeled.

The bottom-up forces of increased demands on infrastructure and generation of waste, as well as dealing with waste, affect Urban Infrastructure. Healthcare Delivery must deal with patients' disease incidence, progression, and preferences, as well as providers' investment decisions. Deep Space Missions is affected by environmental surprises, technological failures, and public support for space exploration. These three examples concern the magnitudes and uncertainties associated with demands on those systems.

Automated vehicle manufacturing is affected by the state of technology for design, development, and manufacturing, as well as the availability of tools, components and materials. Acquisitions Enterprise must address asymmetric threats, changing missions, globalization of technology and, in some areas, the declining defense industrial base. These two examples are laced with changing requirements and both technological and organizational constraints.

Human Phenomena

Behavioral and social phenomena are much more difficult to model than purely physical systems. The five examples differ significantly in terms of the prevalence of human phenomena.

Social and political forces, as well as individual preferences and decisions regarding consumption and use of infrastructure affect Urban Infrastructure. Disease dynamics, patient choice, and clinician decisions affect Healthcare Delivery. Many of the behavioral and social phenomena associated with these examples are not amenable to design changes.

Automated Vehicle Manufacturing is laced with design and development decision making, supervisory control of manufacturing, and operation and maintenance of deployed systems. Deep Space Missions is similarly affected by design and development decision making, as well as ground operations decision making. Acquisitions Enterprise is also affected by decision making at all levels, as well as sustainment of deployed systems. The decision making for these three examples is often amenable to various levels of decision support.

Difficulty of Problem

The difficulty of addressing Urban Infrastructure is exacerbated by fragmented decision making across city, state, and federal agencies, all in the context of severely aging infrastructure. Healthcare Delivery is difficult due to uncertainty of demands for various services, impacts of science and technology advances, and stability of payment models. These two examples face uncertain demands and organizational difficulties.

For Automated Vehicle Manufacturing, the required pace of rapid automation exceeds the state of the art. The level of integration of all needed ingredients is very demanding. Acquisitions Enterprise is beset by a plethora of models, methods, and tools, as well as fragmented and siloed decision making. Deep Space Missions faces harsh environments, extreme distances, communications delays of minutes to hours, and infeasibility of maintenance and repair. These three examples are laced with technological and technical difficulties.

2.2 Crosscutting Issues

In all cases, the problem being addressed must be considered within the broader enterprise context of top-down and bottom-up forces that influence the problem and likely constrain the range and nature of solutions, as well as the choice of the model(s) or simulation(s) to be applied. In other words, what phenomena are internal and external to the model and simulation?

Many models and simulations do not incorporate rich representations of the human behavioral and social phenomena associated with the problems of interest. Yet, human operators and maintainers, as well as citizens and consumers, are central to several of the example problems. Humans provide flexible, adaptive information processing capabilities to systems, but also can make risky slips and mistakes. There is much more uncertainty in systems where behavioral and social phenomena are prevalent.

There are also the human users of models and simulations, ranging from direct model-based decision support to use of model-derived evidence to support organizational decision processes. Technology now enables powerful decision support environments that can empower decision makers to immerse themselves in the complexity of their problem spaces. Evidence of this is increasingly immersive interactive visualizations that prompt expressions like “wow,” but are not well understood in terms of their impacts on decision making.

All of the examples are plagued, to a greater or lesser extent, by the fragmentation and incompatibilities of the ever-evolving range of available tools. Some areas such as computational fluid dynamics, semiconductor design, and supply chain management have achieved a level of standardization, but this is quite difficult in areas where “one off” solutions are the norm. Investing in developing and refining a model and simulation is easier to justify when one is going to produce thousands or even millions of the system of interest. This is more difficult to justify and accomplish well when the target is, for example, a single mission.

Underlying all five examples are implicit assumptions and questions about the model or simulation of interest. Is the credibility of a model or simulation understood, accepted, or implied? Are the effects of uncertainty understood? Can one trust in the results of the model or simulation? Can truly emergent behavior be elicited by the representation(s) chosen? How can one understand the current configuration as the model or simulation evolves? Does the model or simulation conform to exchange standards that enable valid conjunctions of models or simulations?

There is also an assumed demand for interactivity between the users and the model or simulation environment. This is likely to require more intelligence and resilience in the model or simulation to enable valid responses to the range of external stimuli allowed. At the very least, it requires that developers of models and simulations have deep understanding of the use cases the model is intended to support as well as the likely knowledge and skills of the envisioned users.

Finally, a major challenge concerns the necessary regulatory, statutory and cultural hurdles that must be surmounted to actually use a model or simulation, and of the set of phenomena associated with the problem of interest to support making real decisions. This requires that decision makers both trust the model or simulation and be willing to make the decisions being informed by the visualizations of model outputs for the scenarios explored.

2.3 Modeling and Simulation Challenges

The applications cited above are part of an almost infinite space of uses for models and simulations. There are overlaps in the application of models and simulations; overlaps in the necessary characteristics of the model or simulation for the intended use; overlaps in the methods and processes used to develop models or simulations; and overlaps in the challenges with the application of modeling or simulation.

The development of a model, or a simulation execution of a model, as a representation of reality can only go so far. Most problems are complex, and hence are decomposed to enable a solution. Modularization of a problem so that each part can be modeled or simulated is fairly straightforward. What is not straightforward is the understanding of the interdependencies between the system modules being modeled. In part, this is caused by the loss of understanding of these interdependencies when a system is decomposed, or modularized. You cannot validly model or simulate what you do not understand.

Because of the loss of understanding of important interdependencies, it is very difficult to explicitly and adequately represent the interactions in the models of the decomposed system. Because of this, it is not possible to recompose the models or simulation executions into a representation of the original system. Emergent behaviors as a result of the composition may or may not replicate the unidentified relationships between the modules of the original system. In other words, the emergent behaviors may be artifacts of the decomposition rather than reflections of reality.

The challenges with emergent behavior extend beyond the composition of models or simulation executions. These challenges extend into the relationships which exist between the modeled physical and organizational phenomena, and the simulation of the processes in which the models are to be used. This boundary point can be thought of simply as an interface definition.

The concept of an interface is simple; however, the necessary depth of information needed to express the relationship between the physical and organizational phenomena and the system or process that uses them is not easily identified. Methods for identifying the needed depth of information, based on understanding of the interactions, are an area of significant challenge in efficient use of conceptual modeling or execution of conceptual models in a simulation.

Continuing with issues associated with the interactions between modeled parts of a system, or models within a larger system, challenges exist with automated methods for constructing an operational environment from a hierarchical set of model components, for example, within a product line. Considering the needed depth of information, there are challenges in knowing how much information to include in the operational environment. This multi-faceted problem includes identification of the necessary depth of information to properly exercise the model, or gain the necessary data from the simulation execution. There are no known methods for translating between the system, and the environment in which it operates. As stated earlier, you cannot validly model what you do not understand.

Other challenges in conceptual modeling exist in translating the descriptive models from their representational format into executable simulations. These challenges exist in both the essence of model content, as well as the computer environment in which the model will execute. For example, some conceptual models exist in text format. The automated translation of a model expressed in a rich language, into an environment which ultimately is expressed in Boolean expressions is perhaps the largest of the challenges in the translation domain. Less complex, but no-less challenging, is the ability to completely describe the model or simulation so that automated methods can, without loss, translate from one representational format to another.

Additional challenges in modeling and simulation exist within the computational environment in which they exist. Just as there are challenges in modeling the relationships between modeled parts of a system, there are dependencies which exist between the model or simulation, and the infrastructure in which it operates or exists. This is especially true for simulations. An improper execution environment, will introduce unquantified unknowns into the results. Potentially less known are the impacts to the model from the infrastructure in which it exists. The model, as the basic representation of reality, is assumed to be uncorrupted. The model is usually never assessed for representational accuracy or corruption effects when accessed. It is assumed to be in the same state as when it was last 'touched'. The ability to assure that the model is free from infrastructure-induced defects is a gap existing today.

Once the model is put into use, challenges exist due to the need to match the results to the user's viewpoint. Visualization of the model or visualization of the simulation results can be assessed as correct or incorrect simply because the visualization tools used do not represent the results in a manner that is understandable, or useful to the user. Work remains to be done on characterizing the user needs and preferences, as matching that to the visualization effects of the model, or data set resulting from the simulation execution. These challenges can be extended deeper than the visualization tool. Characterizing the user needs, and matching them to the models or simulation execution that fits the problem space in an automated fashion has the potential to significantly increase the efficiency in the use of the model or simulation.

Other challenges exist in the representational format of the underlying phenomena within the model or simulation. There exists a plethora of representational methods for models. Not all of these are known to all model builders or users. Model or simulation users need to be able to assess the applicability of models or simulations to various problems, which exist in formats that are unknown or less known to the users. Methods to translate model or simulation characteristics from one format to another, or represent them in a standard, acceptable format, remain a challenge today.

Challenges existing at the intersection of model and simulation content and the infrastructure in which it exists or executes include the need for methods to identify optimal fidelity or resolution needed for proper application to decision support. Typically, decision makers express their needs in terms of textual or spoken questions. This hides the complexity which exists in matching computational simplicity and rigor to the rich context underlying written or spoken format. Beginning with simple noun verb comparisons will get us part of the way to the match. However, nouns and verbs are not easily matched to mathematical expressions which exist in the computational environment. Methods are needed both to automatically perform the match, as well as to break down the language question into constituent parts which more easily match the computational component, taking care to allow for variability in the language itself. Early steps include allowing the user to base model or simulation selections on the presentation of computational expressions.

Challenges remain in the representation of the natural environment, both internally and externally. Biological and social processes are not easily expressed using logic constructs. As such, a different tactic may be to express what is known in logical constructs, and to quantify what is not known. This serves to reduce the problem to some extent, but leaves unresolved a way to quantify the uncertainty of biological and social systems.

Particularly challenging is a method to express environments that are driven by human behavior, such as socio-economic environments. There is a lack of methods to express, or understand, what is not expressed in systems and environments where humans are involved. Human actions can be unscripted, unpredictable, and often not possible to model in ways comparable to physical phenomena. This is partly because of the unknown relationships, but also because human judgement can be quite subtle.

In order to model or simulate interactions involving biological (human, animal, etc.) inputs, or human-human interactions results, the multi-fidelity, multi-modal, multi-domain models often constructed involve rather mixed precision. The ability to actually do this, and have a repeatable, predictable result is necessary, but methods do not exist today to accomplish this, or validate the composition or decomposition.

The challenges discussed thus far have not included the challenges coming from the application domains themselves. One challenge is with the applicability of the model or simulation beyond the problem space for which it was originally intended. Models and simulations are often reused due to word-of-mouth, with or without the associated documentation. Challenges exist with models or simulations, built for one purpose being validly used in another domain. Just because it was not built for a particular purpose does not mean that it is inherently not usable for another purpose. The challenge is how to validate a model in a different domain.

Modeling and simulation exists for almost every activity today. However, each activity domain retains its own language. This usually underlies the domain's models and simulations. Challenges exist with integrating the domain language and knowledge, extended into the model or simulation manifested. Integration, or interaction between multiple domains is usually accomplished using language. This allows for reasoning and translation of concepts. How can this be extended to facilitate multi-domain model integration?

Many models and simulations are never retired. Such models and simulations evolve through modification. Is it possible to characterize the types of modifications performed to evolve the models? If yes, how? When is it necessary to characterize a model as new? When is it impossible to assume validation due to changes? There exists a need to answer these questions, since evolving models and simulations need to be trusted.

A final challenge remains in understanding and then describing a model or simulation as a complete entity, for future use, for contracting purposes, etc. The methods to completely describe a model or simulation begin with understanding what "complete" means in a domain, as well as use of a model or simulation. The use of a model or simulation within a domain, or ecosystem, needs to be articulated to fully understand the boundary conditions of the model or simulation, the extensibility of the model or simulation, the history of the model or simulation, as well as the current state of use.

	Urban Infrastructure (Crittenden)	Healthcare Delivery (Combs)	Automated Vehicle Manufacturing (Yukish)	Deep Space Missions (Jenkins)	Acquisitions Enterprise (Kraft)
Top-Down Forces	Consequences of climate change, forced migration, macroeconomic trends	Increased demand for services, increased prevalence of chronic disease, changing payment models	Demands for rapid design, development, manufacturing, deployment, and sustainment	Mission requirements for robustness and flexibility, magnitude and timing of budgets	Congressional and services' imperatives, mandates, and regulations; budget pressures
Bottom-Up Forces	Increased demands on infrastructure and generation of waste, dealing with waste	Patients' disease incidence, progression, and preferences; providers investment decisions	State of technology for design, development, and manufacturing; availability of tools, components and materials	Environmental surprises, technological failures, public support for space exploration	Asymmetric threats, changing missions, globalization of technology, declining defense industrial base
Human Phenomena	Social and political forces, individual preferences and decisions regarding consumption and use of infrastructure	Disease dynamics, patient choice, clinician decisions	Design and development decision making, supervisory control of manufacturing, operation and maintenance of deployed systems	Design and development decision making, ground operations decision making	Decision making at all levels; sustainment of deployed systems
Difficulty of Problem	Fragmented decision making across city, state, and federal agencies; aging infrastructure	Uncertainty of demands for various services, science and technology advances, and stability of payment models	Required pace of rapid automation exceeds state of the art, level of integration of all needed ingredients very demanding	Harsh environment, extreme distances, communications delays of minutes to hours, and infeasibility of maintenance and repair	Plethora of models, methods, and tools; fragmented and siloed decision making

Table 2.1. Comparison of Five Applications Examples

3 Conceptual Modeling

Over the past decade, within the modeling and simulation community there has been a growing interest in, and concern about "conceptual modeling." Generally accepted as crucial for any modeling and simulation project addressing a large and complex problem, conceptual modeling is not well-defined, nor is there a consensus on best practices. "Important" and "not well understood" would seem to qualify conceptual modeling as a target for focused research.

Some workshop participants defined conceptual models as "early stage" artifacts that integrate and provide requirements for a variety of more specialized models. In this view, conceptual models provide a foundation from which more formal and more detailed abstractions can be developed, and eventually elaborated into analysis models (e.g., for simulation). However, workshop discussion led us to recognize that "early" and "late" are relative terms that apply within each stage of development. For example, creating an analysis model might involve describing, (i.e., modeling) the analysis independently of software ("conceptually") before implementation and execution. As a consequence, there might be multiple "early" models: conceptual models of reality and conceptual models of analysis; and there may be multiple versions of conceptual models as the understanding of the target system matures and the analysis design and implementation evolves.

These varieties of conceptual models are sometimes distinguished in existing work, with different terminology. In 2013, Robinson used "conceptual model" to mean "a non-software specific description of the simulation model, … describing the objectives, inputs, outputs, content, assumptions and simplifications of the [simulation] model" and "system description" to mean models derived from the "real world," with two stages of computer-specific models derived from the system description (Robinson 2013). In a 2012 tutorial, Harrison and Waite use "conceptual model" to mean "an abstract and simplified representation of a referent (reality)" (Harrison and Waite 2012), instead of Robinson's "system description."

With this context, developing an engineering discipline of conceptual modeling will require much better understanding of:

1. how to make conceptual models explicit and unambiguous, for both the target system (or referent) and the target analysis
2. the processes of conceptual modeling, including communication and decision-making involving multiple stakeholders
3. architectures and services for building conceptual models

Answering the first question (explicitness) requires considering alternative formalisms for expressing conceptual models, and the languages based on these formalisms, which are addressed in section 3.1. The second question (process) is discussed in section 3.2. The third question involves architectures for model engineering, as well as services provided to conceptual modelers, and is covered in section 3.3.

3.1 Conceptual Modeling Language/Formalism

An articulated conceptual model, whether describing the system of interest (the *referent*, in Robinson's terminology) or an analysis model of the system of interest, is expressed using some language, which may be formal or informal, graphical, textual, mathematical, or logical. Today, the situation is that most often, conceptual models are expressed using some combination of sketches, flowcharts, data, and perhaps pseudo-code. Lack of general agreement on the implications of these techniques (i.e., ambiguity) limits the computational assistance that can be provided to engineers. Incorporating conceptual modeling into a modeling and simulation engineering discipline will require more explicit and formal conceptual modeling languages. However, conceptual modeling must be done in a manner accessible to domain engineers, who might not be trained in the necessary formalisms. This is addressed in the first subsection below. In addition, formal conceptual modeling applies as much to analysis as to the referent systems, raising questions about the variety of approaches to simulation, as covered in the second subsection. Formality in model integration is discussed in section 3.3.

Domain-Specific Formalisms

In mathematical logic, formalism is the application of model and proof theory to languages, to increase confidence in inferring new statements from existing ones (Bock, et al 2006). In practice, however, most mathematicians are more informal in their definitions and proofs, with peer review confirming results, or not. We expect conceptual modeling formalisms to be rigorous approaches to studying referent and analysis models, at least in the sense of mathematical practice. Formal approaches have fewer, more abstract categories and terms than less formal ones, facilitating integration across engineering domains and construction of analysis tools. However, by using more abstract language, formal approaches are often too far from the common language of applications to be easily understood by domain experts and too cumbersome to use in engineering practice e.g., in air traffic control, battlespace management, health care systems, logistics, etc. More specific formalisms would be useful not only to domain experts, for describing their systems, but also to technical or modeling experts who must translate the system description into analysis models and maintain them, and to other stakeholders who may need to participate in validation.

Logical modeling is a widely-used approach to formalizing domain knowledge (often called *ontology*, more specifically description logics (Baader, et al 2010)). Ontologies can support acquisition of increasing levels of detail in model structure, and also education and communication. For example, in modeling an ecosystem, one begins with words and phrases, expressed in natural language such as pond, organism, bio-matter, insect, and so forth. Some words will represent categories or classes, while others represent instances falling into those categories. Also, words that connote action will reflect behaviors that are at the core of dynamic system specification. Words and phrases can be connected through relationships forming semantic networks and concept maps. Semantic networks (see, e.g., (Reichgelt 1991)) grew out of theories of cognition around associative memory (Quillian 1968), whereas concept maps (see (Novak 1990)) grew out of a theory of associative networks for the purpose of learning, both essential for capturing expert knowledge. Both are closely related to description logics (Sattler 2010, Eskridge and Hoffman 2012).

Developing explicit and formal conceptual models of the referent will require ontologies and a suitable knowledge representation. Contemporary modeling languages have been proposed and used for modeling software systems (UML (OMG 2015b)), for general systems modeling (OPM (Reinhartz-Berger and Dori 2005), SysML (OMG 2015a)), and for modeling systems in the military domain (UPDM/UAF (OMG 2016), DoDAF (US Department of Defense 2016b), MoDAF (U.K. Ministry of Defense 2016)). Domain-specific modeling languages (DSMLs) also have been developed, for modeling business processes (OMG 2013), for modeling biological systems, SBML (Finney, et al 2006), SBGN (Le Novère, et al 2009), and others. Of course, general purpose languages can be specialized to a domain as well. In addition to using ontologies for domains, methods and processes, DSMLs for representing knowledge along with induced constraints and interdependencies will also help to reduce uncertainty in the modeling process, e.g., to answer questions like what modeling approach, execution algorithm, or steady state analyzer to use. Thus, ontologies and DSMLs for modeling and simulation methods are relevant definitely in the requirements stage, where it is decided which formalism to use and how to execute a model, and also for validating and verifying a large set of methods. Suitable ontologies, if in place, will help in identifying solutions.

While these developments are an important element of establishing an engineering discipline of modeling and simulation, they do not yet go far enough. Ontology is not sufficiently applied to formal and domain-specific modeling languages, leaving a major gap in linking formalisms to engineering domains. Many of the available models of formal and domain languages only categorize terminology rather than semantics of the terms, and consequently cannot utilize domain knowledge to increase the efficiency of formal computations or bring results from those computations back into the domains. For example, ontologies are available for Petri Nets (PN), a widely used simulation formalism, but these only formalize terminology for reliable interchange of PN models, rather than enabling a uniform execution of them across tools (Gaševića and Devedžić 2006). In addition, if an adequate DSML does not already exist within a given domain, each application modeler still must develop a problem-specific ontology and capture problem-specific knowledge in a DSML. Within a particular domain, e.g., logistics, the creation of a domain-specific ontology and modeling framework would support all modelers within that domain (Huang, et al 2008) (McGinnis and Ustun 2009) (Thiers and McGinnis 2011) (Batarseh and McGinnis 2012) (Sprock and McGinnis 2014). Work on modeling formal and domain-specific languages, including semantics as well as terminology and how to integrate them for practical use, are in its early stages (Mannadiar and Vangheluwe 2010) (Bock and Odell 2011), but several results have emerged during the past decade. This is an important area for future research and development.

Language modeling (*metamodeling*) has become a widely used method for precisely defining the abstract syntax of DSMLs (the part of syntax that omits detailed visual aspects of a language). A metamodel is the model of a modeling language (Karsai, et al, 2004), expressed by means of a metamodeling language (Flatscher, 2002). There are several metamodeling languages in practical use today, ranging from informal, graphical languages, such as UML class diagrams and OCL used by the Object Management Group (OMG 2015b) (OMG 2014), the Eclipse Modeling Framework (Eclipse Foundation 2016a) or MetaGME (Emerson 2006). A formal metamodeling language based on algebraic datatypes and first order logic with fixpoint is FORMULA from Microsoft Research (Jackson and Sztipanovits 2009).

Metamodeling can be used to specify diagrammatic syntax of DSMLs, in conjunction with their abstract syntaxes above. For example, languages such as Eclipse's Graphical Modeling Project (Eclipse Foundation 2016b) and WebGME (Institute for Software Integrated Systems 2016) are providing not only a graphical metamodeling environment, but also are capable of auto-configuring themselves into domain specific modeling environments using the created metamodels. Metamodeling of diagrammatic syntax also enables standardized interchange between tools and rendering of graphics (Bock and Elaasar 2016).

Metamodeling has a role in precisely defining the semantics of DSML's. For example, FORMULA's constraint logic programming capability is used for defining semantics of DSMLs via specifying model transformations to formal languages (Simko, et al 2013). The portion of

UML's metamodel that overlaps description logic can be extended to specify patterns of using temporal relation models in UML, providing a basis to formalize the semantics of UML's behavioral syntaxes (Bock and Odell, 2011).

Other approaches to the development of DSMLs include developing a DSML for a subset of the Simulink language, by defining the operational semantics, rather than by creating a meta-model (Bouissou and Chapoutot 2012), or in a similar vein, developing a DSML for systems biology based on an abstract syntax and operational semantics (Warnke, et al. 2015).

A Unified Theory for Simulation Formalisms

Conceptual modeling applies not only to the system of interest, but also to the analysis of that system. Our understanding of a system of interest evolves from our earliest concept of it as we gain deeper understanding through the development of system models. In the same way, our understanding of the analysis itself also may evolve as we better understand the system of interest and begin to elaborate our analysis model. To support conceptual modeling of simulation analysis, it seems reasonable that we should first have the ontology, semantics and syntax to formally define a simulation. Unlike the case of other analyses, such as optimization, this requirement has not yet been satisfied for simulation. Several structures have been studied as simulation formalisms; however, there is little consensus on the best approach. In the same way that various models of computation provide a basis for theory within computer science, considering various simulation formalisms will further the development of a robust theory of simulation.

Some formalisms are available for general discrete event simulation, some adopted industrially and others not. For example, the DEVS language (Zeigler, et al 2000) provides a mathematically precise definition of discrete event systems, and there also are a number of computational implementations, so it is unique in providing both a simulation programming language and an associated mathematical specification. It is not widely used industrially, however, in part, perhaps, because of the requirement to express all behavior using state machines. Popular discrete event simulation languages or environments, such as Arena (https://www. arenasimulation.com), FlexSim (https://www.flexsim.com), Simio (http://www.simio.com), Tecnomatix Plant Simulation (https://goo.gl/XmQGgN), etc., provide a programming language with semantics and syntax, but not a corresponding formal definition. In part, this is due to the intent of many commercial simulation languages to support simulation in a particular domain, such as Tecnomatix Plant Simulation, which is naturally reflected in the semantics of the languages.

Another line of research is to view simulations thru the lens of dynamical systems and computational complexity theory. This is particularly suitable when studying complex socially coupled systems. Formal computational and mathematical theory based on network science and graphical dynamical systems has been studied in (Mortveit and Reidys 2008) (Barrett, et al 2004) (Barrett, et al 2006) (Adiga, et al 2016) (Rosenkrantz, et al 2015). The theoretical framework allows one to study formal questions related to simulations, including: (*i*) computational lower and upper bounds on computing phase space properties, (*ii*) design questions: how does one design simulations to achieve a certain property; (*iii*) inference questions: how does one understand the conditions that led to the observed behavior, etc.

Achieving an engineering discipline for modeling and simulation will require a more complete set of formalisms spanning up from rigorous discrete event, continuous, and stochastic system specification to higher level, perhaps domain-specific, simulation languages. In some areas those domain specific modeling languages that combine a rigorous mathematical semantics with a convenient modeling tool are already in use, e.g., in the area of cell biology, or collective adaptive systems (often based on a continuous time Markov chain semantics). For example, some specialized simulation languages for biology are based on mathematical formalisms, such as ML-Rules (Helms, et al 2014), Kappa (Harvard Medical School 2016), or BioNetGen (BioNetGen 2016), among others. In general, however, this still represents a very significant challenge for the modeling and simulation community.

3.2 Conceptual Model Development Processes

Model development is a challenging and highly intricate process, with many questions needing to be answered, as discussed in this section. Currently, answering these questions in a systematic and informed manner is hampered by a lack of formalized knowledge in the modeling domains and in modeling and simulation in general. Providing these would constrain development decisions and the design of development processes themselves, reducing uncertainty in model lifecycle engineering. The first subsection below gives background on model development processes and analyzes questions about them. The next two subsections (effectiveness and maturity) describe complementary approaches to reducing model defects introduced during the modeling process. These help avoid difficult and high-cost amendments of the model after it is finished. It is impossible to reduce model defects to zero during development, leading to the need for validation after the model is built, the results of which are also useful during model development, as addressed in the last subsection. Taken together, progress in these areas can significantly enhance the credibility of models by improving the quality of processes that produce them.

Motivation and Research Approach

The purpose of modeling and simulation is to improve our understanding of the behavior of systems: an executable model M of a system S together with an experiment E allows the experiment E to be applied to the model M to answer questions about S (Cellier 1991). Simulation is fundamentally an experiment on a model. A conceptual model C is the articulated description of S, upon which both M and E are developed. In science we seek to understand the behavior of natural systems; in engineering we seek to design systems that exhibit desired behavior. Because modeling and simulation facilities are themselves complex systems, it is seldom possible to go in one step from problem to solution. The processes involved in modeling and simulation require different degrees of human interaction, different computer resources, are based on heterogeneous, partly uncertain knowledge defined more or less formally, and involve different types of expertize and users. Data, knowledge, processes, and orchestration vary depending on the system to be modelled, the questions to be answered, and the users. In these processes different versions of models and artifacts are generated, that need to be put into relation to each other.

Model Lifecycle Engineering (MLE) captures the highly iterative process of developing, verifying, validating, applying, and maintaining a model. MLE is an area that requires significant study and exploration to meet society's needs and problems. How is MLE different than Engineering Design or Software Engineering lifecycles? In some instances, it may be possible to build on these related engineering fields in our attempt to forge MLE as a sub-discipline of Modeling and Simulation (M&S). It is expected that MLE will contain phases for constructing models and simulations by beginning with requirements and then proceeding to other phases such as design, analysis, implementation, verification and validation (V&V), and maintenance.

MLE concepts and methods should not be limited to developing M and E; they also should be applied to the conceptual model C, describing S and used in developing both M and E. Clearly, this requires that C be expressed in a form that enables MLE concepts and methods to be applied.

The underlying principle for any type of lifecycle engineering, however, is to ensure that unspent resources (e.g., money, time) are commensurate with work remaining. For complex systems with substantial de novo content, there is typically considerable uncertainty in both the work remaining and the rate of resource consumption. Resources are therefore held in reserve to protect against depletion due to undesired outcomes. Bearing these principles in mind, a lifecycle approach for model/simulation development should include answering the following questions:

- Purpose and Scope Characterization: Who are the stakeholders of the model? What are their concerns? In particular, what are the specific aspects of system behavior we seek to understand through modeling? The answers form the context for the relevant conceptual models. Identification of stakeholders and concerns is a complex undertaking involving a broad spectrum of disciplines, including perhaps the political and behavioral sciences. For example, a macroeconomic simulation of energy production, distribution, and consumption would rightly recognize the public at large as a stakeholder, but it would be counterproductive to ask individual citizens simply to enumerate their concerns since ordinary citizens are not likely to understand the stake they have in atmospheric carbon dioxide or sulfur dioxide. Consequently, it may be necessary to develop methods that combine opinion research with education and outreach to designated proxies for the public interest.
- Phenomenology Characterization: Is the referent a continuous system, discrete event system, or discrete stepwise system? Are stochastic or spatial aspects important? What are the elements of the system which contribute to the behavior of interest? What scientific disciplines address the behavior of interest? Answers to these kinds of questions will help to identify the content of the conceptual model and perhaps how it should be expressed. Having identified concerns, it is not necessarily simple to determine the scope of scientific phenomena to adequately address those concerns. For example, if stakeholders are concerned about the availability of drinking water, it may under some circumstances suffice to consider only hydrological phenomena. Under other circumstances it may be necessary to consider also social, economic, and political phenomena. Decisions will ultimately of course involve judgment, but research may elucidate principles and techniques that might prove useful for such analysis.
- Formalism Characterization: What formulations will be most appropriate to describe the relevant system elements and characterize the phenomena of interest in the form of input-output relations? The conceptual model must support these formulations. The choice of formalism will depend on the nature of the system being modeled—is it continuous, discrete event, discrete stepwise? Are stochastic or spatial aspects important, etc.? Once the nature of the system is identified, how is it best described, e.g., for a continuous system, are block diagrams most appropriate, or systems dynamics, or an object-oriented approach like Modelica (Modelica Association 2014b)? What mathematical formulations will be used to characterize the phenomena of interest in the form of input-output relations? Differential equations? Statistical models? Logical models? A given phenomenon may be mathematically characterized in different ways, depending upon, among other things, the nature of the concerns under consideration. If we are primarily concerned with long-term average behavior, we might choose a lumped-parameter description that assumes all short-term variation self-cancels over time. On the other hand, if we are concerned with infrequent extreme events, we

will require a characterization that captures higher-order dynamics accurately. Research may help us better understand how to infer the possible mathematical formalism from a given referent model, but also how to develop requirements for the referent model from a useful mathematical formalism.

- Algorithm Characterization: What solution algorithms will be selected for computing the input-output relations? What verification test cases are appropriate? Since the conceptual model is a bridge from S to the computational model M, it may be important to understand and accommodate the specific target algorithmic implementation.
- Model Calibration: What data is available to calibrate and later validate the model, M? Is it necessary to calibrate a conceptual model, and if so, how is it done? How does one validate a conceptual model?
- Cross-validation: Do other models exist with which the new model can be cross-validated? If there are other existing conceptual models, how can they be compared to support cross-validation?

These questions need to be addressed during the requirements phase of the model engineering lifecycle. However, answers are likely to be revised during the subsequent phases. From this point on, conventional software development lifecycle considerations apply. In addition, special consideration needs to be given to validation and verification of model variants and their interdependencies. Research is needed to understand how to help answer the above questions: how to manage the evolution process of a model and the data, knowledge, activities, processes and organizations/people involved in the full lifecycle of a model?

Managing the lifecycle process of a model is one of the most important tasks of model engineering. Some research topics should be attacked, for example, how to structurally describe the modeling process, and how to identify the characteristics of activities involved in model construction and management to ensure improvement of model quality and development efficiency and reduction of full model lifecycle cost.

Some decisions, e.g., which execution algorithm to select, might even be supported automatically by exploiting machine learning methods (Helms, et al 2015). However, automatic solutions to these decisions require metrics to clearly distinguish the good choices from the less suitable ones. For some decisions, e.g., selecting the modeling approach, providing suitable metrics is still an open challenge. Knowledge about constraints on applying one method or the other, and interdependencies and implications of using one or the other method on future activities will reduce uncertainties in the overall process.

Within the engineering of models, well-founded answers to the questions of which step to do next and which method to use largely determine the efficiency and effectiveness of the model engineering process. Referring to the first question, and for orchestrating the diverse processes that are involved in modeling engineering, workflow-based approaches might be exploited to make these processes explicit and traceable. These approaches facilitate evaluation of different phases of model lifecycle engineering, including validation and verification of models, and, thus, add to the credibility of M&S. However, this requires a high degree of standardization of these processes. This might be achievable for specific sub-processes of validation or verification, e.g., how to execute and analyze a parameter scan given a specific model. However, the overall process of a simulation study is highly interactive and thus one might only be able to define general constraints on the engineered artifacts, e.g., if the conceptual model (if we interpret conceptual model as a representation of requirements or invariants that refer to the simulation model) changes, so does the stage of the process model, requiring a new validation phase.

Effectiveness Measures

In a model-based engineering (MBE) approach, the development team evolves a set of models throughout the system lifecycle to support design, analysis, and verification of the system under development. These models are intended to express aggregate knowledge about the system to enable communications and shared understanding among the development team and other program stakeholders. Program leadership must continue to determine what knowledge must be acquired at any given point in the lifecycle to maximize the likelihood of program success. The type of knowledge to be acquired can help identify the kind of design and analysis models that should be further developed and updated.

This knowledge can be acquired by performing engineering tasks that involve different kinds of models, such as performing a trade study to select among alternative system architectures, performing an analysis to determine a system error budget, updating electrical, mechanical, or software designs, or analyzing a particular design for reliability, safety, manufacturability, or maintainability. Determining what knowledge is needed becomes more challenging as the complexity of the system increases, and as the complexity of the organization that develops the system increases (e.g., large geographically distributed teams).

The research challenge is to define one or more effectiveness measures that can guide the knowledge acquisition process and associated model development and evolution throughout the system lifecycle. In other words, how do you determine the additional knowledge at each point in time that provides best value to the program stakeholders? The research can benefit from data that has been collected over many years to find a solution. For example, the following figures are typical examples of trends that indicate the impact of collecting certain kinds of knowledge on the overall cost of system development.

In Figure 3.1 the lower curves reflect the percentage of the total lifecycle cost that is expended as a function of the phase of the program lifecycle. As indicated, much of the cost is expended in the later lifecycle phases. However, as shown in the upper curve, the percentage of the lifecycle cost that is committed occurs much earlier in the lifecycle. This finding shows the importance of early design decisions based on the available knowledge.

In Figure 3.2 the cost to fix a defect is shown, and seen to increase exponentially as a function of the phase in the product lifecycle the defect is detected. Acquiring the knowledge to surface defects early can substantially reduce the total system lifecycle cost.

The following are some suggested factors to be considered for research:

- Aggregate knowledge goals at particular milestones in a system development lifecycle.
- Knowledge elements that contribute to the aggregate knowledge.
- Knowledge elements associated with different aspects of the system of interest and its environment.
- A value function associated with acquiring knowledge elements at each point in time, and its impact on the probability of program success.
- Cost to acquire the knowledge elements at a given point in the lifecycle.
- Cost associated with acquiring incorrect knowledge at a given point in the lifecycle.

- Relationship between the effectiveness measure (value vs. cost) and more traditional risk measures.

The acquisition of knowledge across a lifecycle can be thought of as a trajectory whose aim is to maximize program success. The value function of acquired knowledge is dependent on both the knowledge elements and the sequence in which these elements are acquired, since there are dependencies among the knowledge elements. For example, during the concept phase of a vehicle's development, it is often important to acquire knowledge about vehicle sizing and system level functionality to meet mission performance requirements, but it may not be important to acquire knowledge about the detailed software design algorithms.

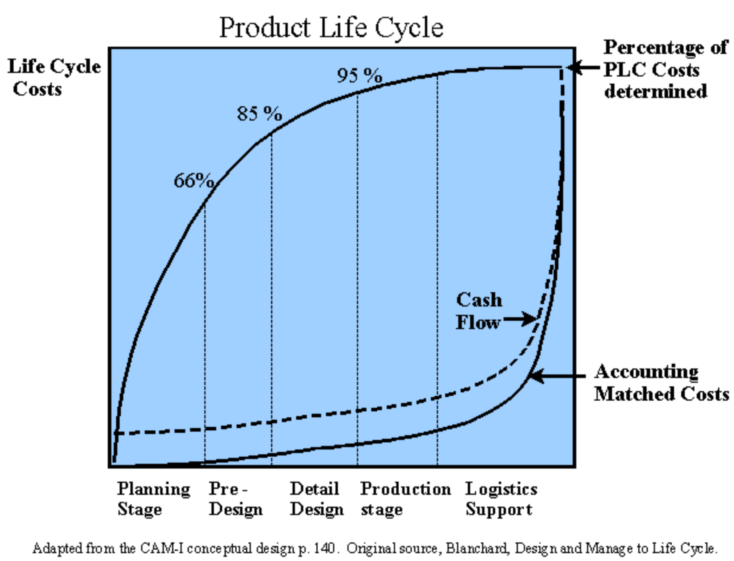


Figure 3.1 Committed and Actual Lifecycle Costs (Berliner and Brimson 1988) citing (Blanchard 1978)

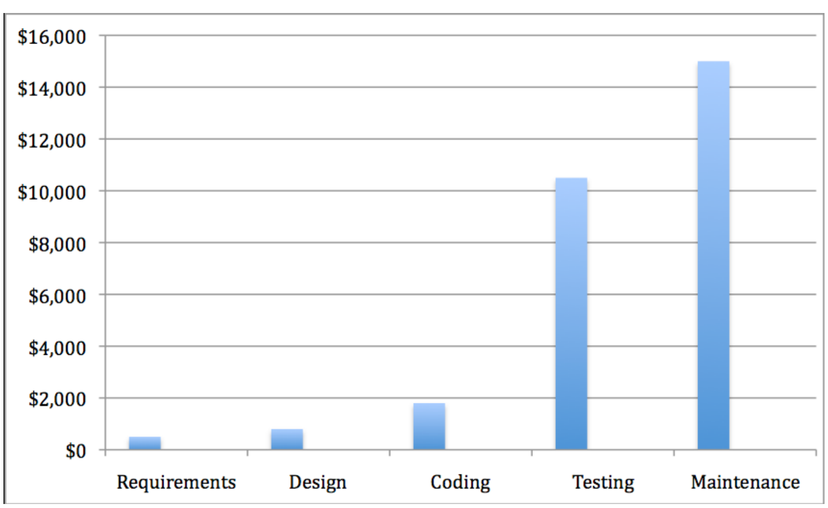


Figure 3.2 Cost To Fix Defect in Stage (McGraw 2006) citing (Boehm 1981)

Maturity Models

The Capability Maturity Model (CMM) for software development has played a key role to guarantee the success of software projects (Paulk, et al 1993). CMM and CMM Integration (CMMI) originated in software engineering, but have been applied to many other areas over the years (CMMI 2016a). However, in M&S, there is no such standardized and systematic assessment methodology developed for M&S processes. Some related research and development results can be used as references to establish the maturity model of M&S:

- Software Lifecycle models describe core processes for software development. Following proven processes for model development begins with an understanding and execution of the core activities in an organization's chosen development path. Software lifecycle models are an example of core proven processes for development. Whether the lifecycle model chosen is the classic waterfall model or more modern iterative versions, all have aspects of requirements development, design, implementation, integration, test, etc. utilized in a way that best fits the size of the organization, the size of the project, or the constraints of the customer and developer.
- Software CMMI or CMMI for Development shows the success of maturity for general software development. CMMI was originally developed at Carnegie Mellon University and the federally funded Software Engineering Institute (SEI). The CMMI Institute reports that thousands of CMMI appraisals are completed every year in dozens of countries (CMMI 2016b). CMMI enables organizations to be viewed and certified as being mature and capable of carrying out intended activities to a certain level or degree of expertise, which lends that degree of credibility to the components developed by those activities. CMMI assigns *capability* levels to process improvement achievement in individual process areas. Therefore, a certain part of an organization may be identified or certified at a level 3 out of 4 for Configuration Management, but capability level 2 out of 4 for Maintenance. CMMI assigns *maturity* levels to process improvement achievement in multiple process areas or a set of process areas and applies to the scope of the organization that was evaluated / certified such as a department, a division, or the entire company – Level 5 being the highest achievable level of maturity.
- The Federation Development and Execution Process (FEDEP) describes core processes for simulation development. FEDEP was initially released in 1996 as the first common process for the development of simulations and was specifically for guidance in creating High Level Architecture (HLA) federations (IEEE Standards Association 2016). These common methodologies and procedures consisted of six steps: 1) Define Objectives, 2) Develop Conceptual Model, 3) Design Federation, 4) Develop Federation, 5) Integrate and Test, 6) Execute and Prepare Results. These six steps included specific work products that were inputs and outputs to each step. These steps and the FEDEP process paralleled the software development process and could serve as the initial draft of the core processes for model and simulation development that would be the basis for an examination of an organization's ability to robustly, reliably and repeatedly develop credible models and simulations, i.e., identify the capability and maturity of organizations or portions of organizations.
- System of Systems describes corollaries that may exist within Systems Engineering (Zeigler, and Hessam 2013).
- DoDAF describes the notion of multiple views of simulations (US Department of Defense 2016b).

Taking CMM/CMMI as a basis, a capability maturity model for modeling and simulation process (MS-CMMI) could be established by:

- Finding the differences and similarities between the processes of modeling / simulation and software development by analyzing characteristics of modeling process and simulation of complex systems, then define indicators and metrics for M&S processes.
- Setting up a MS-CMMI evaluation system (evaluation methods, standards, tools, organizations, etc.) to assess the structured level of capabilities of model developers or model users (use the model to do simulation).

Achieving these goals requires research in:

- Quantitative analysis of the complexity and uncertainties in modeling processes.
- Optimization of modeling processes.
- Risk analysis and control of modeling processes.
- Quantitative measurement of model lifecycle quality and cost.
- Notional mappings with CMMI, etc.
- Identification and description of processes and work products necessary at differing levels of the Modeling and Simulation Maturity Model, when and why they are needed and who performs them.

Validation

As simulation models become more complex, validation of conceptual models and understanding their role in the broader process of validation will continue to be important research areas. Of course, understanding validation of conceptual models is dependent on a precise definition of the terms "conceptual model" and "validation." This section argues that a better consensus is needed on the first term, while a careful review of the validation literature will reveal the same for the second.

This is particularly apparent across M&S communities of practice. For example, the training and engineering communities intersect the broader M&S community, but M&S stakeholders in those communities draw heavily from skill sets based in different scientific disciples and different perspectives of the role of modeling and simulation. The M&S community's challenge is to address universally applicable concepts, like conceptual models in validation, from a holistic perspective with theory that is satisfying to all the stakeholders and technology that is germane to a broad set of problems (in the case of the stated example, simulation theory and technology that is useful for both the social scientist and the engineer).

Consider a few simple questions. What does it mean to validate a conceptual model? 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? Some researchers will see these as easily answered in their particular domains, but will find their conclusions quite different between domains. So, for the discussion in this section we consider terminology in the broadest context possible.

Consider modeling paradigms as equivalence classes on the set of conceptual models. Each paradigm has defining characteristics in terms of conceptual modeling language or formalism. These characteristics define every instance of a conceptual model as belonging to one class or another, or perhaps none. For well-developed theory, further properties and theorems will follow to enable reasoning on all of the elements of each class in general without resorting to building, coding, and executing every instance to understand its properties. As we develop more rigorous and explicit conceptual models that bridge between the referent system and the computer simulation, methods for validation will become even more critical.

Simulation frameworks that include a category for conceptual models permit the side-by-side comparison to and facilitate discussion of related artifacts. For example, (Balci and Ormsby 2007), (Petty 2009), and (Sargent 2013) provide frameworks that include conceptual models in this context. Advances in conceptual modeling will drive the need for new frameworks to explain the properties of conceptual models, and the relations between them, the referent system, and the computer simulation.

Some researchers would consider that the conceptual model is an appropriate artifact to analyze for suitability for use. Although recent work in validation theory is looking hard at the implication of risk in the decision to use particular kinds of simulation, and propagation of error in simulation, more basic research is needed to develop a robust model-based decision theory. Accuracy is well-understood, particularly in the context of physics-based models, but its use in simulation is not well-defined. When deciding on the kind of simulation to inform a particular decision, acceptability criteria are often subjective and little theory exists to objectify the decision analysis. A well-developed model-based decision theory will recast validation in the language of decision theory, defining use in a rigorous way, clearly differentiating objective from subjective elements of the use decision, and providing a defensible basis for using models and simulations to inform decision-making (Weisel 2012).

The logical next step for advances in theory involving validation of conceptual models is to incorporate these advances in simulation development environments. As model lifecycle engineering develops, tools for validation of conceptual models are needed to keep pace. As conceptual modeling languages and formalisms become useful additions to simulation development environments, tools using well-defined conceptual models within the broader process of validation will improve the quality and defensibility of the simulation end product.

It is well-understood that validation is best considered early in the development process (see the previous two subsections) – there should be no difference when considering conceptual models in the mix. As development environments would benefit from rigorous application of conceptual models in the development process, so too would the consideration of validation from the earliest lifecycle stages. New technologies and tools are needed to incorporate validation of conceptual models throughout the simulation lifecycle.

3.3 Conceptual Model Architecture and Services

Many modeling paradigms exist for most kinds of domain problems, applied to knowledge from many engineering disciplines. Understanding complex systems requires integrating these into a common composable reasoning scheme (NATO Research and Technology Organization 2014). The software and the system engineering communities have overcome similar challenges using architecture frameworks (e.g. OMG's Unified Architecture Framework (OMG 2016)), but modeling and simulation does not have a similarly mature integration framework. The first subsection below concerns architectures for conceptual modeling, while the second outlines infrastructure services needed to support those architectures.

Model Architecture

At the foundation of a modeling architecture should be a fundamental theory of models, to enable reusability, composability, and extensibility. What theory of models could support the implementation of a model architecture? An epistemic study of existing modeling and integration paradigms is necessary to develop a theory of models. This should include a taxonomy of modeling paradigms, semantics, syntaxes and their decomposition into primitives that operate under common rules across paradigms, to integrate them as required by complex systems.

Model architecture is needed to unify different classes of models developed using different paradigms. An architecture is the glue specifying interfaces, rules of operation, and properties common across modeling paradigms, enabling models to be interconnected at multiple levels of conceptual abstraction. What is meaningful to connect? What is not? An architecture goes far beyond conventional model transformations and gateways, though these are also essential to comprehension of multi-paradigm modeling processes. An architecture is about persistent co-existence and co-evolution in multiple domains at multiple levels of abstraction. How can a model architecture framework connect models that operate according to different sets of laws? For example, critical infrastructure protection requires connecting country, power grid, internet, economy, command and control, etc. Combat vehicle survivability requires connecting humans, materials, optics, electromagnetics, acoustics, cyber, etc. What mechanisms are required to efficiently interact between different sets of laws (e.g. layered architecture)? What level of detail is required to observe emerging behaviors between different sets of laws when integrated? How should a model architecture be implemented, in which format, using which tools? As a model architecture matures, successful design patterns should emerge for the most common reusable interconnections between disciplines. What are these design patterns in each community of interest?

Model architecture sets the rules to meaningfully interconnect models from different domains. Generalizing and publishing rules for widespread modeling paradigms would allow composing and reusing models that comply with the architecture and complex system simulations will become achievable. As an example of interconnected models across domains, start with a Computer Aided Design (CAD) model representing a physical 3D object in terms of nodes and facets. In the CAD paradigm, objects can be merged to interconnect. A related Finite Element Model (FEM) represents continuous differential equations for physical laws between boundary layers. It can be used to compute the fluid dynamics during combustion. FEM models can interconnect at the level of physical laws to compute the temperature distribution from the combustion products distribution for instance. They also interconnect with a CAD model at the mesh level. A computer graphics model enables display of objects as seen from particular viewpoints. It interconnects with CAD and FEM models to map materials and temperature to facets for the purpose of generating an infrared scene image in the field of view of a sensor. A functional model of a surveillance system can represent discrete events involved in changing a sensor mode as a function of the mission. The functional model interconnects with the computer graphics model at the sensor parameter level. Finally, a business process model can represent a commander's mission planning. It can interconnect with a functional model by changing the mission.

Figures of merit must be developed to demonstrate how well a model architecture facilitates composition of multi-paradigm, multi-physics, multi-resolution models. The performance of a model architecture must be checked against interdisciplinary requirements using metrics for meaningfulness and consistency. How can we test a particular integration for validity? How can it be done efficiently over large-scale complex simulations? How can it be done by a non-expert? What mechanisms should a model architecture framework include to support checking for conceptual consistency?

Integration complexity and coupling between the degrees of freedom of individual components and the degrees of freedom of the integration are yet to be understood. When integrating a model in a complex simulation, what details can be ignored and still ensure a valid use of that model? What details cannot be ignored?

Reliable model integration depends on sufficient formality in the languages used, as described in section 3.1. In particular, formal conceptual models of both the system of interest (referent) and analysis provide a basis for automating much of analysis model creation through model-to-model transformation. As an example, consider the design of a mechanical part or an integrated circuit. The CAD tools for specifying these referents use a standard representation, with a formal semantics and syntax. For particular kinds of analyses—such as response in an integrated circuit—simulations are essentially available at the push of a button. Formalism in the specification of the referent enables automation of certain analyses. This pattern is well-demonstrated, e.g., in the use of BPMN (Business Process Modeling Notation) to define a business process, and then automating the translation of this model into a hardware/software implementation specification. The Object Management Group has developed standard languages for model-to-model transformations. At present, there are only limited demonstrations of applying this approach to systems modeling. Automating this kind of model-to-model transformation captures knowledge about how to create analysis models from referent models, so perhaps the most fundamental question is: where should this knowledge reside—should it be captured in the referent modeling language, in the analysis modeling language, in the transformation, or perhaps spread throughout? Formalization of mappings between conceptual models of a referent and its analysis models is critical to building reliable bridges between descriptions of the referent and specifications of a simulation model and its computational implementation.

Services

The success of large-scale integration of knowledge required by complex systems fundamentally depends on modeling and simulation infrastructure services aggregated into platforms. These enable affordable solutions based on reusing domain-specific models and simulators, as well as integrating them into a multi-model co-simulation. For example, understanding vulnerabilities and resilience of complex engineered systems such as vehicles, manufacturing plants, or electric distribution networks requires the modeling and simulation-based analysis of not only the abstracted dynamics, but also some of the implementation details of networked embedded control systems. Systems of such complexity are too expensive to model and analyze without reuse and synergies between projects.

Services need to enable open model architecture development and sharing of model elements at all levels. How can a common conceptual modeling enterprise be launched involving many stakeholders? How can a conceptual model be augmented with knowledge from different contributors (e.g., wiki)? How does it need to be managed? What structure should the conceptual model have? What base ontologies are required (e.g. ontology of physics)? How can conceptual model components be implemented in executable model repositories and how can components plug and play into simulation architectures? Guiding principles must also be defined and advertised. What guidance should modelers follow to be ready for a collaborative conceptual modeling enterprise in the future? Standard theory of models, architecture, design patterns, consistency tests, modeling processes and tools will arise naturally as the modeling science matures.

Services can be aggregated into three horizontal integration platforms:

- In *Model Integration Platforms*, the key challenge is to understand and model interactions among a wide range of heterogeneous domain models in a semantically sound manner. One of the major challenges is semantic heterogeneity of the constituent systems and the specification of integration models. Model integration languages have become an important tool for integrating complex, multi-modeling design automation and simulation environments. The key idea is to derive opportunistically an integration language that captures only the cross-domain interactions among (possibly highly complex) domain models (Cheng, et al. 2015).
- *Simulation Integration Platforms* for co-simulation have several well-established architectures. The High Level Architecture (HLA) (IEEE Standards Association 2016) is a standardized architecture for distributed computer simulation systems. The Functional Mockup Interface (Modelica Association 2014a) for co-simulation is a relatively new standard targeting the integration of different simulators. In spite of the maturity and acceptance of these standards, there are many open research issues related to scaling, composition, large range of required time resolution, hardware-in-the-loop simulators and increasing automation in simulation integration.
- *Execution Integration Platforms* for distributed co-simulations are shifting toward cloud-based deployment, developing simulation-as-a-service use model via web interfaces and increasing automation in dynamic provisioning of resources as required. More will be said about this in the next chapter.

4 Computational Challenges in Modeling and Simulation

Computational algorithms and software play a central role in all computer models and simulations. A computer simulation can be viewed as a collection of state variables and data structures that represent the state of the system under investigation and algorithms that transform that state to capture the evolution of the system state over time. The algorithms encode the rules that govern the behavior of the system. In many cases the basis for these behaviors are specified through mathematics, e.g., differential equations derived from physical laws. In other simulation models, the behaviors are specified in logical rules that encode the causal relationships among the components making up the system. These computational rules may be used to determine the new state of the system in the next "clock tick" or time step of the simulation computation. In other simulations the changes in system state may occur at irregular points in simulation time, governed by the occurrence of "interesting" events such a doctor finishing a consultation with a patient, or a machine finishing the processing of a part in a manufacturing system. Regardless, computational methods and software are critical elements in modeling and simulation.

New challenges are arising in computational methods for modeling and simulation that create new research problems that must be addressed. This is because application requirements are changing on the one hand, and the underlying computational platforms are changing on the other. For example, reliable simulation models are essential to determine the impact of new policies and technologies on the evolution of cities, an area of increased interest with phenomena such as global warming creating new challenges. The infrastructures making up a city such as water, transportation, and energy are highly dependent on each other. For example, electrification of the vehicle fleet will clearly have a direct impact on vehicle emissions. But electrification has other impacts as well. The demand for electricity in households will increase, which in turn impacts the emissions produced by power generation plants as well as the amount of water they consume. In some cases, this is the same water used for food production, resulting in other impacts on the economy. When one considers other emerging technologies such as household generation of power through solar panels and more broadly smart homes, the introduction of automated vehicles, commercial use of drones for package delivery, the introduction of smart electrical power grids, and changing human behaviors resulting from these innovations, the emerging phenomena resulting from the confluence of these interactions are not well understood.

At the same time, the computing platforms on which simulations execute are undergoing a different kind of revolution. For decades the performance of computer hardware doubled every 18 months in accordance with Moore's Law. These improvements derived largely from increases in the clock rate used to drive computer circuits. These improvements in clock speed stopped around 2004 due to an inability to dissipate heat from these circuits as they were clocked at a higher rate. Now, advances in hardware performance are being derived almost entirely from exploitation of parallel processing. The number of processors or cores in computing devices has been increasing rapidly across all platforms, from high performance supercomputers down to computers in handheld devices such as smart phones. Another related phenomenon dramatically changing the hardware landscape is the emergence graphical processing unit (GPU) devices for a much broader range of application than rendering graphics, for which they were originally designed. The high volume production of these devices has lowered their cost, making them increasingly attractive for computationally demanding tasks. A third major hardware trend is the explosion of mobile computing devices that continue to increase in power and sophistication. These hardware changes have great implications in the development of computational algorithms for computer simulations, which are among the most computation intensive applications that exist. There are many research challenges that call for the development of novel computational methods, as will be discussed later in this chapter.

Other major trends in computing include cloud computing, “big data,” and the Internet of Things. Each of these developments have major ramifications in modeling and simulation. Cloud computing provides a platform that can make access to high performance computing facilities as straightforward as having access to the Internet, opening broader opportunities for exploitation of computation intensive simulations. Modeling and simulation has long utilized data analysis techniques for tasks such as characterizing inputs and specifying relevant parameters for simulation models. Big data technologies offer new capabilities that simulations can readily exploit. While big data and advances in artificial intelligence is creating unprecedented capabilities for situation awareness, i.e., characterizing and interpreting the state of operational systems, modeling and simulation offers a predicative capability that cannot be achieved through data analysis algorithms alone. In addition, the Internet of Things creates many new rich sources of data that are again synergistic to modeling and simulation offering unprecedented opportunities for modeling and simulation to be embedded in the real world and to have enormous impacts in society. These emerging platforms and computation technologies offer exciting new opportunities to increase the impact of modeling and simulation in the context of managing operational systems. Lastly, Dynamic Data Driven Application Systems (Darema 2004), a paradigm that encompasses real-time data driving computations and simulations, are used in a feedback loop to enhance monitoring and/or aid in the management of operational systems.

This chapter describes important computational challenges that must be addressed for modeling and simulation to achieve its fullest potential to address the new requirements of contemporary applications, and to maximally exploit emerging computing platforms and paradigms. The first section of this chapter focuses on emerging computing platforms and computational challenges that must be addressed to effectively exploit them. These range from massively parallel simulations executing on supercomputers containing millions of cores, to effectively exploiting new platforms with heterogeneous computing elements such as GPU accelerators, to field programmable gate arrays (FPGAs), cloud computing environments, and mobile computing platforms. Radical, new computing approaches such as neuromorphic computing that are loosely modeled on the human brain are also discussed. The section that follows focuses on challenges arising where simulations become pervasive, and appear everywhere utilizing paradigms such as DDDAS mentioned earlier and cyber-physical systems. Creating, understanding, and managing large-scale distributed systems of simulations interacting with each other to manage operational systems and subsystems present major challenges, and raises important concerns in privacy, security, and trust. Research is required both to identify fundamental principles concerning such simulations as well as establishing a theory behind their operation.

The third section raises the question of how the modeling and simulation community should manage the plethora of models that already exists, and continues to expand as new modeling approaches are developed. Complex systems often involve many subsystems, each of which may be a complex system in its own right. Understanding systems such as these will inevitably require a host of different modeling approaches to be integrated, including not only different types of models, but models operating across vastly different scales in time and space. The relationship among these different modeling approaches is poorly understood, as is determining computational methods to best combine them to address key questions in large, heterogeneous, complex systems.

Are there underlying theories that can be used to combine traditionally distinct areas such as continuous and discrete event simulation? What computational methods and algorithms are required to successfully exploit this plethora of models? Many simulation trials will be required in any study. Are there new techniques to improve the execution of so-called ensemble simulations?

The section that follows explores the relationship between modeling and simulation and big data, and highlights the synergies that naturally arise between these technologies. Simulation analytics represents a new paradigm expanding and exploiting these synergies. Key research questions concerning model and data representation, challenges in managing large-scale data and live data streams, and an approach termed qualitative modeling are discussed.

In summary, there are numerous computational challenges that must be addressed for modeling and simulation to achieve maximal impact in light of new application requirements and emerging hardware and software computing platforms. This chapter highlights areas where advances are required to maximize the effectiveness and impact of modeling and simulation in society.

4.1 Exploiting Emerging Computing Platforms

The general computing architectures used for most large-scale simulations have been similar for the last 30 years: shared memory multicore or multiprocessor systems and tightly coupled distributed memory clusters. But computing platforms have undergone dramatic changes in the last decade, changes that are only modestly exploited by modeling and simulation technologies today. Examples of computing platforms requiring greater attention for modeling and simulation applications include massively parallel supercomputers, heterogeneous computing systems including graphical processing unit (GPU) accelerators, and field programmable gate arrays. The growing, widespread adoption of cloud and mobile computing create new opportunities and challenges for modeling and simulation. Effective exploitation of these platforms requires careful consideration of how simulation computations can best exploit, and operate under the constraints imposed by the underlying platform while meeting execution time and energy consumption goals for contemporary applications. Research challenges for each of these new, emerging computing platforms are discussed next, and discussed in greater detail in (Fujimoto 2016).

Massively Parallel Simulations

The number of processors (cores) in the most powerful supercomputers has exploded in the last decade. While the number of processors in the most powerful machines remained relatively stable, ranging from a few thousand in 1995 to ten thousand in 2004, this number began increasing dramatically in 2005. In November 2015 the Tianhe-2 machine, rated the most powerful supercomputer in the world, contained over 3 million cores. Effective exploitation of the computing power provided by these machines for large-scale simulation problems requires a paradigm shift in the modeling and simulation community.

This trend is exemplified by experimental data reported in the literature in the parallel discrete event simulation field (Barnes, et al. 2013). Performance measurements of telecommunication network simulations indicated supercomputer performance of approximately 200 million events per second using 1,536 processors in 2003. This number increased to 12.26 billion events per second on 65,536 processors in 2009, and 504 billion events per second in 2013 using almost 2 million cores. However, over this 10-year span, the performance *per core* increased by only a factor of two. Performance increases are being driven almost entirely by the exploitation of parallel processing.

Exploitation of massively parallel computer architectures presents many critical challenges to the modeling and simulation community. Perhaps the most obvious is the fact that the simulation computation must be developed in a way to exploit finer grains of computation, i.e., the atomic unit of computation that cannot be subdivided into computations that are mapped to different cores must become smaller. For example, in numerical simulations involving large matrix computations, rather than mapping entire rows, columns, or sub-matrices to individual cores, new approaches that consider mapping individual elements of the matrix to different cores are beginning to show promise, thereby exposing much higher levels of parallelism in the computation. The simulation computations and associated algorithms must be rethought to consider such fine grained parallelism.

Once the simulation has been formulated as a fine grained parallel computation, a key challenge concerns efficient execution of the simulator. Communication latency has long been a principle impediment to efficient execution of parallel simulations; keeping the numerous cores busy with useful computations becomes very challenging if the delay to transmit information between cores increases. The reason is because many computations will have to remain idle, waiting for results computed on other cores to arrive. This problem becomes even more challenging in fine grained simulation computations where the amount of computation between communication actions becomes small. Latency hiding techniques that can mask communication delays become even more critical in order to successfully exploit large-scale parallel computers. Further, effective exploitation of memory system architectures become increasingly more important. When the state size encompassed by the simulator increases, efficient use of cache memory systems becomes increasingly more challenging and important.

Another key question concerns how to map the parallel simulation model to the parallel architecture, especially for simulations that are modeling highly irregular physical systems. For example, consider a simulation of a large network, such as the Internet. Many networks such as these that arise in natural and engineered systems are highly irregular, and often contain “hub nodes” with high interconnectivity relative to other nodes in the network. The amount of activity, and thus simulation computation can vary by several orders of magnitude from one network node to another. Partitioning and mapping large-scale irregular network simulations to execute efficiently on modern supercomputers is a challenging task that requires further exploration.

Parallel Simulation on Heterogeneous Computing Platforms

Modern computers ranging from supercomputers to mobile devices are increasingly being composed of combinations of general purpose processors coupled with hardware accelerators, e.g., GPUs. A GPU is a hardware accelerator that off-loads computational tasks from the central processing unit (CPU). They derive their name from the fact that they were initially developed to render graphics for display devices on workstations and personal computers. GPUs have since found broader application as a means to accelerate data intensive numerical computations. High volume manufacturing of GPUs have driven their hardware cost down, making them attractive components for high performance computing systems.

GPUs are designed for data parallel computations, i.e., computations where the same operations are applied to large volumes of similarly typed data. Computing elements are organized to implement single-instruction-stream, multiple-data-stream (SIMD) operations, i.e., a common program is executed by the many computing elements (cores) but operating on different data. This data-parallel processing is the main source of performance improvement in these hardware platforms.

A significant body of work has emerged in developing methods to exploit GPU architectures for numerical simulation applications. Such applications are often formulated as matrix computations, making them well suited for the exploitation of these architectures. Other computations such as discrete-event simulations are typically not structured as matrix computations. Rather, they often utilize much more irregular data structures which are more challenging to map to GPU accelerators. It is especially significant that the next generations (at least) of the highest-end supercomputers will be designed as clusters of nodes, each of which is composed of a small number of multicore processors and advanced GPUs that share memory. The GPUs will offer the vast majority of the computational parallelism in these platforms.

To illustrate some of the challenges associated with executing irregular simulations on GPUs, consider a large discrete event simulation program that consists of many event computations. To execute efficiently in the SIMD style used in GPU architectures the simulation should consist of relatively few, and ideally only one, type of event, a restriction that applies to a limited number of discrete event simulation applications. SIMD code is also most efficient when it is mostly straight line code with few branches, and when loops running in parallel take (almost) the same number of iterations. This is a problem for discrete event simulations, whose control flow frequently branches. Also, code running on GPUs, for at least the next few generations of them, will not be able to execute Operating System code, perform I/O, or send or receive messages without involving the CPU. This last restriction is also a major problem for discrete event simulation since, on average, each event has to send one event message. This will almost certainly cause the CPU to be a performance bottleneck in any discrete event simulation that attempts to run events in parallel on the GPUs. The traditional multicore/multiprocessor architectures will likely remain more efficient for these simulations, until such time as there is more convergence between CPU and GPU architectures than is currently specified in the technology roadmaps. Making efficient use of GPUs for highly irregular, asynchronous parallel discrete event simulations will be, to say the least, a major challenge.

Concurrent execution can be obtained by partitioning the state variables of the simulation into objects, and processing the same event computation concurrently across these objects. Further, as mentioned earlier, each event computation should contain few data dependent branch instructions because if the program is executed over different data, the execution of different program sequences resulting from different branch outcomes must be serialized in the SIMD style of execution. The future event list used in discrete event simulations, a priority queue data structure, is similarly challenging to distribute for concurrent access on existing GPU architectures. Thus, restructuring irregular simulations for execution on GPUs remains challenging.

Further, once the computation has been reformulated for execution on a GPU, other computational challenges must be addressed. Specifically, the memory available within the accelerator remains limited, and moving data in and out of the GPU's memory can quickly become a bottleneck. Techniques to hide the latency associated with data transfers are essential to achieve efficient execution. Memory systems are typically organized as banks of memory, with concurrent access to memory distributed across different banks. However, accessing the data residing in the same bank must be serialized. Care must be taken to map the simulation's state and other variables to the memory system to avoid creating bottlenecks.

Effective exploitation of GPU architectures today requires careful programming that is tailored to the specific target architecture. This makes codes relatively brittle – performance optimizations designed for one architecture may no longer be valid when the next generation architectures appear. Tools to automate the mapping of simulation computations to GPU architectures are needed to alleviate this task from the programmer. Moreover, software development on GPU architectures can be burdensome. Application specific languages or advances in parallel compilers may offer ways to simplify the programming task.

Array Processors as a Platform for Modeling and Simulation

Advances in field programmable gate array (FPGA) technology have improved their speed, performance, and connectivity with other devices while lowering their power consumption, leading to their emergence as array processors for use in high performance parallel computing platforms. These processors combine the features of application-specific integrated circuits with dynamic reconfigurability, especially during runtime, to provide a suitable system for performing massively parallel operations. These systems have a sufficient number of processing units to provide large-scale parallelism, higher processing power, and shorter reconfigurability time, even during the execution of the same program. Their performance is better than microprocessors by a factor of 100 and more (Tsoi and Luk, 2011).

The suitability of array processors as a parallel processing platform has been and is being investigated in data-intensive applications, such as signal and image processing, database query, big data analysis, and applications that are compute and memory intensive, such as high-speed network processing, large-scale pattern matching, influence-driven models for time series prediction from partial observation, model-based assessment, and many more (Dollas, 2014).

In array processor architectures, a single instruction controls the simultaneous execution of data in the processing units (SIMD) which is efficient when data sets in the processing units don't rely on each other. The topology of the array processor is heavily influenced by the structure of the interconnection network, its speed of connectivity, and its configurability for a specific application. Because of this dependency, efficient partitioning (mapping) algorithms are needed.

Array processors have good potential for big data processing models and good results have already been shown for some unique applications. However, their suitability for general applications and for modeling and simulation of complex systems needs to be studied. One of the reasons for the limitation of array processors is the coupling of prefetch instructions with the execution unit. Decoupling, along with the development of methodologies to properly map data dependency, needs to be researched.

Development of user-friendly programs for mapping models into the array architectures, creation of tools for dynamic reconfiguration of general application models, development of efficient dynamic routing algorithms to accelerate the routing phase specific for array processors, and production of an open-source hardware design to enable research into novel reconfigurable architectures are all very important. Selecting an appropriate memory model, such as shared, distributed, or hybrid, to develop an efficient programming interface for the selected memory models needs to be researched, especially for complex compute bond simulation models.

Developing hardware solutions for data processing that support high degrees of parallelism is challenging because as core counts increase, the average on-chip distance between arbitrary communication points also grows. Thus, enforcing scalable communication patterns is crucial. For example, an algorithm can be parallelized by replicating a task over many processing elements and organizing them into a feed-forward pipeline.

The creation of more high-level development environments, such as OpenCL, in place of low-level ones (VHDL, Verilog), for high-level abstractions will allow array processors to be developed more efficiently independent of the technical advances of modern synthesizers and provide fundamental trade-offs between speed and chip space. Furthermore, appropriate tradeoff analyses between speed and generality, clock speed and power consumption, chip area and accuracy, expressiveness, and (runtime) flexibility need to be made. In addition, while OpenCL provides programming portability, it doesn't provide performance portability. Therefore, the portability issue also needs to be resolved. Thinking outside the box while researching porting data processing algorithms from software to hardware and accurately abstracting the underlying operations of a given task, including synchronization, to achieve high degrees of parallelism and flexibility are also important (Woods 2014).

Other challenges include speeding up the tools for mapping a model description (which is in the range of hours to days) using existing parallel programming languages, such as OpenCL, CUDA (compute unified device architecture and programming model to increase the computing performance-restricted for a certain hardware), and SystemC.

Modeling and Simulation in the Cloud

Cloud computing offers a means to make modeling and simulation tools much more broadly accessible than was possible previously. Cloud computing provides the ability to offer modeling and simulation tools as a service that can be readily accessed by anyone with an Internet connection. In principle, users of such tools need not own their own computers and storage to complete the simulations. This feature can be especially beneficial for simulation computations requiring high performance computing facilities because the cloud eliminates the need for simulation users to manage and maintain specialized computing equipment, a serious impediment limiting widespread adoption in the past. The “pay-as-you-go” economic model for the cloud is attractive when computational needs are heavy during certain periods of time, but much less during others. However, there are certain challenges that must be overcome for the modeling and simulation community to maximally exploit cloud computing capabilities.

Cloud computing is built upon a computational technology called virtualization. Virtualization enables one to create a “private” computational environment where resources such as CPU, memory, and operating system services appear to be readily available to applications as virtualized components. Virtualization provides isolation between applications, thereby enabling physical computing facilities to be shared among many users without concern for programs interfering with each other.

Cloud computing presents certain technical challenges, especially for parallel and distributed simulations. A significant issue that has impeded greater exploitation of public cloud computing services concerns communications delay. Both latency and latency variance, i.e., jitter, may be high in cloud computing environments and significantly degrade performance. This problem could be alleviated by improved support from cloud providers for high performance computing. Another approach is to design parallel and distributed simulations with better ability to tolerate latency and jitter in the underlying communications infrastructure.

A second issue concerns contention for shared resources in cloud computing environments, as users are typically not guaranteed exclusive access to the computing resources used by their programs. This can lead to inefficient execution of parallel and distributed simulation codes. An approach to addressing this problem is to develop mechanisms to make these codes more resilient to changes in the underlying computing environment during the execution of the simulation. For example, dynamic load adaption is one method that can been applied to address this issue.

Cloud computing introduces issues concerning privacy and security. These are issues that are well-known in the general computing community and are equally important if cloud computing is to be successfully exploited by the modeling and simulation community.

There is a trend to recognize that groups of software services require different facilities and support from cloud computing, virtualization and service-oriented architectures. Arguably this is also true in this area and is emerging as "Modelling and Simulation as a Service" (MSaaS). This could cover modeling and simulation applications ranging from "online" simulation, where multiple users can access the same simulation (and potentially share information between them), to simulations requiring various high performance computing support, to groups of interoperable simulations to pipelines of simulations and supporting services (real-time data collection, simulation analytics, optimizers, etc.) These in turn make novel demands of cloud and service-oriented architecture concepts such as workflow, orchestration, choreography, etc.

Mobile Computing Platforms

As discussed in the next section, the number of mobile computing devices dwarfs the number of desktop and server machines, the traditional platform used for modeling and simulation codes, and this gap is rapidly increasing. The increasing computing power of mobile devices means simulation codes need not be limited to remote servers or execution in the cloud. Rather, simulations can be embedded within a physical system itself. Increased use of mobile platforms such as drones provide many new opportunities for the use of simulation to monitor and assist in managing operational systems in real time. For example, simulations operating in drones may be used to predict the spread of forest fires or toxic chemical plumes, enabling one to dynamically adapt the monitoring process or institute approaches to mitigate damage. Transportation represents another important application where simulation embedded within the traffic network may be used to project traffic congestion arising after an incident, and to explore alternate courses of action.

Embedding the simulation computations within the physical system being monitored or managed offers the opportunity for the computations to be used in tighter control loops using disaggregated data compared to approaches using back end servers or the cloud. Further, placing the computations nearer to data streams lessens reliance on long-range communications capabilities, and can mitigate privacy concerns by eliminating the need to communicate and store sensitive data on centralized servers.

Data-driven online simulations are growing in importance. Sensor data and analytics software process live data streams to construct or infer the current state of the system. Simulations are then used to project future system states, e.g., to improve the monitoring systems to better track the physical system as it evolves, or to be used as a means to optimize or improve the system. These simulations must run much faster than real time to be useful. Paradigms such as DDDAS can be expected to grow in use into the foreseeable future.

Mobile computing platforms present new challenges for simulation applications. The simulations must be able to produce actionable results in real time. This necessitates automation of many of the steps in a modeling simulation study. For example, input data must be analyzed and processed rapidly to parameterize and drive the simulation models. Experimentation plans for analyzing possible future outcomes must be rapidly created and executed. Simulation runs must be mapped to available computing resources, and analyses of output data must be completed and interpreted with minimal delay, and translated into action plans. Data from the physical system offers the opportunity to automatically calibrate, adapt, and validate simulations by comparing observed system behaviors with those predicted by the simulations.

Energy consumption is another area of increasing concern. In mobile computing platforms reducing the energy required for the computation will increase battery life, and/or can allow smaller, more compact batteries to be used. However, most of the work to date in energy consumption has focused on low-level hardware, compiler, and operating system issues. Relatively little work has been completed to understand the energy consumed by simulations. Better fundamental understandings of the relationship among energy consumption, execution time, data communications, and model accuracy are needed. These relationships must be better understood for both sequential and parallel/distributed simulations. Approaches to optimize energy consumption consistent with the goals and constraints of the simulations in terms of timeliness in improving results are needed.

Neuromorphic Architectures

Neuromorphic computers are a radical departure from the traditional von Neumann computer architectures. They are essentially the hardware realization of neural nets, modeled loosely on animal nervous systems, and are capable of doing tasks such as image processing, visual perception, pattern recognition, and deep learning vastly more quickly and energy efficiently than is possible with traditional hardware.

At this point it is too early to do more than speculate about how neuromorphic computation will be incorporated into simulations once they become better understood and more widely available. But one possible use case might be in autonomous vehicles such as self-driving cars or aerial drones which may need extensive image processing in embedded simulations to predict in real time the behavior of other nearby vehicles. Those tasks may not be directly programmed in a traditional rule-based manner, but may instead make use of the learning capability inherent in neuromorphic chips to adapt to local conditions and to the world as it changes over time. Another example is a simulation of a system where visual processing is critical, such as satellite aerial surveillance. The systems themselves may make use of neuromorphic computation, but *simulations* of those systems will likely need it as well, since otherwise the simulation will probably run many times slower.

4.2 Pervasive Simulation

Embedding Simulations (into literally everything)

A key observation in the "post digital revolution society" is that information and communication technologies (ICT) have become *pervasive*, i.e. interwoven with human behavior, or in other words: the "fabric of everyday life" to such an extent, that the separating view of a "physical world" being connected with a "digital world" is ceasing. Today we talk about one "cyber-physical" world (Cyber-Physical Systems, an NSF program developed by Helen Gill in 2006), referring to the tight entanglement of real world physical objects (things, appliances) and processes (services), with their digital data representation and computations in communication networks (the "cyber"). Embedded, wirelessly connected tiny compute platforms equipped with a multitude of miniaturized sensors collect data about phenomena, analyze and interpret that data in real time, reason about the recognized context, make decisions, and influence or control their environment via a multitude of actuators. Sensing, reasoning and control, thus, are tightly interconnecting the physical and digital domains of the world, with feedback loops coupling one domain to the other. Connecting the "physical" with the "digital" based on embedded electronic systems, which in addition to executing preprogrammed behavior also execute simulations we call *pervasive simulation*. Pervasive simulations have clear synergies and overlaps with mobile and dynamic data driven application systems discussed earlier.

Collective Adaptive Simulations

Taking the plenty-hood of todays embedded platforms with their computational, sensory, reasoning, learning, actuation and wireless communication capacities (smart phones, autonomous vehicles, digital signage networks, stock exchange broker bots, wearable computers, etc.), it is not just considered possible, but already a reality that these are programmed to operate cooperatively as planet scale ensembles of collective adaptive computing system (CAS). CAS research asks questions on the potential and opportunities of turning massively deployed computing systems into a globe-spanning "super-organism," i.e. compute ensembles exhibiting properties of living organisms such as displaying a "collective intelligence." Essential aspects of CAS are that they often exhibit properties typically observed in complex systems, such as (i) spontaneous, dynamic network configuration, with (ii) individual nodes acting in parallel, (iii) constantly acting and reacting to other agents, and (iv) highly dispersed and decentralized control. If there is to be any coherent behavior in the system, it must emerge from competition and cooperation among the individual nodes, so that the overall behavior of the system is the result of a huge number of decisions made every moment by many individual entities. Pervasive simulation raises CAS to *collective adaptive simulations*.

Massive Scale Pervasive Simulations

The International Telecommunication Union (ITU) predicts there will be 25 billion devices online within the next decade, outnumbering connected people 6-to-1 (International Telecommunication Union 2012b). This will lead to a pervasive presence around us of objects and things (e.g., RFID tags, sensors, actuators, mobile phones), which will have some ability to communicate and cooperate to achieve common goals. This paradigm of objects and things ubiquitously surrounding us is called the Internet of Things (IoT). The ITU defines IoT as a "global infrastructure for the information society, enabling advanced services by interconnecting (physical and virtual) things based on, existing and evolving, interoperable information and communication technologies" (International Telecommunication Union 2012a). The IoT covers different modes of communication, including: between people and things, and between things (machine-to-machine or M2M). The former assumes human intervention, and the latter none (or very limited).

A primary aim of IoT is to deliver personalized or even autonomic services by collecting information from and offering control over devices that are embedded in our everyday lives. The reliance of IoT on simple, cheap, networked processors has implications for security; the potentially invasive nature of the information gathered has implications for privacy; and our reliance on machine-to-machine systems to make decisions on our behalf makes mechanisms for expressing and reasoning about trust essential. The need for trust has long been recognized, as stated recently by Moulds (2014), the "… pivotal role in … decision making means it is essential that we are able to trust what these devices are saying and control what they do. We need to be sure that we are talking to the right thing, that it is operating correctly, that we can believe the things it tells us, that it will do what we tell it to, and that no-one else can interfere along the way."

Privacy, Security and Trust

As pervasive simulations become more commonplace, it is essential that they be secure or at least tolerant of cyber threats. Privacy and trust issues must be adequately addressed to realize widespread adoption.

As the world becomes more connected, we will become dependent on machines and simulations to make decisions on our behalf. When simulations use data from sensors, devices and machines (i.e., things) in the network to make decisions, they need to learn how to trust that data as well as the things with which they are interacting. Trust is the belief in the competence of a machine or sensor to act dependably, securely and reliably within a specified context (Grandison and Sloman 2000). Trust is a broader notion than information security; it includes subjective criteria and experience. Currently securing sensors and devices is accomplished through information security technologies, including cryptography, digital signatures, and electronic certificates. This approach establishes and evaluates a trust chain between devices, but it does not tell us anything about the quality of the information being exchanged over time.

As the number of sensors connected to the network grows, we will see different patterns of communication and trust emerge. If we assume a hierarchical connection of components: sensors are at the end-nodes, which communicate data to aggregators. Sensors may be unintelligent (sense environment and send data to aggregator) or they may be intelligent (sense environment, reason about the data, and communicate with aggregators). Aggregators are capable of collecting data from sensors, reasoning about that data, and communicating with other aggregators. Having aggregators communicate with each other enables trust decisions to be made in a more distributed manner, reasoning about trust across geographic areas.

Data from the sensors and aggregators will be fed into models and simulations that are making predictions and/or decisions that will impact our lives. Data from sensors or aggregators may be in conflict with each due to: malfunction, bad actors, tampering, environmental conditions, context conditions, and so on. Whether or not the simulation should trust this data must be established by an agent that is capable of a trust evaluation prior to it being deemed useful as information. Further, if simulations have a role in controlling or giving commands to some sensor, actuator or device in the IoT system (i.e., a cyber-physical system) then the data the simulation uses from external sources in which to make those decisions, must be trustworthy such that it is not purposely misled into issuing malicious commands.

Foundational Research Concerns

In order to develop a deep scientific understanding of the *foundational principles of pervasive simulations,* we need to understand the trade-offs between the potentials of top-down (by design) adaptation means and bottom-up (by emergence) ones, and possibly contributing to smoothing the tension between the two approaches. We need to understand how and to what extent pervasive simulations – when involving billions of components – can create a "power-of-masses-principle," and possibly express forms of intelligence superior than that of traditional artificial intelligence.

Furthermore, understanding properties concerning the evolutionary nature of pervasive simulations, e.g. open-ended (unbounded) evolutionary simulation systems, the trade-off and interaction between learning and evolution, and the effect of evolution on operating and design principles are of foundational importance. Understanding the issue of pluralism and diversity increase in *complex pervasive simulation systems* as a foundational principle of self-organization, self-regulation, resilience and collective intelligence is needed. Last but not least, laying down new foundations for novel complex *pervasive simulation theories* for complex, adaptive, large-scale *simulation super-organisms* (including lessons learned from applied psychology, sociology, and social anthropology, other than from systemic biology, ecology and complexity science) remains a key challenge for the scientific community.

Systems Research Concerns

In order to develop principles and methods for the design, implementation and operation of *globe-spanning simulation super-organisms* we identify systems research concerns such as (i) Opportunistic Information Collection: Systems need to be able to function in complex, dynamic environments where they have to deal with unpredictable changes in available infrastructures and learn to cooperate with other systems and human beings in complex self-organized ensembles. (ii) Living Earth Simulation: The provision of a decentralized planetary-scale simulation infrastructure strongly connected to the worlds online-data sources (search engines, power grids, traffic flow networks, trade centers, digital market places, climate observatories, etc.) is needed as a means to enable a model-based scenario exploration in real time - at different degrees of detail, varying time-scales, integrating heterogeneous data and models. (iii) Collaborative Reasoning and Emergent Effects in Very-Large Scale Pervasive Simulations: Reasoning methods and system models are needed that combine machine learning methods with complexity theory to account for global emergent effects resulting from feedback loops between collaborative, interconnected simulations. (iv) Value Sensitive Simulations: Research is needed on ethics, privacy and trust models for simulations that are robust and resilient to common threat models in planetary scale simulations.

Towards *pervasive simulation applications*, we have to look at the specifics of design, implementation and operational principles rooted in the very nature of application domains of societal relevancy: e-health eco-systems, fleets of self-driving vehicles, reindustrialization (Industry 4.0), physical internet (intelligent logistics), digital economy, energy management and environmental care, citizen science, combinatorial innovation, liquid democracy, etc.

4.3 New and More Complex Simulation Paradigms: A Plethora of Models

As we simulate ever larger and more complex systems, from thousands of interacting components to millions and billions, the complexity of the models we must build and execute also dramatically increases at all levels in the layered stack of simulation software. Large simulations must frequently combine different modeling paradigms and frameworks, at different temporal and spatial scales, and different synchronization and load balancing requirements. They must interface with other non-simulation software, such as databases, analysis packages, visualization systems, and sometimes with external hardware systems or humans. And a single execution of a model is not sufficient. We always need a structured ensemble of many independent executions in a proper simulation study. Among the greatest R&D challenges we face is the creation of simulator platforms, frameworks, tool chains, and standards that allow this diversity of paradigms to interoperate in a single simulation application. The software challenges are made even greater because of the hardware computing architectures on which complex simulations run are also changing rapidly, as was discussed earlier.

Complex Simulations

Simulations are becoming ever more complex as they are applied to new domains and grow in scale and fidelity required. The additional complexity is multidimensional, often with multiple kinds of complexity in the same model, leading to a variety of architectural requirements beyond correctness, fidelity, and performance. Examples of this complexity include:

- *Federated models* — models composed (recursively) of separately developed submodels that are then coupled in structures that mimic the way the real systems being simulated are composed of coupled subsystems.
- *Multi-paradigm models* – models that contain subsystems designed according to different paradigms, e.g. queuing models coupled to Petri net models and numerical differential equation models.
- *Multiscale models*— models with significant phenomena occurring at different time or space scales, often differing by orders of magnitude.
- *Multiphysics models* — models in which multiple different physical phenomena, e.g. fluids, solids, particles, radiation, fields, etc., all coexist and interact.
- *Multi-resolution models* — models in which it is necessary to be able to adjust a resolution parameter to allow a trade-off between time- and space-resolution or degree of detail for improved performance.
- *Multi-synchronization models* — parallel models that use multiple synchronization paradigms, e.g. a hybrid or federation of different time-stepped, conservative event-driven, and/or optimistic event-driven synchronization algorithms.
- *Mixed discrete and continuous models* — models in which some parts are described by numerical equations describing state changes that are continuous in time, while other parts are discrete, in which all state changes are discontinuous in time.
- *Real time models* — models that must produce results by specific real time deadlines, often in embedded systems.
- *Hardware-in-the loop (HWIL)* — a special case of a real time model in which a simulation is coupled to a physical device with which it must synchronize and communicate at a real time speed determined by the needs of the device.
- *Human-in-the-loop* — a simulation that interacts with humans in real time, at speeds and with response times keyed to human behavior and reaction times, and with I/O keyed to human sensory and action modes.
- *Models as components of other computations* — models that are subsystems of a larger computation that is not itself a simulation, e.g. an animation system, or a control system.
- *Models containing large non-simulation components* — for examples models that run whole (parallel) speech understanding or visual systems inside a single event.
- *Virtual machines as model components* — an important special case in which the system being simulated involves computers or controllers that run particular software, and the execution of that software has to be faithfully duplicated, including timing, for the simulation to be correct.

Some of these complexity dimensions are reasonably well understood, at least in principle. But others are poorly understood even theoretically, and considerable research will be required to clarify them. In most of these dimensions there are no widely accepted standards and no *robust tool chains* for building, executing, debugging or validating them. When such models are built today, they are usually one-offs that are dependent on the specific details of the particular application needs and are likely to contain *ad hoc* design decisions and engineering compromises that make the simulation brittle, unportable, and/or unscalable.

Abstraction Layer	**Function**
model layer	The code of a particular model (or component).
model framework layer	Collection of model classes, components, and libraries for a single application area, such as network simulation, or PDE solution, etc.
simulator layer	Provides a single paradigm for simulation time, space, naming, parallelism, and synchronization for use in one component of a (possibly) federated simulation.
component federation layer	Provides interface code to allow independently-created submodels, possibly written in different languages, to communicate, synchronize, and interoperate in various ways to become a single federated model.
load management layer	Within one parallel model execution, measures resource utilization (time, energy, bandwidth, memory) at runtime and dynamically manages or migrates loads to optimize some performance metric.
ensemble layer	Runs many instances of the same model as an ensemble in a single large job, for such purposes as parameter sensitivity studies, parameter optimization, variance estimation, etc. Handles scheduling, failures, accounting, and time estimates, allocates file directories, decides on ensemble termination, etc.
operating system / job scheduler layer	Runs independent jobs in parallel. Provides processes, interprocess communication, I/O, files systems, etc.

Table 4.1 Abstraction Layers of a Simulation Software Stack.

To manage this kind of simulation complexity, we need to develop simulation-specific software engineering standards, abstractions, principles and tools. For example, one step might be to define *standards* for simulation software as a stack of software layers, in which each layer provides and exposes additional services for use by the layers above, and abstracts or hides some features from the layers below. This follows the pattern set by the layering of general purpose system and application software, or the TCP/IP and OSI protocol stacks. Table 4.1 shows a set of abstraction layers that might crudely exemplify such a simulation software stack.

Presumably there could be various alternative systems at each layer, just as there are different protocols at each layer of the TCP/IP stack. The point is not to suggest this particular organization for the simulation stack. Any such standard should be the result of lengthy and careful consideration among the stakeholders in the simulation community, perhaps under the auspices of professional societies such as the Association for Computing Machinery (ACM). But there is an urgent need for software engineering principles specific to simulation to help manage the complexity that currently limits the kinds of simulations we can realistically attempt.

Unification of Continuous and Discrete Simulation

One of the basic simulation questions that will require considerable research to clarify is the relationship between continuous and discrete simulations. On the surface they seem strikingly different. Continuous simulations treat state changes as *continuous* in time, whereas discrete simulations treat state changes as *discontinuous*. The fidelity of continuous simulation is dominated by numerical considerations (error, stability, conservation, etc.), whereas for discrete models it is dominated by detailed correspondence with the system being modeled and also by statistical considerations. The two kinds of simulation are sufficiently different that there are very few people who are expert in both.

Despite the differences, it is common for complex models to combine aspects of both discrete and continuous submodels. Frequently, for example, one part of a system, e.g., electric power distribution, or aircraft aerodynamics, is described by differential equations and represented by a continuous simulation, but the digital control system for those same systems (power grid, aircraft) is better represented by discrete models. The entire coupled simulation is thus a mix of continuous and discrete models.

The problem in coupling continuous models to discrete ones is that the continuous side is usually programmed as a time-stepped simulation, while the discrete side is likely to be event driven, and the two do not share a common synchronization mechanism. To start with, we need robust, high performance parallel integration algorithms on the continuous side of the coupling that can freely accept inputs from the event-driven discrete side at arbitrary (unpredictable) moments in simulation time falling between two time steps. Some, but not all, integration algorithms have the property that at any simulation time one or more new, shorter time steps can be interpolated between two pre-planned ones without loss of accuracy or other key properties. However, in practice, even if the integrator has that property, the actual integration codes were not developed with that capability in mind and they do not incorporate the necessary interpolators and synchronization flexibility.

A more ambitious research agenda is to *unify* the theory and practice of parallel continuous and parallel discrete event simulation. A few dozen scattered papers have been published related to this theme, but the issue is still not widely recognized and it will certainly require a major international research and development effort to clarify the issues and build appropriate tools. Unification would require development of a variety of scalable parallel variable rate integrators, both explicit and implicit, that are numerically stable. They need to support variable, dynamically changing spatial resolution as well (in the case of PDE solvers). To execute optimistically, or couple efficiently to an optimistically synchronized model, a unified discrete and continuous simulator will have to support rollback as well.

Co-simulation and Virtual Simulation

Co-simulation stems from modeling embedded systems where verification of hardware and software functionality as a system is performed simultaneously before and during the design phase to ensure the final manufactured system will work correctly. The approaches developed for co-simulation, as well as the tools developed for describing the models and simulating the correct functionality, use VHDL, VERILOG, and SystemC. The use of these tools and methodologies for co-simulation of embedded systems is rather mature. Although some of the existing tools such as VHDL and Verilog do not have standard interface features for communication between hardware and software, SystemsC and some industry-developed tools used in the design of this type of system have been in practice for some time.

Compared with the digital realm, hybrid modeling and co-simulation of continuous and discrete systems and their synchronization haven't been addressed to the level necessary to provide accurate results when used for the design of mixed and hybrid complex systems. The complexity of continuous/discrete systems makes their co-simulation and validation a demanding task and the design of heterogeneous systems challenging. The validation of these systems requires new techniques offering high abstraction levels and accurate simulation from a synchronization and intersystem communication point of view. This is especially necessary for the development of cyber-physical systems, which are a combination of continuous components that may be defined by a set of ordinary or partial differential equations, discrete components (such as microcontrollers) for control purposes, and embedded software for local and remote operation via the Internet.

Appropriately sharing design parameters between discrete and continuous subsystems for access by either subsystem at the correct time, occurrence of the correct event, and initiation of events by either subsystem are among the issues needing to be researched. In addition, the following issues require further research: scheduling events to occur at a specific time (time events) or in response to a change in a model (state events); events that are described with predicates (Boolean expressions), where the changing of the local value of the predicate during a co-simulation triggers the event; modeling abnormal behavior, such as those caused by a random event, such as faults or misuse; and defenses against the misuses including fault tolerance mechanisms for protection against them.

One of the most important difficulties in continuous/discrete co-simulation is the time synchronization between the event-driven discrete simulation and the numerical integration into the continuous solver which influences the accuracy and the speed of the simulation. The exchange of events between the discrete and the continuous models is especially critical for co-simulation. The continuous model may send a *state event*, whose time stamp depends on its state variables (e.g., a zero-crossing event); and the discrete model may send events, such as *signal update events,* that may be caused by the change of its output or the *sampling* events (Nicolescu, et al, 2007 and Gheorghe et. al, 2007).

Since designs are becoming more complex, it is expected that some of the methodologies developed for co-simulation of embedded systems will be adaptable for co-simulation of cyber-physical systems and will verify the stability, controllability, and observability of such systems under various operating environments. Challenges in this area particularly include the development of a single tool for co-simulation of continuous, discrete, and embedded software components of cyber-physical systems to ease synchronization events needed among these three subsystems.

Simulation Ensembles

A complex model code will almost always have inputs that describe initial conditions, parameters that control or modulate the system's behavior during simulation time, and random seeds that initialize random variables controlling stochastic behavior. A serious simulation study involves hundreds, thousands, or even more executions of the same model code, i.e. an *ensemble* of simulations, to explore and quantify the behavioral variation that the model can produce.

Ensembles of simulations are required in at least these circumstances, and others as well:

- to broadly explore and survey that space of behaviors that the model produces with different inputs and parameters;
- to examine the sensitivity of model behavior to perturbations of inputs or parameters;
- to find optimal input parameter values that maximize some output metric;
- to measure the mean, variance, correlation, and other statistical properties of the models' outputs over a large number of executions with different random seeds;
- to search for or measure the frequency of rare events that can occur in the behavior of the model;
- to conduct uncertainty quantification studies;
- to guide and track training progress in human-in-the-loop training simulations;
- to do runtime performance studies, including scaling studies.

Because ensemble studies are almost universal, the simulation community should recognize *ensemble studies as the fundamental unit of simulation*, rather than concentrate primarily on the single execution. It is the resources and costs required of the ensemble that matters, not those required for any individual run. Thus, to reduce resource utilization it is often much more important to optimize the number of simulations in the ensemble rather than the performance of individual simulations. Likewise, if time-to-completion of the entire study is critical, then it is more important to design the study so that more parallelism is derived from running simulations in parallel, even if that means reduced (or no) parallelism within a single simulation.

Methods to automate the creation and execution of simulation experiments from job submission to resource allocation to execution of computational experiments including multiple runs are needed. We need to define standards and build tools to support the ensemble-level of simulation. We should be able to run a *single job* in a form portable to multiple platforms, to conduct an entire ensemble study, or at least a good part of it. It should choose inputs, parameter values, and random seeds, dynamically allocate nodes on a parallel machine as needed, launch individual simulations on those nodes, calculate their time estimates, allocate file system space for their outputs, monitor their normal or abnormal termination, and decide as some simulations terminate and free nodes, which next simulations to run. The code or script that manages the ensemble may be interactive, or may conduct the entire sensitivity or optimization or variance estimation study autonomously, deciding what simulations to run, in what order, and when to stop.

4.4 Beyond Big Data: Synergies Between Modeling, Simulation and Data Analytics

Data analytics and machine learning algorithms provide predictive capabilities, but are fundamentally limited because they lack specifications of systems behavior. Modeling and simulations fill this gap, but do not exploit new capabilities offered by new machine learning algorithms. Approaches that synergistically combine these methods offer new approaches for system analysis and optimization.

Simulation Analytics

Traditional simulations compute aggregated statistics that are reported back to analysts. Recently, new HPC-based approaches for analysis of disaggregated data and sample paths through simulations exist, potentially providing much finer grained analysis results. As an example, large-scale high fidelity multi-agent simulations are being increasingly used in epidemiology, disaster response, and urban planning for policy planning and response. These simulations have complex models of agents, environments, infrastructures, and interactions. The simulations are used to develop theories of how a system works, or carry out counter-factual experiments that entail the role of various "system level interventions." In this sense simulations here can be thought of as theorem provers. They are also used for situation assessment and forecasting. The eventual goal in each case is to design, analyze and critique policies. The policies can be viewed as decisions taken by policy makers ranging from small groups to local and national government agencies. To use simulations in this setting one often resorts to carrying out statistical experiments; these experiments can be factorial style experiments, but they can also be sequential experiments and use adaptive designs. Computation trees are examples of this. Even a moderate sized design leads to a large number of runs; this coupled with simulations of systems at scale produce massive amounts of data.

As simulations become larger and more complex, however, we encounter a number of challenges. First, if a simulation is too computationally intensive to run a sufficient number of times, we do not obtain the statistical power necessary to find significant differences between the cells in a statistical experiment design. Second, if the interventions are not actually known ahead of time, we do not even know how to create a statistical experiment. This can be the case, e.g., when the goal of doing the simulation is to find reasonable interventions for a hypothetical disaster scenario. Third, as the system evolves in time, it is often necessary to incorporate new information leading to interactive systems with certain real-time requirements. New methodologies and new techniques are needed for the analysis of such complex simulations. Part of the problem is that large-scale multi-agent simulations can generate much more data in each simulation run than goes into the simulation, i.e., we end up with more data than we started with. Although we have discussed these issues in the context of multi-agent simulations of large socially-coupled systems, they are applicable to other classes of biological, physical and informational simulations as well. Additional discussion can be found in (Marathe, et al. 2014, Parikh, et al. 2016).

A broad challenge is that of *sense-making*. The basic issue is actively studied in artificial intelligence (AI). Broadly, there are three parts to the problem: *Simulation analytics pertains to developing new algorithmic and machine learning techniques that can be used to support the* *above tasks.* They involve: (i) how to design a simulation that computes the right thing and summarization of simulation data, (ii) find interesting patterns in the data sets, (iii) discovering potentially new phenomenon - how to analyze simulation results to extract insights and (iv) integrating the data with real world observations to provide a consistent partial representation of the real world under study. We discuss each of these topics below; also see (Barrett, et al. 2011, Barrett et al. 2015).

- Summarization: Summarization of simulation data is needed as massive amounts of data are being produced by these systems; it is expected that the simulated data can be orders of magnitude larger than the data that was used to drive the simulations. What does summarization mean in this context? How does one summarize the data? How does one retain important information and find it in the first place? The challenges here lie in developing and adapting statistical science and machine learning techniques on one hand and algorithmic techniques on the other. The basic topic of summarization has now been studied in the data mining literature. Summarizing simulation based data can of course use these techniques but also has aspects that might facilitate the development of specific methods.
- Finding Interesting Patterns: An important question arising within the context of simulation analytics is to identify interesting patterns. These patterns might point to anomalies or help with summarization or help discover potentially new phenomenon. The question here revolves around data representations and pattern representations, and efficient and provable algorithmic techniques to find these patterns.
- Discovering Potentially New Phenomenon: This is related to the previous problem but takes into account the problem semantics to discover a potentially new phenomenon. For example, a good pattern finding algorithm might be able to find clusters of a certain size repeated in certain simulations. Knowing that these simulations pertain to epidemiological outbreaks or star formation might provide new clues on super spreaders in a social network.
- Information Synthesis: An overarching problem is to try and synthesize the simulated information produced by different simulation components. The synthesis of data is an important issue and one could view simulations as an approach to build a coherent view of bits and pieces of data, i.e. gathered by measuring aspects of the real world (either systematically or as a part of convenience data). In this context, the notion of information needs to be broadened not just as numerical data but also procedural and declarative data; information that pertains to how things work or how things behave. Indeed, simulations provide a natural way to both interpolate sparse data to form a coherent view but also allow us to extrapolate this data to develop potential possible worlds. Information synthesis comes up in physical systems but is most apparent when dealing with modeling and reasoning about biological, social and information systems; e.g. urban transportation systems, public health, banking and finance.
- Believability: Why should one believe simulation results? There is much discussion of this topic in other sections and hence the focus here is on developing methods that can allow policy analysts a way to see patterns produced by simulations that can increase confidence in the simulation results. For instance, stochastic simulations might produce many possible branches as the simulation evolves. Is there a way to summarize these branches so that we can make sense of why this might have happened?

Model and Data Representation

Integrating algorithms for simulation and data raises questions concerning the most effective representation of models and data. Representations are needed to facilitate use of formal methods. Another challenge concerns the creation of domain specific languages and efficient translators to accelerate the creation and exploitation of models. Data and model representations have been

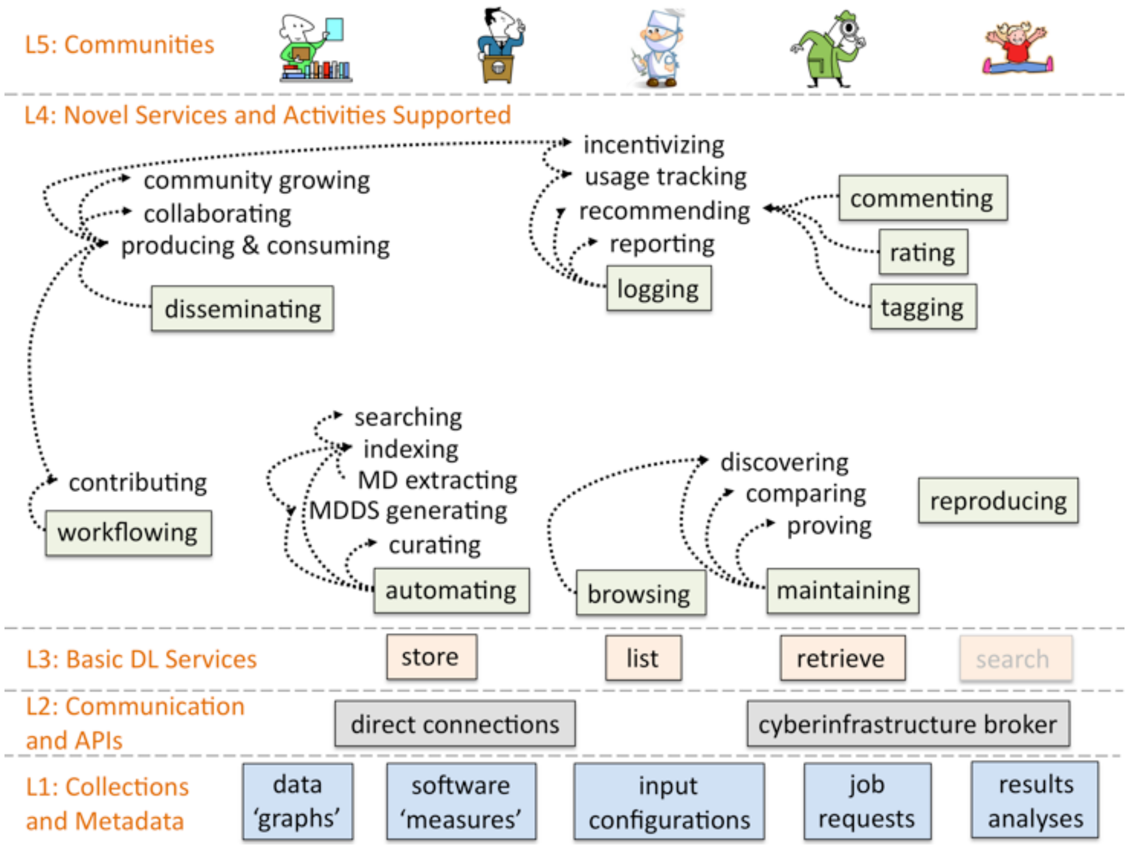


Figure 4.1: Conceptual layers based on 5S framework for a digital library to support simulations

studied in other contexts as well, including: databases, digital libraries, semantic web, etc. Many of the concepts studied there are equally applicable. We will focus on the following topics: (*i*) the physical and logical way to store and represent numerical, declarative and procedural data, (*ii*) formal methods to reason about the data and models within the simulation environment, (*iii*) data and model synthesis for coherent system representation. The digital library and semantic web community has made significant advances in this area. Informally digital libraries refer to systematic organization of data and associated data along with methods to coherently access these data sets. In this sense digital libraries are different from traditional databases. They are usually built on top of a logical representation of data in the form structured or semi-structured data; see (Ledig et al., 2011a, Ledig et al., 2011b).

An important research direction is to develop digital library concepts and frameworks to support simulation and modeling. This would require (*i*) logical and physical organization of data from raw data sets that may be distributed across different locations to structured (e.g. RDBMS) and semi-structured data sets that provide a logical organization of data using the Resource Description

Framework (RDF) and its extension; (*ii*) a hierarchy of progressively rich services for content generation, curation, representation and management and (*iii*) languages and methods to describe and develop complex workflows for integrating raw and simulated data sets, and manipulating these data sets while keeping the efficiency of system in mind. See figure 4.1.

Logical methods based on traditional database concepts have been useful in this context. Jim Gray and his colleagues make an excellent argument to used databases to organize the input as well as output data (Hey, Tansley and Tolle, 2009). This context can be extended to support not just organization of the data but to actively guide simulation during execution; these database-driven simulations provide a new capability in terms of expressiveness and human efficiency without compromising overall system efficiency. The use of RDF and its extensions to store and manipulate data are very promising – indeed graph databases have become extremely popular for storing certain kinds of data sets. The tradeoffs among extensibility, expressiveness and efficiency between these representations is a subject of ongoing research (beyond purely theoretical terms).

Services: As discussed in (Leidig, et al. 2011a, Leidig et al., 2011b, Leidig et al., 2011c, Hasan, et al. 2014), minimal digital libraries (DL) are expected to provide a set of DL services that meet the anticipated use case scenarios. User groups will be comprised of domain scientists who will use these services to generate complex work flows to support policy designs. Metadata structures and provenance information connect input data and simulation data along with policy related experimental metadata. A list of services is shown in Figure 4.2. The idea is that these services form a rich and composable set of APIs that are in a sense organized to progressively support higher-level services within the list.

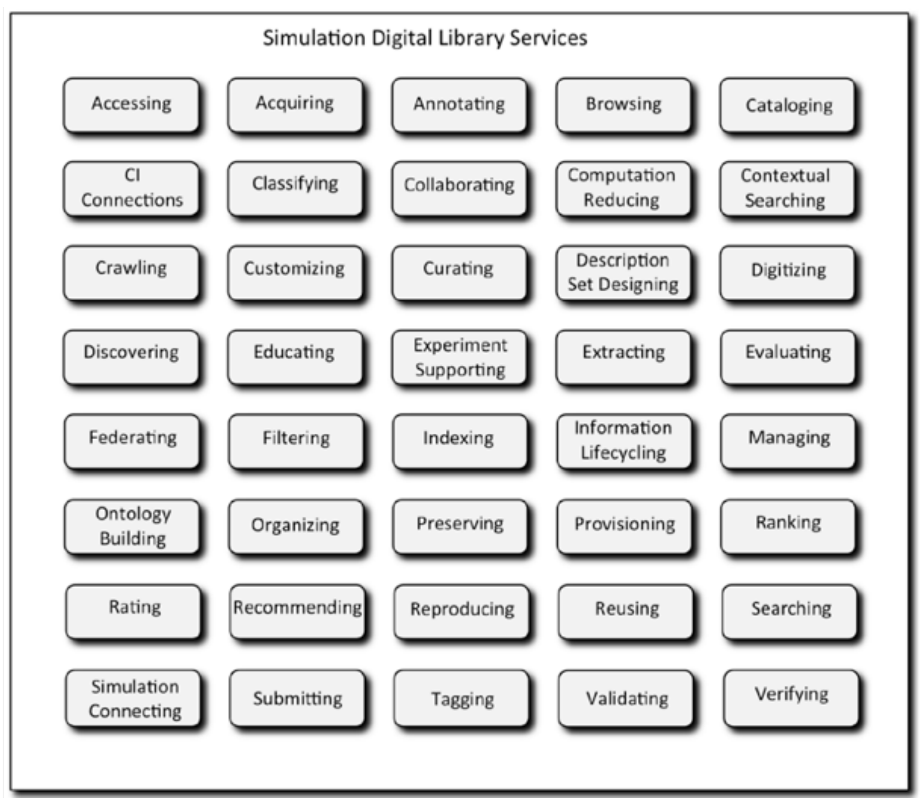


Figure 4.2. Examples of digital library services needed to support complex simulations.

Large-Scale Data and Stream Management

The introduction of large-scale data and data streams within simulations present new data management challenges. Completing this work is a recent initiative on this topic (see streamingsystems.org/finalreport.html). Four basic topics were identified: (*i*) programming models, (*ii*) algorithms, (*iii*) steering and human in the loop, (*iv*) benchmarks. Much of the discussion applies to issues pertaining to the current document and as a result, we will keep the discussion brief.

As such streaming in the context of M&S applies to streaming data that might be used to feed the simulations, e.g. data arriving for sensors as a part of the IoT vision that measure attributes of a social or a physical system. But streaming also applies to computing and reasoning about simulated data; often the size of these data sets is prohibitive. As a result, they are best viewed as streams and need to be processed on the fly to produce meaningful summarization.

Qualitative Modeling

Modeling physical systems and the decision making process based on the results of simulations using those models are, for the most part, based on numerical quantities which quantitatively describe the relationship between inputs and outputs of the system. While such models are adequate for physical systems, they fail to meet the needs of the simulation community in regard to modeling and simulation of complex systems, such as those in cognitive science, knowledge engineering, health sciences, artificial intelligence, and many more. In these systems, models that describe the relationship between the inputs and observed outputs are in qualitative or linguistic form. This class of models is closer to human thinking than quantitative models and is easy to understand.

While the properties of these models are a better fit with human thinking and diagnosis in human terms, no efficient computational algorithms for the construction and execution of these models currently exist. Efficient tools to support the development of these models for qualitative data mining and feature extraction, pattern recognition, sensors, and sensor networks are in their infancy, especially when complex systems are considered.

Designing complex dynamic systems that require skills obtained through experience and the issues involved in translating human skills into the design of automatic controllers are challenges that remain. The transfer and reconstruction of skills may be performed using traces that were collected from an operator's actions (Bratko and Suc 2003). However, such transfer has only been tried for simple systems; and their suitability for complex systems needs to be tested.

Similar to skill transfer, the characterization of intuitive knowledge of the physical world, advanced methods for reasoning which use that knowledge to perform interesting and complex tasks, and development of computational models for human common sense reasoning need to mature through efficient and better tools.

Discretization is used to convert things which can be represented and reasoned about symbolically. It provides a means of abstraction to develop models for situations involving only partial knowledge where few if any details are known. In these cases, qualitative models can be used for inferring as much as possible from minimal information. For example, "We are at McDonalds" versus "We are at McDonalds at Manhattan Ave," (Forbus 2008). Challenges remain in developing models which can represent such partial knowledge in more descriptive form, and the tools for building models capable of understanding analogies and metaphors still needs to be researched.

Some of the approaches to qualitative modeling include qualitative mathematics which are simple and can build the right model for a given situation (Bratko and Suc 2003). However, these models lack generality (i.e., each case requires a new model); and not all of the model-building skills are captured in the characterization.

The other challenges which remain in qualitative modeling are related to relevance, ambiguity, ontology modeling, and mature qualitative mathematics for complex system modeling. Ontology modeling based on traditional mathematics tends to be informal where informal decisions are used to decide what entities should be included in a situation, what phenomena are relevant, and what simplifications are sensible. Qualitative modeling will make such implicit knowledge explicit by providing formalisms that can be used for automating (either fully or partially depending on the task) the modeling process itself.

The ontological frameworks for organizing modeling knowledge, research on automatically assembling models for complex tasks from such knowledge, and application of qualitative models of particular interest to cognitive scientists, including how they can be used to capture the expertise of scientists and engineers and how they can be used in education, remain to be addressed. Open questions focusing on the relationships between ideas developed in the qualitative modeling and other areas of cognitive science need to be addressed.

Still challenges remain for accurate and precise mixed quantitative/qualitative modeling and simulation for applications in complex systems, such as those in health sciences (e.g., the cardiovascular system) and cognitive science, which require further basic and fundamental research (Nebot, Cellier and Vallverdu 1998).

5 Uncertainty in M&S

5.1 Mathematical Foundations of Uncertainty in M&S

Modeling and simulation of complex real-world processes has become a crucial ingredient in virtually every field of science, engineering, medicine, and business. The basic objectives of model development are commonly two-fold. The first objective is to explain from a scientific perspective relationships between independent/controllable model input variables and dependent responses or other Quantities of Interest (QOIs). The second objective is to use the models and simulation for prediction and decision making. Whether used for explanation or prediction, a model can never fully explain (partially observed) past events or predict future events. It is therefore of central importance to understand the epistemological limitations of models and the uncertainty inherent in their predictions.

The workshop participants agreed that probability theory is the only theory of uncertainty consistent with the established normative tenets of epistemology. Probability is defined as a finite measure on a general space. Normative principles, which underlie the Kolmogorov axiomatization of probability measures (Alexandrov et al. 1999), provide the philosophical and analytical justification that will agree with the tenets of mathematical analysis. Thus, probability theory is unique and serves the specific purpose of quantifying uncertainty via the measure theory that underlies modern philosophy and mathematics. There was a general consensus among the workshop participants that non-probabilistic approaches such as those based on intervals, fuzzy sets, or imprecise probabilities, lack a consistent theoretical and philosophical foundation.

Even when the workshop participants agreed on Bayesian probability theory as a mathematical foundation for uncertainty in M&S, there were differences in the philosophical interpretation of this theory. In the engineering and M&S communities, much emphasis has been placed on Validation and Verification (V&V) and Uncertainty Quantification (UQ) (ASME 2016; NAS 2012). V&V consists of activities that aim to ascertain whether a model is "correct" and "credible." Similarly, UQ aims to quantify the uncertainties inherent in using a model and examine how these uncertainties are reflected in the model's predictions. Some workshop participants pointed out that the treatment of uncertainty in the engineering and M&S community often starts from a perspective of objective probability (or statistical analysis), which is inconsistent with the Bayesian perspective. Such treatment stems from the premise that uncertainty can be quantified objectively, and that such quantification can be based on data from repeated (past) experiments. From a Bayesian probability theory perspective, the notion of a probability as the limit of a relative frequency in a large number of repeated experiments cannot be justified. This is particularly the cases when "extrapolation" is needed in prediction or when data about experiments cannot be collected, for instance, as in an engineering design context in which human and economic factors play an important role, and the artifact being designed does not yet exist. Instead, it is important to recognize that probabilities express subjective beliefs. Even when these beliefs are sometimes strongly informed by large amounts of related and relevant data, and when this data has been incorporated through Bayesian updating, they remain an expression of subjective beliefs.

The workshop participants argued that even though UQ practice in engineering is gradually being influenced and enriched by rigorous methods drawn from modern statistics, probability, and philosophy, and the problem is increasingly being approached from a Bayesian perspective (Kennedy and O'Hagan 2001; Oden et al. 2016), some existing V&V and UQ literature appears to stylize ad hoc methods and lacks a consistent theoretical and philosophical foundation. One such example is the identification of uncertainty in the UQ and V&V literature in promoting a taxonomy that includes various definitions of both *aleatory* and *epistemic* uncertainty. Drawing distinction between aleatory and epistemic uncertainty, for the purposes of predictive modeling is important only if the modeler seeks to employ classical Fisherian (frequentist) methods where the quantification of aleatory uncertainty is the focus. Over the last five decades, Fisherian methods, which are philosophically aligned with objective probability as interpreted by von Mises, have been largely replaced by Bayesian approaches. This overcomes the philosophical shortcomings of classical methods (e.g., Bayesian confidence replaces Fisherian hypothesis testing). From a Bayesian perspective, there is no need to delineate between aleatory and epistemic uncertainty as both are readily characterized within modern probability theory. Similarly, the UQ and V&V literature has introduced various ad-hoc metrics of model validity. Since predictive models are developed as an aid to decision making, it would seem logical to define the notion of validity in a decision-making context. One would then base the treatment of uncertainty on value rather than validity as is further elaborated in Section 5.2.

The workshop participants would like to point out that, although probability theory provides the foundation for dealing with uncertainty, there are practical challenges in the application of probability theory in M&S. While physical processes (e.g., thermal, electrical, chemical, mechanical, multi-physics) are understood through models constructed from the laws of physics, our "certainty" about predicting the fidelity of physics-based models has no such foundation—no "physics of uncertainty" exists. Instead, uncertainty is a subjective assertion. The only physics-based assertions available for the characterization of uncertainty are "independence" (often stated through "conditional independence") and stationarity. Independence (along with stationarity) is a key ingredient of those few stochastic processes that yield to analysis (e.g., Brownian motion, Levy processes, regenerative processes, Markov processes, extreme value processes, branching processes) for which we have (perhaps functionally retrievable) probability laws. However, independence is rarely justified in engineered systems. This becomes a more daunting issue in M&S of complex systems, where sophisticated physics-based models when viewed as trajectories in a stochastic domain have insufficient independence structure to yield a functional characterization of probability law.

In summary, there is a need to unify behind a Bayesian perspective on uncertainty in M&S. Currently, activities such as model calibration, validation, uncertainty propagation, experimental design, model refinement, and decision making under uncertainty are seen as an afterthought to model development. While agreeing on Bayesian probability theory as a foundation and on the mathematical models that should be applied in practice, there were philosophical differences regarding the meaning of probability. This has led to a significant fragmentation in the community where new ad-hoc algorithms and models are continually proposed, but result in very little reuse by other practitioners. It is therefore important for the M&S community to be well-informed consumers of the available probability theory (as developed and accepted by philosophy, mathematics, and science) as opposed to developing competing methods that are at best redundant with existing methods or at worst invalid.

5.2 Uncertainty in the Context of Decision Making

Most often, M&S is ultimately used to guide decisions in engineering, medicine, policy, and other areas. Systems engineers make risk-informed design decisions. Medical professionals consider uncertainty when designing treatment strategies. Uncertain climate models influences policy decisions. It is clear that consistent consideration of uncertainty results in better decisions.

If model development were carried out independently of its eventual use in decision making, then one would conclude that reducing uncertainty is always better. In such a scenario, the modeler develops the best possible model under the budget constraints, and provides it to the decision maker, whose task is to bring in value judgments and make a decision using the available model. However, this is an inefficient approach for addressing uncertainty. It was explicitly recognized during the workshop that M&S must be considered in the eventual context of use (COU), which defines the role and scope of the model in the decision-making process, and the resources available. Modelers must decide how much effort and resources to expend based on the potential impact on the decision. Based on the impact, they may then decide to refine the model with the goal of reducing uncertainty. In making these decisions, the role of the modeler is not simply to quantify model uncertainty, but to *manage uncertainty*. Uncertainty management (UM) is a broader activity in M&S that involves (i) establishing the decision COU and the modeling goals, (ii) identifying the effects of uncertainty on the decision, (iii) determining options for reducing uncertainty and the associated cost, (iv) evaluating the effects of these options on the goals, and (v) use of rigorous techniques to make consistent modeling decisions.

M&S processes are purpose-driven activities. The value of a modeling activity depends on the specific COU for which a model is developed. If the goal is to support selection among different alternatives, then information should be gathered only to the point that the best alternative can be determined. Within engineering design, for example, the primary COU of models is to help designers select among multiple design alternatives that maximize the designer's inputs. Therefore, the choice of model fidelity is dependent on designer's values, which are quantified by his or her preference function.

Various approaches have been well established within decision theory for modeling preferences. One of the approaches for quantifying preferences and value tradeoffs under risk and uncertainty utilizes utility theory (Keeney and Raiffa 2003), which is based on axioms initially presented by von Neumann and Morgenstern (vonNeumann and Morgenstern 1944). Utility theory forms the basis for rigorous approaches for estimating preference structures based on principles such as certainty equivalence. It is a foundation of microeconomics, and is increasingly being adopted by many application domains such as engineering design and systems engineering.

Although utility theory can be used to formalize the preferences of a decision maker for whom a model is being developed, this can be challenging due to a number of reasons. First, the model developer may not have direct access to the decision maker or his/her preference structure during the model development process. This is particularly true when a model, initially developed to support one decision, is used for a different decision. Second, the preferences of the decision maker may evolve over time, or as more information becomes available. Third, modeling efforts may be driven by multiple uses, and hence, multiple target decisions. Fourth, modeling efforts may sometimes be driven by external factors, unrelated to the target decision. These challenges prevent direct application of the existing approaches, and need further investigation by the research community.

After quantifying the preference structure, the next step is to evaluate the impact of modeling choices on the target decision. Models can improve the value of decisions, but also incur cost. They require time as well as computational, monetary, and human resources. The tradeoff between the value of a model and associated costs leads to a broad question: *How much effort should be put into modeling activities to support decision making?* This question can be addressed by modeling uncertainty management itself as a decision-making process. Different models, at different fidelities, result in different accuracies and costs. The choice of model will have an impact on the expected outcome of the decision. More accurate model predictions tend to lead to more valuable decision outcomes but also cost more. If the increase in the expected value or utility of the decision outcome is larger than the expected cost of modeling, the modeling activity is worth pursuing. One can think of this process as efficient information gathering: Choose the information source (e.g., a model and corresponding simulation) that maximizes the net value of information (Lawrence, 1999).

While this criterion for making modeling decisions is easy to state, implementing it during the model development process may be challenging. The criterion requires a comparison of cost and improvement in the decision. It may be difficult to quantify both of these quantities in the same units. The cost is generally related to (i) cost of collecting data, (ii) computational effort required to characterize the uncertainty in the predictions, and (iii) cost of employing subject matter experts to provide uncertainty assessments. Methods are needed for combining these cost attributes within a single measure. In addition, other modeling choices that influence the expected value of information need to be made: deciding from which model to sample, deciding how much experimental data to gather, deciding whether to refine a model or not, choosing the level of model fidelity, selection of general modeling approach (e.g., continuous simulation, agent based simulation, etc.), deciding a model validation strategy, deciding whether to reuse existing models or to develop new customized models, choosing the level of abstraction for a model, deciding which multiscale models to integrate, deciding to compose models at different scales, etc. Each decision can be modeled from the perspective of value of information maximization. This general strategy has been utilized in techniques such as Bayesian global optimization based on sequential information acquisition (Jones et al. 1998), for model selection decisions (Moore et al. 2014), and for making different model calibration and verification decisions. Bayesian approaches are gaining particular importance due to the ability to integrate different sources of uncertainties (parameters and data) and to incorporate prior knowledge (Farrell et al. 2015).

The decisions listed above are usually made sequentially rather than in a single step. For example, the level of abstraction of the model is chosen before specifying the details of the parameter values. The decision-making process can be modeled as a decision network, where different decisions may be made by different individuals, perhaps within different teams, or even different organizations. In addition to the individual decisions, the structure of the decision network also affects the outcomes. The key question from the uncertainty management standpoint is: *How can resources for M&S activities be allocated efficiently to maximize the value gained from the network of decisions?* This is itself a computationally challenging, dynamic decision making problem.

The organizational context in which M&S activities are framed presents additional challenges. For instance, M&S may be part of the systems engineering process, which in turn is a part of the overall business process. Therefore, modeling activities may compete for resources with many other activities within the organization, or time constraints may be imposed based on external factors such as market competition. There is therefore a need to establish techniques for partitioning the budget for different activities and targets within the context of organizational goals.

In summary, there are three key decision-related research challenges in M&S. The first challenge is to consistently deduce the preference functions for individual uncertainty management activities from overall goals within organizations where multiple entities are involved in decision making and their preferences may be conflicting. The second is related to mapping uncertainty in physical quantities to the utility functions. The third is due to the complexity of sequential decision-making processes with information acquisition. Addressing these challenges would help in partitioning and allocating organizational resources for modeling and decision making under uncertainty.

5.3 Aggregation Issues in Complex Systems Modeling

Aggregation of information is an integral part of M&S of complex systems. The common approach for managing complexity is to follow a divide-and-conquer strategy, which involves partitioning the modeling activity based on various criteria, such as type of physical phenomena, level of detail, expertise of individuals, and organizational structure. The models of the partitioned system are then integrated into system-level models to provide a holistic representation of the system behavior. Based on the criteria used for partitioning the modeling task, the techniques are referred to as multi-physics, multi-disciplinary, multi-fidelity, and multi-scale techniques. These techniques are gaining increasing attention in many application domains ranging from computational materials science to critical infrastructure design (Felippa et al., 2001). In computational materials science, for example, models are developed at multiple levels including continuum, meso- and micro- scales and atomistic levels.

Aggregation of information is associated with a number of challenges in M&S. First, composition of models requires an understanding of physical phenomena at different levels, and how they can be seamlessly integrated across different levels. This is referred to as scale bridging within the multiscale modeling literature, and strategies ranging from hierarchical to concurrent modeling are being developed (Horstemeyer 2010). Second, there is a need for rigorous approaches for modeling uncertainty across different scales. Since different individuals, teams, and organizations develop models, the sources of uncertainty and the domain of applicability of individual models may be different. Modeling assumptions may not be consistent across different models. These inconsistencies across models can result in erroneous predictions about the behaviors at the aggregate level.

A greater challenge in such divide-and-conquer strategies is that even if consistency across different models is achieved, the fundamental nature of aggregation can result in erroneous results due to the path dependency problem. Saari (2010) shows that multilevel methodologies can be treated as generalizations of aggregation processes. Although each lower-level model provides strong evidence for seemingly logical outputs, the conclusions at the aggregate level can be incorrect. The aggregate level output could merely reflect the way in which lower-level models are assembled rather than the actual system behavior (Saari 2010, Stevens and Atamturktur 2016). The primary cause of the inaccuracy is that separation caused by divide-and-conquer strategy loses information.

The potential inaccuracies resulting from aggregation have been studied in detail in relation to aggregation of preferences for group-decision making. It has been shown that aggregation procedures can result in biases in decisions (Saari and Sieberg 2004; Hazelrigg 1996). The implication for simulation-based design is that commonly used decision-making methods based on normalization, weighting, and ranking are likely to lead to irrational choices (Wassenaar and Chen 2003). This is particularly important in M&S because, as discussed in Section 5.2, the model development process involves many decisions made by different decision makers. The aggregate system-level model represents an aggregation of beliefs and preferences of individual lower-level model developers. Therefore, the inaccuracies resulting from preference aggregation is a fundamental challenge in M&S of complex systems. In summary, there is a need to recognize and address the challenges associated with aggregation of physics-related and preference-related information in modeling complex systems.

5.4 Human Aspects in M&S

Human aspects in M&S are important for two reasons. First, humans are integral parts of socio-technical systems, such as electric power grids, smart transportation systems, and healthcare systems. Therefore, accurately modeling human behavior is essential for simulating the overall system behavior. Second, the developers and users of models are human decision makers. Therefore, the effectiveness of the model development and usage process is highly dependent on the behavior of the decision makers.

With the rapid rise of smart networked systems and societies (Simmon et al. 2013), which consist of people, internet-connected computing devices, and physical machines, modeling humans within the overall system has become an essential part of M&S activities. Within such cyber-physical-social systems, humans receive information over the network, interact with different devices, and make decisions that affect the state of the system. The key challenge in modeling such systems is to determine how to incorporate human behavior into formal models of systems. Modeling human behavior is challenging because of complex and uncertain physiological, psychological, and behavioral aspects. Humans are generally modeled with *attributes* such as age, sex, demographic information, risk tolerance, and *behaviors* such as product and energy usage. Such an approach is common in agent-based models. Another class of models is human-in-the-loop models, where humans are part of the simulation.

As discussed earlier, M&S is a decision-making process, and the decision makers are humans. Humans are known to deviate from ideal, rational behavior. For example, decision makers exhibit systematic biases in judgment of uncertainty (Kahneman et al., 1982), inconsistencies in preferences, and in the process of utilizing the process of expected utility theory. These deviations from normative models can be attributed to a number of factors such as cognitive limitations, performance errors, and incorrect application of the normative model (Stanovich 1999).

The gap between normative and descriptive models of human decision making has been well documented within the fields of behavioral decision research and psychology. Behavioral experiments have provided insights into how humans deviate from normative models, which have been used to develop psychological theories to explain these deviations. These deviations have been modeled in descriptive theories such as prospect theory, dual process theory, and many others. Alternate theories about decision making based on simple heuristics have also been proposed (Gigerenzer et al. 1996). These heuristics extend from simple one-step decisions to multi-step decisions with information acquisition at each step. Behavioral studies have also been extended to interactive decisions modeled using game theory (Camerer 2003). Recently, psychologists have started exploring neuro-science as a way to understand human behavior in general, and decision making in particular (Camerer et al. 2005).

While there has been significant progress on understanding humans as decision makers, the utilization of this knowledge in M&S activities has been limited. There are a number of open questions such as (i) how do these biases affect the outcome of modeling decisions? (ii) how can these biases be reduced? (iii) how can the effects of these deviations from rationality be reduced within the M&S process? (iv) what is the best way of presenting and communicating uncertainty information to the decision makers? (v) what is the effect of domain specific expertise and knowledge on deviations from rational behavior? and (vi) are there differences in biases between novice and expert modelers?

From an organizational standpoint, there are multiple individuals involved in the modeling process. Different individuals may have different beliefs, may be driven by different values, and may be influenced differently by different types of biases. These values, beliefs and biases get embedded in their individual models. Further research is necessary to establish how these interact within an organization, to ensure consistency across values and beliefs, and to overcome biases of individuals. This is clearly not a comprehensive list, but it highlights the importance of considering human aspects in M&S, and provides some pointers for further investigation.

In summary, human considerations are important for creating better models of systems involving humans, and for simulation of social-technical systems. Additionally, human considerations are important for better understanding of biases that exist during the modeling decisions made by humans. Addressing human aspects within M&S would help in designing better control strategies for smart networked systems and societies, better M&S processes, efficiently allocating organizational resources, and making better model-driven decisions. Research towards answering these questions would require collaboration between domain-specific modeling researchers and researchers in social, behavioral, and psychological sciences.

5.5 Communication and Education of Uncertainty in M&S

An additional challenge regarding uncertainty in M&S is: how to effectively communicate model predictions among various stakeholders? Especially in model reuse or when passing the models from model developers to decision makers, it is important to state clearly the key underlying assumptions along with their potential impact on the predicted QOIs. Sensitivity of key outcomes to the alternative modeling assumptions should also be assessed and presented effectively. Visualization tools need to be developed for illustrating the uncertainty sources, how they propagate, and their impacts over the entire domain of interest.

Related to the topic of communication of uncertainty is education for both students and faculty. At present, undergraduate students are typically taught the existing models related to each course subject without being introduced to the significance of the modeling process or a critical assessment of associated assumptions and uncertainties. For example, in engineering design courses, students are most often introduced to ad-hoc approaches to deal with uncertainty, such as the use of "safety factors." Courses on probability and statistics are often elective but not required, and students often take advanced science and engineering courses before they have gained exposure to probability and statistics. Moreover, probability and statistics courses for engineering undergraduate students deal largely with data analysis and do not introduce many concepts that are important to prediction and decision making under uncertainty.

A modern curriculum on probability in engineering and science is therefore needed to equip students with the foundation to reason about uncertainty and risks. A modern curriculum should foster an appreciation of the role that M&S could play in addressing complex problems in the interconnected world. The curriculum should also address effective communication of uncertainty and risk to modelers, decision makers, and other stakeholders.

5.6 Other Issues: Integration of Large-Scale Data

The advent of ubiquitous and easy-to-use cloud computing has more readily enabled simulations to leverage huge real-world datasets, i.e., "big data." Naturally, real-world datasets may be used to inform the models of the simulated system and its inputs, or could also be used to validate these models by comparing output behavior with real-world observations. A challenge of big real-world datasets is that they may be incomplete or noisy and include samples taken in different contexts so that they need to be "detrended" based on covariate information (contextual metadata). Moreover, many or most of the sample-features available may be superfluous to the simulation objectives. Noisy and superfluous features may result in inaccurate (e.g., overfitted) and needlessly complex models, again considering the specific simulation objectives. Techniques have been developed by data scientists to reduce or combine features of a sample dataset, e.g., using the classical methods of multidimensional scaling or principal component analysis. Future work in this area includes model-specific techniques of feature selection. Note that large datasets may not only have large numbers of samples but samples with enormous numbers of features (high feature dimension), so that future work in this area also includes scalable (low complexity) and adaptive techniques, the latter for dynamic, time-varying settings.

Large-scale data sets are often also used for deriving complex empirical relationships, using machine learning algorithms. Overfitting is a common concern in such scenarios. Cross-validation or hold-out testing provides a direct demonstration of a model's ability to predict under new conditions not encountered in the training set. Such methods use a majority of the data to calibrate or correct a model while holding some data to predict experimental or observational outcomes that were not used in the model calibration process. Characterizing uncertainty in extrapolative settings and rare events are challenging topics that require new research approaches that incorporate rigorous mathematical, statistical, scientific, and engineering principles.

6 Model Reuse, Composition and Adaptation

The motivations for the reuse of models are well-founded. Models are *knowledge artifacts*, and as such their reuse provides the opportunity for scientists, engineers and educators to "stand on the shoulders of giants." Models are also typically manifest as *software* that has been developed with significant effort and subjected to rigorous testing and verification and validation. The attractiveness of the potential cost and labor savings associated with the reuse of this software is quite understandable.

The reuse of models is confounded, however, by the fact that they are peculiarly *fragile* in a certain sense – they are typically context-sensitive, highly purposeful abstractions and simplifications of a perception of a reality that has been shaped under a possibly unknown set of physical, legal, cognitive and other kinds of constraints by a modeler, or modeling team; quite often a model's function is sensitive to many unstated assumptions. The end result is that model reuse can be fraught with significantly more complexity than, say, reusing the implementation of a sorting routine.

While some communities of practice (e.g., micro-electronics design, defense training) can arguably be viewed as success stories in the development and adoption of both the technologies and business practices for model reuse, general solutions to this important problem remain elusive.

There has been much significant work in the area of model reuse, and in software reuse more broadly. While it is beyond the scope of this effort to provide a comprehensive survey, several notable works are cited herein. In this report, we focus on three distinct areas for recommended further study:

- *Advancements in the theory of reuse*. Without a firm theoretical foundation, we cannot fully know the fundamental limits of what we can hope to accomplish with reuse. Properly formulated, good theory may also be exploited to produce robust and reliable reuse practices.
- *Advancement in the practice of reuse.* In this context we consider: (1) modeling and simulation (M&S) broadly, (2) data, and (3) discovery and knowledge management.
- *Advancements in the social, behavioral, and cultural aspects of reuse.* Here we consider how incentives may stimulate or impede reuse.

6.1 Advancements in the Theory of Reuse

Reuse has been defined as "Using a previously developed asset again, either for the purpose for which it was originally developed or for a new purpose or in a new context" (Petty, Morse, Riggs, Gustavson, & Rutherford, 2010) and *reusability* as "the degree to which an artifact, method, or strategy is capable of being used again or repeatedly" (Balci, Arthur, & Ormsby, 2011). In the former definition, an *asset* is "a reusable collection of associated artifacts". Assets may be software components, data sets, documentation, design diagrams, or other development artifacts, but for brevity and simplicity we use the term here primarily to refer to software components.

In the context of modeling and simulation, an asset may be either a software component that implements all of part of a model (e.g., a software component that implements a physics-based model of a jet aircraft engine) or all or part of the software needed to support a model (e.g., a component that implements an XML-based scenario initialization operation); when a distinction is needed, the former category will be referred to as *model components* and the latter as *support components*.

Metadata is supplemental information about a component that may be used for a number of purposes. In modeling and simulation, a model component's metadata may describe the model's function, intended use, assumptions, and uncertainties, in a way that enables appropriate reuse and reduces inappropriate reuse of the component (Taylor S. J., et al., 2015).

A theory of reuse for M&S does need to be formed from "whole cloth." Several theories from computing and mathematics support the development of a theory for M&S reuse. These theories include computability theory, computational complexity theory, predicate logic, algorithmic information theory, model theory, and category theory.

Prior Theoretical Work Relating to M&S Reuse

Past theoretical work relating to modeling and simulation reuse is briefly summarized, and several key results are described next.

Composability

Composability is the capability to select and assemble simulation components in various combinations into simulation systems to satisfy specific user requirements (Petty & Weisel, 2003). In a system of composable components the different simulation components can be composed from different sets of models, each suited to some distinct purpose, and the different possible model compositions will be usefully valid. Here *valid* is meant in the modeling and simulation sense, i.e., a valid model replicates the desired aspects of the phenomenon or system it models with sufficient accuracy to be useful (Balci, 1998). Although composability and reusability are not the same idea (Balci, Arthur, & Ormsby, 2011) (Mahmood, 2013), composability can be an important enabler for reuse. For close to two decades, composability has been an important objective for simulation developers, especially in the defense-related modeling and simulation community; it was identified as such at least as early as 1999 (Harkrider & Lunceford, 1999) and was recently described as "still our biggest simulation challenge" (Taylor S. J., et al., 2015). Composability applies to both model components and support components, but much composability research has focused on mechanisms for composing models and the validity of the resulting composite models.

In parallel with software engineering efforts attempting to implement frameworks for composability, theoretical work in the early 2000s produced some elements of a theory of composability based on formal definitions and reasoning. Starting from mathematical logic and computability theory, the goal of that work was to develop a deductive theory that would enable the determination in a mathematical, algorithmic way of certain characteristics of interest of a composition of models, especially whether their combined computation was valid. That work achieved several results:

- Based on an examination of existing composability terminology and levels of composable components, common definitions of composability and related terms were proposed (Petty & Weisel, 2003).
- Formal definitions of *model*, *simulation*, and *validity* consistent with their common informal meanings were developed to serve as the basis for the theory (Petty, Weisel, & Mielke, 2003).

- For several classes of models and forms of validity (including the general cases), the question of whether models that are separately valid remain valid when composed was resolved (Weisel, Mielke, & Petty, 2003).
- The computational complexity of selecting models to be composed was determined (Page & Opper, 1999) (Petty, Weisel, & Mielke, 2003).
- Software engineering approaches to achieving composability in practice were surveyed (Balci 2016).
- A simple form of composition was shown to be theoretically sufficient to assemble any composite model (Petty, 2004).

Two key results from the preceding list will be discussed in more detail in this section, and one in the next section:

- It is a common assumption, sometimes made intentionally and sometimes unintentionally by simulation developers, that if two models have been separately determined to be valid, then those models (or the components implementing them) may be composed and the resulting composition will also necessarily be valid. This is in fact not true. To address this specific question a series of related theorems were developed that considered several different classes of models, including a "computable" class that contains all models that can be executed on a digital computer, and that considered several different formal measures of validity, including a "trajectory metric" that formalizes the typical practitioner's notion of error accumulating over a simulation execution. It was proven that in all but the most trivial cases the composition of two (or more) separately valid models cannot be assumed to be valid (Weisel, Mielke, & Petty, 2003). In other words, two models that are individually valid may nevertheless produce invalid results after they are composed. To be clear, this result does not show that compositions of separately valid models cannot be valid; rather it shows that they cannot be assumed to be valid. The implication of this result is simple, and is generally understood at an intuitive level by experienced simulation practitioners; even if the components of a composite model are known or assumed to be valid, the overall composite model must also be validated as a whole.
- Software developers have produced sophisticated software frameworks for combining, or composing, models, with the intention of making such compositions easier to assemble and execute (Petty, Kim, Barbosa, & Pyun, 2014). Similarly, there are a number of different mathematical forms of function composition. The parallel is more than an analogy; recall that from a theoretical viewpoint, any model that executes on a digital computer is a computable function. It would be reasonable to assume that different software frameworks or mathematical forms of model composition would make a difference in what can and cannot be achieved in terms of model composability. In fact, they do not, at least at a theoretical level. In a theorem that uses induction on the number of models to be composed, it was proven that simple composition, i.e., composition with the mathematical form of $f(g(x))$, or more generally, $f_1(f_2(\ldots f_n(x)\ldots))$, is sufficient to assemble any composite model (Petty, 2004). The implication of this result is that theoretical investigation of model composition can consider simple composition without any loss of generality.

Composability and the related concepts of *interoperability* and *integratability* have been distinguished, with the first focused on modeling semantics and the other two focused on technical connectivity at the software and hardware levels respectively (Page, Briggs, & Tufarolo, 2003). These concepts have been subsumed in a single framework, known as the Levels of Conceptual Interoperability Model, that reinterprets the issues in terms of the degree to which models can exchange and consistently understand simulation data (Tolk & Muguira, 2003). The verification of a composition of components with respect to its requirements specification was examined in (Mahmood, 2013). In that same work, the notion of *pragmatic composability* considers the context within which a composition executes. The role of conceptual models in achieving reuse and composability was described in (Balci, Arthur, & Ormsby, 2011).

Component Selection

If a set of models, or equivalently, the components implementing those models, are to be composed, they must be available in a repository of components, and the components to be composed must be selected from among those available in the repository (Clark, et al., 2004). This is known as *component selection*. Component selection is the computational problem of selecting from a repository containing a set of available components a subset of those components to be composed so that the resulting composition will satisfy a given set of objectives for a simulation system. This deceptively simple-seeming problem arose during the study of composability previously mentioned, but it is treated separately here because it is a general software engineering issue, applicable to any repository of components, whether or not those components are model components or support components (Kaur, Singh, & Singh, 2014).

Note that there are actually two computation problems in component selection. The first and implicit problem is to determine which requirements a component satisfies, either in advance of component selection or on request when a set of requirements are presented. The second and explicit problem is to select a set of components to meet a given set of requirements. Both of these problems are well-known in software engineering; (Pressman & Maxim, 2015) summarizes them as "How do we describe software components in unambiguous, classifiable terms?" and "[H]ow do you find the [components] that you need?" respectively.

Work on component selection from a theoretical perspective proceeded in two stages. The earlier and seminal work defined four variants of the component selection problem based on two forms of objectives computability and two forms of composition (Page & Opper, 1999). Follow-on work identified two additional variants of the problem and defined a general form of it that subsumed all six variants (Petty, Weisel, & Mielke, 2003). This work led to two key results:

- To select components to compose that collectively meet a set of objectives, the objectives met by each component must be determined. Unfortunately, it is easy to see that such a determination may be problematic. Suppose a desired objective for a component is that it complete execution (rather than enter an infinite loop) for all inputs. This is the well-known "halting problem", which has been proven to be incomputable in general. Even objectives that in principle can be algorithmically decided may require a computation time that is superpolynomial and thus infeasible in practice (Page & Opper, 1999). The implication of this result is that the determination of the objectives met by a component may have to be done by means other than purely algorithmic, such as heuristic examination of the components themselves or by external labeling with metadata that identifies the requirements the component satisfies.

- Even if the objectives met by each component in the repository are somehow known, component selection remains difficult. In (Page & Opper, 1999), the specific form of component selection most similar to the practical application was shown to be NP-complete by reduction from SATISFIABILITY. In (Petty, Weisel, & Mielke, 2003), a general form of component selection was shown to be NP-complete by reduction from MINIMUM COVER. The implication of this result is the same as any NP-complete problem; the computational problem (in this case component selection) cannot be solved algorithmically in general, and heuristics that produce acceptable selections for most instances of the problem will have to be developed.

Research Topics in M&S Reuse Theory

Three research topics related to advancing the theory of modeling and simulation reuse and applying that theory in practical settings are proposed. They are listed from "most theoretical" to "most practical," and a set of relevant research questions for each topic is listed.

Composability Theory

Understanding the theoretical limits of composability, i.e., the composition of models and the validity of such compositions, is essential. Work has been started, but a fully coherent, comprehensive, and mature theory of composability has not yet been developed. Relevant research questions include:

1. *What are the theoretical characteristics or attributes of a model or component composition, beyond simply a composition of computable functions, and how do they affect reuse?*
2. *What theoretical formalisms are most effective at describing and analyzing composability?*
3. *Can models at different levels of abstraction or based on different modeling paradigms be composed without loss of validity?* (Fujimoto, 2016)
4. *Can the operations and problems of modeling and simulation reuse be recast in the terms and concepts of algorithmic information theory, category theory, and model theory, and if so, what insights would that provide?*
5. *Although as noted earlier the overall validity of a model composition is not assured simply by the validity of the model components, can anything about the validity of the composition be inferred from the components and the way in which they are composed?* (Tolk, et al., 2015)

Metadata and Reuse

Metadata is often described as enabling reuse, and a rigorous theoretical approach to metadata is conjectured to be more likely to succeed that *ad hoc* specifications. Predicate logic is arguably most often among the formalisms proposed for metadata, but it has not yet been demonstrated to be usable in practical settings. Theoretical limits proven in (Overstreet & Nance, 1985) may constrain what can be expected from metadata, but this warrants further investigation. Relevant research questions include:

1. *What formalism(s) are suitable for expressing component metadata?*
2. *What characteristics of a model should be expressed in metadata?*
3. *Can developing a standard vocabulary, perhaps defined using some form of ontology, increase the effectiveness of metadata?*
4. *Can component metadata be algorithmically or heuristically generated from or verified against a component?*
5. *How can the assumptions made in a model be expressed in metadata and used in component selection and model composition?*

Reuse Automation

Algorithms and frameworks that automate reuse operations, including component selection and composition verification and validation would likely expand the frequency and value of reuse. Relevant research questions include:

1. *Can model selection, composition, and code generation be automated?* (Fujimoto, 2016)
2. *What forms of theoretical composition correspond to practical reuse patterns?*
3. *Can reuse patterns themselves be reused, in the manner of design patterns?*
4. *Can the validity of a proposed composition of models be algorithmically confirmed?*
5. *Can heuristics be developed to circumvent theoretical obstacles and provide reasonable performance in most practical situations?*
6. *Can constraints imposed on model development (e.g., standards) improve the composability of the models once developed?* (Fujimoto, 2016)

6.2 Advancements in the Practice of Reuse

In this section, we consider some of the challenges to the day-to-day practice of reuse in a modeling context. We separate the discussion into three distinct areas:

- Modeling and simulation – in which we deal with issues confronting the reuse of representations of models and their implementation in simulation languages and frameworks.
- Data – in which we deal with the issues confronting the reuse of those elements that are consumed and produced by models.
- Knowledge management and discovery – in which we address the issues involved in archiving and discovering artifacts (models, simulations, data) that may be reused.

Challenges in the Practice of Reuse of Models and Simulations

We identify research challenges associated with the reuse of model representations and their implementation as simulations in four areas: (1) multi-formalism, multi-scale modeling, (2) reuse across communities of interest and the implementation spectrum, (3) exploitation of M&S web services, and (4) quality-centric approaches to component evaluation. Each of these is discussed below.

A.	Based on Model Representation		Development Approach
	1.	Discrete M&S	Logic
	2.	Continuous M&S	Differential equations
	3.	Monte Carlo M&S	Statistical random sampling
	4.	System Dynamics M&S	Rate equations
	5.	Gaming-based M&S	Logic
	6.	Agent-based M&S	Knowledge, "intelligence"
	7.	Artificial Intelligence-based M&S	Knowledge, "intelligence"
	8.	Virtual Reality-based M&S	Computer generated visualization
B.	Based on Model Execution		
	9.	Distributed / Parallel M&S	Distributed processing / computing
	10.	Cloud-based M&S	Cloud software development
C.	Based on Model Composition		
	11.	Live Exercises	Synthetic environments
	12.	Live Experimentations	Synthetic environments
	13.	Live Demonstrations	Synthetic environments
	14.	Live Trials	Synthetic environments
D.	Based on What is in the Loop		
	15.	Hardware-in-the-loop M&S	Hardware + Simulation
	16.	Human-in-the-loop M&S	Human + Simulation
	17.	Software-in-the-loop M&S	Software + Simulation

Table 6.1. M&S Areas (Types) (Balci, Introduction to Modeling and Simulation, n.d.) (Balci, Arthur, & Ormsby, Achieving Reusability and Composability with a SImulation Conceptual Model, 2011)

Multi-Formalism, Multi-Scale Modeling

As a topical matter, M&S is incredibly broad. It spans dozens of disciplines and countless potential objectives and intended uses (ACM SIGSIM, 2016). To our knowledge, a definitive, exhaustive taxonomy for M&S has not been formulated. For the purposes of this report, we adopt the characterization given in Table 6.1. While necessarily incomplete, it is indicative of the breadth of M&S. Each area noted in the table possesses its own characteristics and methodologies, is applicable for solving certain classes of problem, and has its own community of users. Many M&S areas have their own societies, conferences, books, journals, and software tools.

The current era of "net-centricity" has produced a proliferation of "systems of systems" in which disparate systems with diverse characteristics are composed and integrated over networks, e.g., the Internet, virtual private networks, wireless networks, and local area networks.

We face serious technical challenges in achieving reusability, composability, and adaptability for developing simulation models representing such network-centric systems of systems. Different systems or system components may be required to be modeled by using different M&S types and/or at vastly different spatial and temporal scales. For example, one component may be modeled using discrete M&S, another using Computational Fluid Dynamics, another in Finite Element, and still another using system dynamics. Achieving interoperability across these modeling approaches is an open problem.

New methodologies, approaches, and techniques must be created to enable the development of an M&S application or component by way of reusing, composing, and adapting different types of M&S applications or components.

Artifact Reuse Across Communities of Interest and the Implementation Spectrum

Many different types of M&S applications are commonly employed in a Community of Interest (COI) such as air traffic control, automobile manufacturing, ballistic missile defense, business process reengineering, emergency response management, homeland security, military training, network-centric operations and warfare, supply chain management, telecommunications, and transportation. Reusability, composability, and adaptability are critically needed to facilitate the design of any type of large-scale complex M&S application or component in a particular COI, and significantly reduce the time and cost of development.

An M&S application or component is developed in a COI under a certain terminology (e.g., agent, job, missile). In another COI, the same M&S application or component may be developed from scratch without any kind of reuse because the terminology does not match although they are basically the same applications or components.

Challenges in reuse across the wide spectrum of implementations are also important. In M&S application development, we should aim to reuse, compose, and/or adapt an artifact, development process, design pattern, or framework such as: (1) a simulation program subroutine, function, or class, (2) a simulation programming conceptual framework, (3) a simulation model/software design pattern, (4) a simulation model component or submodel, (5) an entire simulation model, or (6) conceptual constructs for simulation in a particular problem domain.

Figure 6.1 depicts how well reusability can be achieved at different levels of M&S application development.

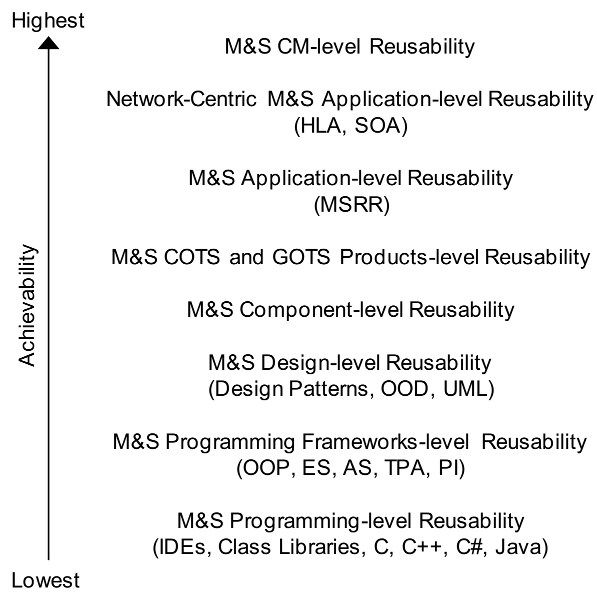


Figure 6.1. Levels of Reusability versus Achievability (Balci, Arthur, & Ormsby, Achieving Reusability and Composability with a SImulation Conceptual Model, 2011).

At the programming level, classes (under the object-oriented paradigm) and subroutines/functions (under the procedural paradigm) are extracted from a library using an Integrated Development Environment (IDE) such as Eclipse, NetBeans, or Microsoft Visual Studio. However, reuse at this level is extremely difficult due to the many options in programming languages (e.g., C, C#, C++, Java), differences in operating systems (e.g., Unix, Windows), and variations among hardware platforms (e.g., Intel, SPARC, GPU, FPGA) supporting language translators. An artifact programmed in Java and executing under a Unix operating system on a SPARC workstation cannot be easily reused in an M&S application being developed in C++ under the Windows Operating System on an Intel-based workstation.

M&S programming frameworks may be categorized according to the underlying programming paradigm, e.g., Object-Oriented Paradigm (OOP), Procedural Paradigm (PP), Functional Paradigm (FP), and so forth. Balci (Balci, 1988) describes four conceptual frameworks under the PP for simulation programming in a high-level programming language: event scheduling (ES), activity scanning (AS), three-phase approach (TPA), and process interaction (PI). A simulation programmer is guided by one of these frameworks by reusing the concepts supported in that conceptual framework. However, an artifact programmed under one framework cannot be easily reused under another.

Reuse at the design level is feasible if the same design paradigm is employed for both the M&S application development and the reusable artifacts or work products. The reuse is also affected by the design patterns employed. For example, an M&S application being designed under the Object-Oriented Design (OOD) approach can reuse work products created under the OOP. Unified Modeling Language (UML) diagrams are provided as an international standard to describe an OOD. UML diagrams assist an M&S designer in understanding and reusing an existing OOD.

However, reuse at the design level is still difficult since it requires the reuse of the same design paradigm. For example, a continuous simulation model consists of differential equations, and may not integrate easily with OOP components. Monte Carlo simulation is based on statistical random sampling. A System Dynamics simulation model represents cause-and-effect relationships in terms of causal-loop diagrams, flow diagrams with levels and rates, and equations. An agent-based simulation model represents agents and their interactions. Different types of simulation models are designed under different paradigms, and one paradigm cannot be easily accommodated within another. Yilmaz and Ören (Yilmaz & Oren, 2004) present a conceptual model for reusable simulations under the conceptual framework of a model-simulator-experimental frame.

M&S component level reuse is intended to enable the assembly (composition) of a simulation model by way of employing already developed model components in a similar fashion as an automobile is assembled from previously produced parts. A component may correspond to a submodel or a model module. Reuse at this higher level of granularity is beneficial because it reduces development time and cost over that of reuse at the class or function level. However, this approach to reuse still poses difficulties since each reusable component can be implemented in a different programming language intended to run under a particular operating system on a specific hardware platform.

M&S Commercial Off-The-Shelf (COTS) (e.g., Arena, AutoMod, and OpNet) and Government Off-The-Shelf (GOTS) products enable reuse of components within their IDEs. Such an IDE provides a library of reusable model components. A user can click, drag, and drop an already developed component from the library and reuse it in building a simulation model. However, such reuse is specific only to that particular COTS or GOTS IDE, and portability to another IDE would become a user's responsibility.

Reuse at the application level is feasible if the intended uses (objectives) of the reusable M&S application match the intended uses of the M&S application under development. For example, the U.S. Department of Defense (DoD) provides the DoD M&S Catalog (Modeling and Simulation Coordination Office (MSCO), 2016) containing previously developed M&S applications. Some of these applications are independently certified for a set of intended uses. Some are not well documented and come in binary executable form only. Even if the source code is provided, understanding the code sufficiently well to modify the represented complex behavior is extremely challenging. Reusability of earlier developed M&S applications is dependent on run-time environment compatibility and the match between intended uses.

A network-centric M&S application involves M&S components interoperating with each other over a network, typically for the purpose of accommodating geographically dispersed persons, labs, and other assets. The High Level Architecture (HLA) is a DoD, IEEE, and NATO standard for developing network-centric M&S applications by way of interoperation of simulation models distributed over a network (IEEE, IEEE Standard 1516, 1516-1, 1516-2, and 1516-3). If a simulation model is built in compliance with the HLA standard, then that model can be reused by other models interconnected through the HLA protocol over a network.

Service Oriented Architecture (SOA) is yet another architecture based on the industry standard web services and the eXtensible Markup Language (XML). SOA can be employed for developing a network-centric M&S application by way of reuse of simulation models, submodels, components, and services over a network. For example, Sabah and Balci (Sabah & Balci, 2005) provide a web service for random variate generation (RVG) from 27 probability distributions with general statistics, scatter plot, and histogram of the requested random variates. The RVG web service can be called from any M&S application that runs on a server computer over a network using XML as the vehicle for interoperability. Reuse, composability, and interoperability are fully achieved regardless of the programming language, operating system, or hardware platform. However, this type of reuse is possible only for network-centric or web-based M&S application development.

New methodologies, approaches, and techniques must be created to enable the development of an M&S application in a COI by way of reusing, composing, and adapting other M&S applications or components created in other COIs. New methodologies, approaches, and techniques are needed to enable the development of an M&S application through reuse, composition, and adaptation of M&S applications or components across the spectrum of implementation levels.

M&S Web Services

This research challenge deals with *how* to reuse, compose or adapt. Initiated in the early 2000s. the U.S. National Institute of Standards & Technology (NIST) Advanced Technology Program (ATP) cited many advantages of component-based development that could be realized conditioned on the following (NIST, 2005):

1) Establishment of a marketplace for component-based software development so that the technology users can realize significant economic benefits through
    a) reduced software project costs,
    b) enhanced software quality, and
    c) expanded applicability of less expensive technology.
2) Increased automation and productivity in software development enabling
    a) improved software quality characteristics,
    b) reduced time to develop, test, and certify software, and
    c) increased amortization of costs through software component reuse.
3) Increased productivity of software project teams by
    a) permitting specialists in the application domain to create components incorporating their expertise, and
    b) providing a focus on discourse in development at a level far more higher-level than a programming language.
4) Expanded markets for software applications and component producers by promoting
    a) the creation of systematically reusable software components,
    b) increased interoperability among software components, and
    c) convenient and ready adaptation of software components.

More than a decade later, many of the advantages NIST ATP identified have not been realized in spite of significant research investments. Component-based software development remains an "unsolved problem" largely due to the vast and varied landscape of programming languages, operating systems, and hardware available.

Component-based development of M&S applications may also be considered an "unsolved problem" due to several factors:

1) Components that need to be assembled with each other are coded in different programming languages intended to run under different operating systems on different hardware platforms.
2) The level of granularity and fidelity (degree of representativeness) provided in a component is not compatible when assembled with other components having different levels of granularity and fidelity.

3) A component available only in binary form with no source code and documentation creates uncertainties when conducting verification and validation processes.
4) The intended uses of a component do not match the intended uses of the other components when the components are assembled together.
5) A component providing much more functionality than needed degrades execution efficiency.

The U.S. Department of Defense has created a number of M&S repositories (APL, 2010). Reusing, composing, or adapting resources from these repositories has been hindered because of (1) the differences in programming languages, operating systems, and hardware, (2) classified nature of many models and simulations and associated data, (3) lack of organizational push for reuse, (4) lack of contractors' interest in reuse, and (5) lack of effective documentation.

Within the software engineering community, reuse is considered by many to be a "solved problem" for *cloud-based software development* under the Service-Oriented Architecture (SOA). A software application can be implemented as a web service and other applications can reuse via XML or JSON communications. The programming language used in developing the software application, the operating system it runs under, and the server computer hardware it runs on are transparent to the calling application.

To effectively engender reusability, composability, and adaptability problems, the M&S community should pursue the web services paradigms that have been successfully applied within the general software arena.

Quality-Centric Approaches to Component Evaluation

An existing M&S application can be reused without any change if and only if its credibility is substantiated to be sufficient for the intended reuse purpose.

An existing submodel (model component) can be reused without any change if and only if

(a) its credibility is substantiated to be sufficient for the intended uses for which it is created, and

(b) its intended uses match the intended uses of the simulation model into which it will be integrated.

Any change to the M&S application will require it to be verified, validated, and certified again. Any change to the existing submodel will require not only the submodel, but also the entire simulation model to be verified, validated, and certified again.

Traditionally, Verification and Validation (V&V) are conducted to assess the *accuracy* of a model. However, *accuracy* is just one of dozens of quality indicators affecting the overall usefulness of an M&S application. Arguably, *accuracy* is the most important quality characteristic; however, we cannot ignore the importance of other quality indicators such as *adaptability, composability, extensibility, interoperability, maintainability, modifiability, openness, performance, reusability, scalability, and usability.*

It is crucially important that M&S application development be carried out under a *quality-centric approach* rather than just the traditional *accuracy-centric approach*. It should be noted that a quality-centric approach embodies the accuracy-centric approach since accuracy is a quality characteristic by itself.

New methodologies, approaches, and techniques must be created under a quality-centric paradigm for assessing the overall quality of an M&S application by employing quality indicators such as accuracy, adaptability, composability, extensibility, interoperability, maintainability, modifiability, openness, performance, reusability, scalability, and usability.

Data Reuse in Practice

The increasing volume, velocity, and variety of available data present both great opportunities and challenges. This is true across all areas of government, academia, industry, and is equally true of models and simulations. The value of M&S can rely heavily on the availability and quality of input data. Similarly, M&S can be prolific sources of output data. The United Nations Economic Commission for Europe (UNECE) projects global data to reach 40 Zettabytes (that is 40 Billion Terabytes) by 2019 (see Figure 6.2 below). The business and culture of government at large, the defense industry, and Modeling and Simulation domain are suffering under the weight of this data "glut". Organization's existing practices for managing, analyzing, and sharing data are becoming increasingly ineffective in the face of the mountains of data they must contend with on a daily basis. New strategies, approaches, and technologies are needed to meet this challenge.

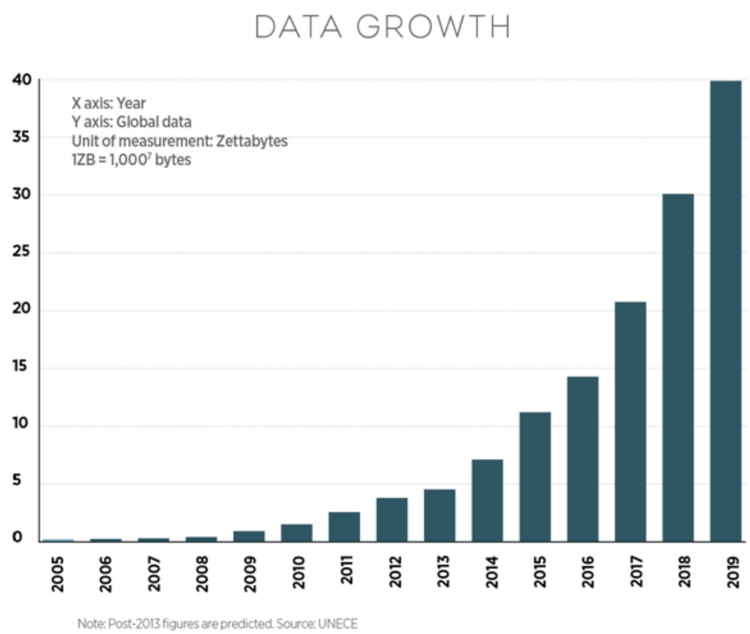


Figure 6.2. United Nations Global Data Growth Projections in Zetabytes.

During a recent address, President Obama noted that, "Understanding and innovating with data has the potential to change the way we do almost anything for the better" (Strata + Hadoop World 2015). This begins by thinking about data differently. Data is the foundation of information, knowledge, and wisdom (see Figure 6.3 below). Within the U.S. Army, data are an enterprise asset, information is an enterprise currency, and knowledge is an enterprise resource (Office of the Army Chief Information Officer/G-6, Feburary 2016). How we manage, analyze, and share data is what allows us to work our way up the information pyramid, such that we are using data and "technology to make a real difference in people's lives" (White House Office of Science and Technology Policy (OSTP), May 2012).

Today's amazing mix of cloud computing, ever-smarter mobile devices, and collaboration tools is changing the consumer landscape and bleeding into government as both an opportunity and a challenge. Challenges from data can be thought of in terms of managing, analyzing and sharing. In turn, these challenges drive research opportunities that have the potential to change how we think about data.

Managing Data

Data management practices refer to the storing, identifying, organizing, correcting and validating data. Vast amounts of data are produced across government, defense and modeling and simulation (M&S) organizations. Currently, many models and simulations use a series of inconsistent *ad hoc* data structures to log and store data based on legacy files and formats. These data structures range from flat files to relational/hierarchical databases across a multitude of formats and from an even wider variety of sources. In addition, the data structures for each simulation event are unique, and do not include meta-data descriptions making direct comparison of data between events extremely difficult and highly problematic. Consider the challenge of *ad hoc* data structures that are inconsistent from simulation event to simulation event and how it would impact model and/or simulation scenario development, integration, analysis, verification and validation of the models, simulation and data generated for a single system. Now imagine this challenge across a system of systems. It could quickly turn into a time intensive effort that produces questionable results of limited value that impact the credibility of the models, simulation, and data produced.

Traditionally, after simulation events, users of models and simulations employ a technique called *data reduction*. The concept of data reduction is to reduce large amounts of multi-dimensional data down to a corrected, ordered, simplified form. This is typically done by editing, scaling, summarizing, and other forms of processing into tabular summaries. In this process, the raw data is often discarded along with the hidden knowledge one may obtain from it.

As data storage costs have approached zero, data management opportunities have exploded. Society has started to shift away from minimal data storage concepts to now storing everything, including all of the raw data produced such that we are now in an era of big data. This has magnified the need and opportunity for more robust and advanced technologies in metadata identification, organization, and validation. This produces a data set with properly formed data, sorted for processing, and the data model required for the analysis and sharing components of data reuse.

Effective active data management practices will promote data reuse, data integrity, complex analytics, and is the foundation of data science. This allows for data scientists to use these rich data sources and apply advanced analytic techniques to derive additional insights that traditional analysis techniques fail to uncover.

Analyzing Data

Data analysis refers to the process of inspecting data with the goal of discovering useful information, suggesting conclusions, and supporting decision making. In other words, how to most effectively move decision makers to the top of the knowledge pyramid where wisdom can be applied to accomplish goals by making decisions. *Exploratory, inferential*, and *predictive* data analytics are the three main bodies of analysis used in modeling and simulation.

In exploratory data analysis for simulations, the goal is to describe the data and interpret past results. These are generalizations about the data that are good for discovering new connections, defining new M&S scenarios for testing and grouping observed events into classifications. Examples include the number of successes vs. number of attempts in a simulation, census data, and number of times events occurred when conditions are met.

In inferential data analysis for simulations, the goal is to make inferences about the systems behavior based on a limited number of simulation events. This is critical due to the complexity and computational resources required to test every variable parameter for every possible condition within a complex system or system of system simulation. Examples of this include polling and failure rate analysis.

In predictive data analysis for simulations, the goal is to use previously collected data to predict the outcome of a new event. This helps with gaining deeper understandings of the interactions of the complex systems or system of systems. This involves measuring both the quantity and the uncertainty of the prediction. Examples of this include credit scores, behavior predictions, and search results.

Data reuse can help organizations be more effective at data analysis and deriving wisdom from data; this can be due to cost savings associated with complex system tests, in addition to leveraging system experts external to organizations. An enabler of efficiently traveling upwards in the knowledge pyramid is Data Science. Data science is an interdisciplinary field about processes and systems to extract knowledge and insights from data by employing techniques and theories drawn from computer science, mathematics, and statistics. Algorithm and Statistical based techniques such as data mining are leveraged in order to transition from data to the information and ultimately the knowledge components of the pyramid.

As our systems become more interconnected, and the models and simulations of these systems become more sophisticated, richer and richer data sets are produced. These systems are often loosely coupled, composed of multi-mission and multi-role entities, across organizations and often display nonobvious behaviors when operating in a complex environment. Exploring these relationships is a key component of a technique called data mining. Data mining complex simulations typically involves four common classes of tasks: anomaly detection, clustering, classification, and regression. Anomaly detection is focused on data errors or outliers that may be interesting to an analyst, e.g., failure modes. Clustering is a method of assigning similarity scores to groupings of like events. Classification is the task of generalizing known structures to apply to new data, for example, predicting causes and effects on system performance. Regression attempts to find a function, or simplified model, that can describe the behavior of the system with the least amount of error.

The opportunities to leverage these data science techniques within government, defense, and the M&S domain are vast. Research opportunities include data visualization for analysis and cloud computing, impact on analysis spawned by big data, and data developed for one purpose to be reused in order to support another purpose. An example of this is where given a large enough data sets from a simulation suite, stochastic techniques such as metamodeling can produce a function or simplified model that can be used to predict certain behaviors. These metamodels can be used as low cost alternatives to the large scale simulation for certain activities. By combining classification and clustering, correlated behaviors and second and third order effects can also be discovered within your data sets. Anomaly detection can help identify corner cases, off-nominal system states, and provide the ability to focus expert analysis on the cases that are more interesting.

Sharing Data

The sharing component covers the entire knowledge pyramid. It also plays a special role in decision making – especially as decision making becomes increasingly data-driven. The level of preparation necessary for data (e.g. data, information, knowledge, wisdom) to be used for the decision making to take place will vary, but one thing that is required is that it must be discoverable and accessible. Modern information technology architectures build upon the years of success of great technologies such as indexing and federated search, many perfected by companies like Google. Therefore, this section will focus on the remaining challenges of sharing.

Sharing of data, information, knowledge and wisdom across the pyramid has several different challenges. One which may be immutable is culture. Cultures of not sharing contribute to examples of events such as 9/11. Artificial cultural boundaries between agencies within the intelligence community created a serious impediment to protecting the country. Post 9/11 the intelligence community was reformed, restructured, and given a mandate to share information in an effort to change the culture. As a sharing culture pertains to M&S data, many would posit that despite existing mandates to share M&S data (even data which has been characterized for limitations and constraints) within a single government department does not consistently occur let alone consistently occur across the entire federal government. Such can be the challenges of policy versus implementation. For example, within the Department of Defense, sharing is mandated by DoD Directive 8320.02, yet rarely or consistently is M&S data published (i.e. made accessible) to anyone beyond the very focused end user. The unintended consequence of not sharing across the M&S domain is the reproduction of data and results which may already exist elsewhere that could have been made available and accessible for reuse. Opportunities exist to foster a culture of sharing which can be addressed through education as an opportunity to avoid repeating the failures of the past across our community and M&S domain. Initiatives such as the National Institute of Health's Big Data to Knowledge (BD2K) launched in 2012 that seek to facilitate the broad use of biomedical data assets by making them discoverable, accessible, and citable are great models of how to encourage more data sharing.

The technical domain presents another obstacle to M&S data sharing. The sharing component covers the entire knowledge pyramid, but plays a special role in both the raw data and wisdom components. In order to produce decision quality knowledge, data has to be converted into at least information or knowledge, but preferably wisdom. A good illustration of the processing in terms of transformations and outcome states is shown in Figure 6.3 below.

This illustration shows the work an organization should do on its data but does not show the sharing implications. One implication is that organizations are unaware of the fact that they do not have good visibility into their own data. They do not know what they do not know. As Figure 6.4 (a) shows, a majority of an organization's data typically remains either unused (discovered but not used) or with unknown (not discovered and not used) value. Once this shortcoming is overcome sharing can begin by achieving enterprise wide attributes of visibility, accessibility, and understandability (see Figure 6.4 (b)).

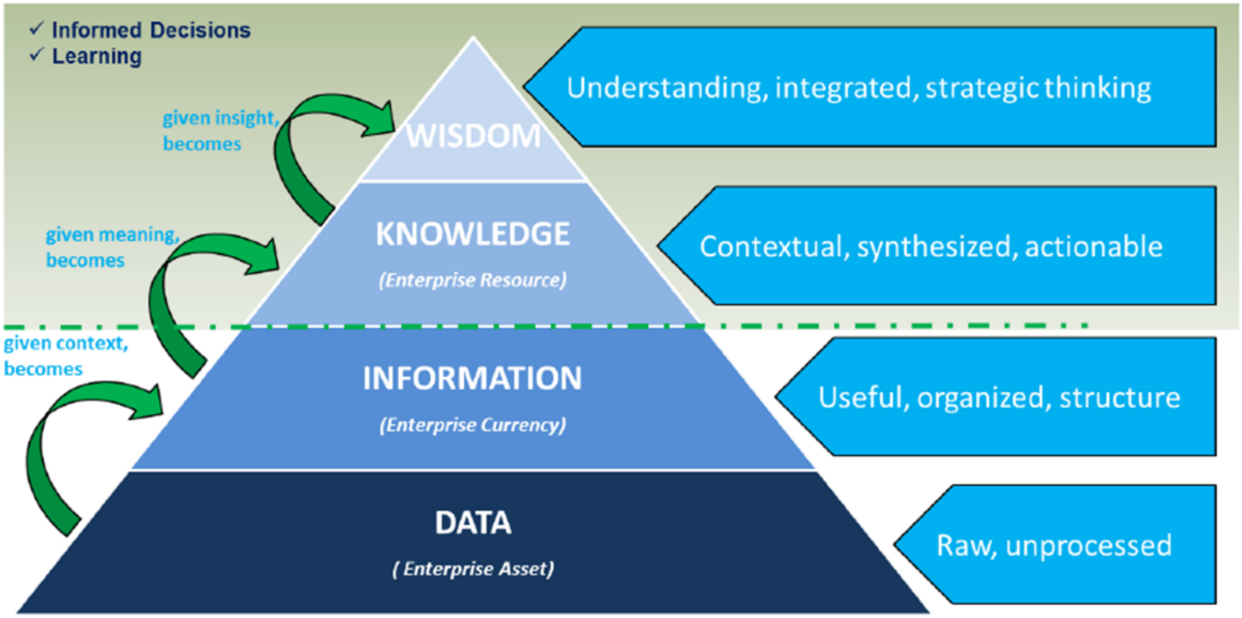
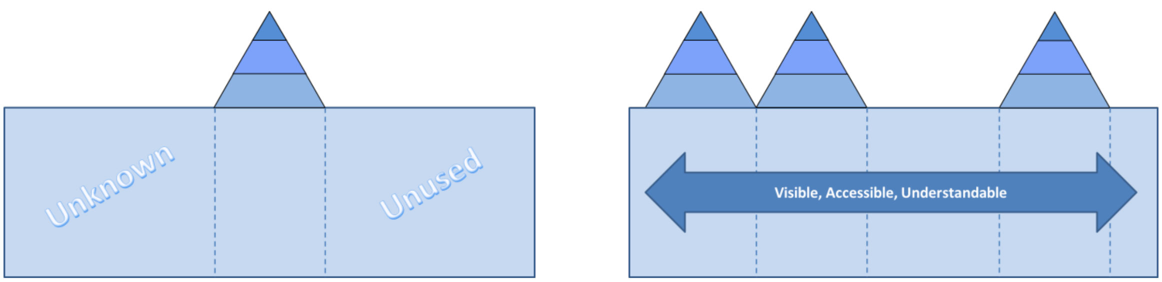


Figure 6.3. DIKM Pyramid Levels of Processing (Wikipedia, n.d.).



(a.) DIKM Pyramid limited visibility into data.

(b.) Sharing is having achieved visibility, accessibility, and understandability.

Figure 6.4. DIKM Pyramid Implications for Sharing (Wikipedia, n.d.).

Conceptually, sharing of data defined as the data becoming visible, accessible, and understandable is quite simple and most organizations can tap the technology to achieve at least visibility and accessibility with commonly available information technology tools at their disposal. However, understandable data is more difficult to achieve. As mentioned previously, analysis is the gateway to understanding data beyond statistical summary, but it is not the solution for everything. The missing ability for universally understandable data is automatic semantic exchange across systems which access data. To share is to communicate. C.E. Shannon accurately identified the challenge (Shannon, 1948):

> *"The fundamental problem of communication is that of reproducing at one point either exactly or approximately a message selected at another point. Frequently the*

messages have meaning; that is they refer to or are correlated according to some system with certain physical or conceptual entities. These semantic aspects of communication are irrelevant to the engineering problem."

In other words, the challenge of automated semantic data exchange (i.e. sharing of messages with meaning) not only depends on the data being shared but being properly interpreted contextually and properly used. The National Science Foundation is pursuing universal internet data models. Other approaches being taken includes work on automatic generation of taxonomies and reasoning mechanisms. This area is ripe for additional research opportunities.

As sharing and collaboration gain traction within a community of interest, data security and privacy challenges naturally emerge. To understand the implications of data security it is important to consider the states in which data exists. Data can be defined as being in motion (data transmitted over a connection), at rest (persistent for any length of time in any form), or in memory (in use by any program, tool, operating system, etc.). Threats to data in these forms can generally be classified into categories of privacy (unauthorized disclosure), integrity (alteration), and destruction (permanent deletion).

Although destruction is always a concern for data in any setting, of particular concern in a data sharing paradigm is Privacy and Integrity. The key emergent risk even in a 'secure' sharing environment in a sharing paradigm becomes misuse. Data producers have an inherent concern that simulation data will not be used within the scope for which they pertain. Additionally, data producers may have a concern that if not kept private, its misuse could reflect poorly on the producer themselves (inaccurate embarrassment). Data integrity concerns arise for data producers with any reuse fearing alteration of original data. For these reasons in a data sharing paradigm; security is a key area of present day and future research interest as the complexity extends far beyond general business use cases to highly technical scenarios. Consider for example, that a transport security layer may be implemented to protect data in motion between two servers, as accessed by several different authenticated role-based users from different geographic locations, and that same data might also become vulnerable over the net by a distributed cache; secure in two ways (in motion and private) yet vulnerable in a third (in memory).

Data security and privacy need to be considered throughout the data lifecycle in all of its mediums (as exampled above), and as technology around data is quickly changing such that security/privacy technology need to adjust to keep pace. Data security and privacy need to be considered as a part of risk management processes as well in such a way that they are not statically defined, but allow for continual evaluation for adapting new technologies ensuring they provide proper protections and safeguards to prevent improper collection, retention, use or disclosure of data. Opportunities exist to research and develop capabilities for architecting for openness such that trust, accountability, and transparency about how data is collected, used, shared, secured can be determined.

In conclusion, data is fundamentally changing how we conduct business and live our lives through advances in data quality, availability, and storage capacity. A key component of successfully working with data is having the proper data science background and education. Research opportunities abound in the data sciences; from metadata generation, organization, and validation within each data management category, to data analysis visualization, cloud computing impact on analysis, to data reuse in data analysis category, to automatic generation of taxonomies and reasoning mechanisms, effective security and privacy in a sharing category just to name a few.

Data enabled by technology (current and future research areas) for managing, analyzing, and sharing will drive new strategies and approaches empowering users to connect the dots and provide the right data anytime and anywhere to make more informed decisions. We can now ask questions of the data that we never could before; even questions about the data itself such as should we throw data away and if so, when? The understanding and motivation to embrace this reality across government, defense business and culture needs to be applied to the M&S domain.

Discovery and Knowledge Management of M&S Assets

Knowledge management is a key area for M&S reuse with the recognition that models and simulations are encapsulations of knowledge. Although not generally considered in those terms, a model is a representation or interpretation of an object or physical phenomenon which engenders the understanding of the original. The applicability of models lies in a consistent and coherent representation of the knowledge about the thing or process being modeled.

Luban and Hincu (Luban & Hincu, 2009) emphasize the coupling between simulation and knowledge management. In referencing some earlier work, they state that "although the literature separates simulation and knowledge management, a more detailed analysis of these areas reveals that there are many links between them. More knowledge about the system can be discovered during simulation modeling process, and model development can be facilitated by collaborative knowledge management tools."

The following sections will consider some potential research areas related to knowledge management as an enabler of modeling and simulation.

Applications of Machine Learning

The complexity of modern simulations makes it increasingly difficult for a human being to adequately understand the interconnections and dependencies to assure that the model or the simulation is a correct implementation. As models and simulations become adaptive, assessing validity will require another application to monitor and analyze the running system. Although this may sound counter to the purpose, the use of machine learning may offer possible solutions.

Monitoring and assessment of running simulations

Simulations are generally used to answer a question about the outcome of a process under investigation. Whether the method is discrete event, Monte Carlo, mathematical or just statistical models, the aim is to provide an answer to a question.

Although very useful, that approach assumes that the intermediate stages of the simulation are incidental. However, if you take an example such as the erosion of a river bank due to changing hydrologic action, the intermediate erosion processes might be useful in understanding the end result. Astrophysical simulations such as the collision of galaxies are captured as sequential time steps. Harel and Rumpe (Harel & Rumpe, 2000) call this "snapshot" approach a "frozen situation at any given time during the system's execution."

Research topics include non-intrusive monitoring; visualization of simulation process from multiple perspectives; and understanding interaction dependencies in distributed computing environments

Model specification, construct validity, selection and credibility

Models are a substitute for the actual system which the researcher is interested in understanding. As such, the models have a degree of abstraction that requires some assessment of the quality of the model for the intended purpose. Balci (2004) describes quality assessment as "situation dependent since the desired set of characteristics changes from one M&S application to another. M&S application quality is typically assessed by considering the M&S application requirements, intended users, and project objectives."

The Capability Maturity Model Integration (CMMI) defines a process that is intended to assure that the resultant modeling and simulation application is well defined and documented. Of course this assumes that the CMMI process was followed and executed by individuals that were trained and followed the proscribed procedures. Assigning a level of validity based on the model construct would generally require a test or demonstration that the model is consistent with the actual object or process. The specification and construction validity of a model or simulation is therefore highly dependent on the process and underlying assumptions used in the formulation of the model.

The selection of a model by a user is therefore based on the confidence of the user that the model was designed, constructed, and assessed by a set of reasonable criteria including a quality control process. Since there is generally no currently accepted numerically defined method for applying a confidence figure (e.g. 95%), it is left to the user to determine if the model or simulation is sufficient for their purposes. The confidence that the user has in the model is also reflected by the validity associated with that model. Research topics include numerical confidence of quality and measures of appropriateness.

Attribute labeling with authoritative vocabulary

In the area of reuse of models the major stumbling block is generally language. A simple example would be building a model car. The instructions for assembly might include the phrase "attach the hood to the support on the firewall." This phrase is perfectly understandable to someone familiar with American English however the term "hood" in the United Kingdom would be replaced with "bonnet." The same piece serves the same function but utilizes different labels.

When someone constructs a model which does not use the language of mathematics, attribute labeling, descriptions, etc. become problematic. In addition, the modeler is influenced by their domain expertise which shapes a person's view of the world. Looking at a stream bed, a hydrologist considers the erosion factors due to grazing impacts while the geologist considers the subsurface geology as a contributing factor.

Model reuse will be a consistent problem if there is no agreed upon way of describing a particular component of the model or the model itself. Research in this area focuses on the attribute labeling through the use of an authoritative or controlled vocabulary.

Patricia Harping (Harping, 2010) with the Getty Research Institute provides a good example of the need for a controlled vocabulary for managing their art collections and the need for both descriptive and administrative data.

> "Data elements record an identification of the type of object, creation information, dates of creation, place of origin and current location, subject matter, and physical description, as well as administrative information about provenance, history, acquisition, conservation, context related to other objects, and the published

> sources of this information. […] Art and cultural heritage information provides unique challenges in display and retrieval. Information must be displayed to users in a way that allows expression of nuance, ambiguity, and uncertainty. The facts about cultural objects and their creators are not always known or straightforward, and it is misleading and contrary to the tenets of scholarship to fail to express this uncertainty. At the same time, efficient retrieval requires indexing according to consistent, well-defined rules and controlled terminology."

How does the above relate to models and simulations? Models, as with art, require descriptions of what they are and how they are intended to be used as well as what inputs and outputs are required. The use of an authoritative vocabulary that would allow both within-domain and cross-domain identification and usage would be exceedingly useful for model reuse. It must be recognized that a controlled vocabulary such as used in many database applications would be inadequate for model development. As stated above, the domain of the user influences choice in the modeling process. The vocabulary should therefore be derived from the model domain while providing consistency in the description or labeling. Research topics include the development of ontologies and authoritative vocabularies.

Syntactic and Semantic Consistency

The development and use of models is dependent on the language elements of syntax and semantics. Although often misunderstood, syntax and semantics express different aspects of a model.

Model syntax specifies the allowable expressions that are used in the construction of the model. When developing a model, the modeler must follow a set of rules that provide well-formed expressions. These rules form the basis of an abstract syntax such as one defining a data structure. By following the syntactic rules, a model instance can be constructed using a logical set of elements expressed in a modeling language. The language might be mathematical, graphical, or an artificial language (e.g. programming language such as FORTRAN).

Semantics supplies the meaning of the model. The relationships between the things or processes being modeled is known as the semantic mapping. The second aspect of semantics is being able to determine how other models might be derived from the current model. This is known as semantic derivation but in general usage, many still use the term semantic mapping. The relationship between things is of major importance to the modeling and simulation community from a reuse standpoint.

As an example, computer-aided design (CAD) drawings are descriptive models of a physical object. For complex systems such as an aircraft, the relationship between the various component models and the system is critical. The specification of a voltage level for a component (e.g., a radar) will have a cascading effect on other components, such as a battery, wiring, connectors, and also in other calculations such as center of gravity and mass.

Semantic associations of a model which could be derived or interrogated by the user would increase the reusability of models by providing insight into the relationship of one model to another.

Syntax and semantics also have a major influence on the model and simulation consistency. Kuester and Engels (Kuester & Engels, 2004) describe the issue of consistency with the syntactic and semantics aspects. The authors stated that they "… can make a distinction between syntactic consistency and semantic consistency. Concerning horizontal consistency problems, syntactic consistency ensures that the overall model consisting of submodels is syntactically correct. With regards to vertical consistency problems, syntactic consistency ensures that changing of one part of the model within the development process still results into a syntactically correct model. With respect to a horizontal consistency problem, semantic consistency requires models of different viewpoints to be semantically compatible with regards to the aspects of the system which are described in the submodels. For vertical consistency problems, semantic consistency requires that a refined model is semantically consistent with the model it refines."

In the increasingly common use of distributed simulation, consistency becomes more problematic. Anthony, et al. (Anthony, et al., 1994) state that "it is generally more difficult to check and maintain consistency in a distributed environment. Forcing consistency tends to restrict the development process and stifle novelty and invention. Hence, consistency should only be checked between particular parts or views of a design or specification, and at particular stages, rather than enforced as a matter of course." The semantic relationship of the models in the distributed environment might provide a pathway for developing consistency checking in this simulation domain. Research topics include ontological model descriptions and relationship mapping.

Context Management

Context as defined by the Merriam-Webster dictionary is the interrelated conditions in which something exists or occurs (e.g. environment, setting). For the development of models and simulations, there should exist a contextual framework which captures key model and simulation attributes. From a reuse standpoint, the contextual framework is essential for proper understanding of why the model was developed and how it was expected to be used.

A potential list of attributes that make up a contextual framework for a model might include:

1. Assumptions: what has been taken to be true?
2. Constraints: what conditions or restrictions have been applied to construction or use?
3. Intention: what was the purpose for which the model was developed?
4. Usage risk: what are the established and generally accepted application boundaries?
5. Model fidelity: what is the accuracy with which the model replicates the original?
6. Trust / Confidence: what measure can be used to assure the user of proper operation?
7. Pedigree / provenance: who constructed or altered the model, what was changed, why was it changed, how was it changed, when was it changed?

The contextual framework provides the user community with enough information to make informed decisions and this is a critical aspect in model reuse. In general, very little information is available with models, including ones which might be used to determine a life or death situation. It is an anecdotal assumption that many models in use today were developed by someone who is dead and no one knows how the model was constructed. Reconstruction of the contextual framework can be done to some extent, but will only result in a partial set of knowledge. Techniques for automatic context generation are needed.

Domain Knowledge Extension for Collaboration and Enhanced Decision Making

The primary use of models and simulation is to understand or convey information concerning a thing, process, or theory. The end product is a decision by the user as to the credibility of the model or simulation. The decision maker, whether an individual or group using models and simulations as a decision aid must therefore believe that the results are reflective of the domain of interest. In cases where the model is obviously incorrect (e.g., water flows uphill), the results would be discarded by the decision maker. However, when the model or simulation provides what appears to be a correct result or at least a result which on the surface appears correct, how much credibility should be attributed to the model output?

Blatting, et al. (Blatting, et al., 2008) make the case that "… since credibility is subjective, different decision makers may well assign different degrees of credibility to the same M&S results; no one can be told by someone else how much confidence to place in something. The assessment of M&S credibility can be viewed as a two-part process. First, the M&S practitioner makes and conveys an assessment of the particular M&S results. Then, a decision maker infers the credibility of the M&S results presented to them in their particular decision scenario."

The previous sections have outlined areas in which the practice of modeling and simulation might be improved by research in certain areas. Knowledge management is an important aspect of the use and reuse of models and simulation as a decision making process.

Reuse Through Model Discovery

Scudder, et al. (Scudder, Gustavson, Daehler-Wilking, & Blais, March 23-27 2009) made the case that discovery would be achieved only through consistent and relevant metadata which in turn requires consistent labeling and a markup syntax. The basic concept is similar to other data discovery approaches which rely on the developer community to adhere to a defined set of rules for describing their models. A problem with standardizing model descriptions is getting agreement across modeling domains.

One definition of a model is representation of something (e.g., a system or entity) by describing it in a logical representation (e.g., mathematical, CAD, physical). The nature of the representation leads to the problem of discoverability as a form of the description. For example, how would you embed the necessary information in a mathematical model that would allow for discovery? The use of an indirect association (think of a catalog) would provide an access point but would also require a governance process that would maintain the associations as more models are added or if the models change.

Taylor et al. (Taylor S. , et al., 2015) identified another aspect of reuse which is that some models would require specialized knowledge to use. As models have become more ubiquitous, the model interfaces have become easier to use. When the user was required to construct a very specific formatted file of input data, they had to understand the data and how it would be used in the model. With the graphic interface, it is easy to construct a model that anyone could run, but that doesn't insure that the output results would be valid. In addition, if the user discovered six models purporting to provide the same answers, how would the user determine which model is the best or most accurate?

The same authors make the case for reuse through standard ontologies and data models. The development of ontologies can be problematic due to the need for consensus among the domain subject matter experts. The initial barrier of developing the ontologies is outweighed by the significant gain in reuse and composability due to inherent relationship mapping.

6.3 Advancements in the Social, Behavioral and Cultural Aspects of Reuse

Even when all the strictly technical challenges of reuse have been resolved, social, behavioral and programmatic barriers may still prevent realization of the full potential of reuse. The social and behavior challenges identified in this subsection must be addressed with, if not ahead of, the technical challenges identified in the rest of this section of the report. There will be no substantive progress against the reuse challenge as a whole if the current workforce members who are most successful or influential within their respective domains are not concerned about M&S as a larger discipline. All of which is unlikely to happen unless funding comes to pay people to work the larger, broader, philosophical, and theoretical understanding of models, what they are, and how they work.

This subsection addresses identifying and teaching the skills necessary for a model or simulation producer to increase the ease of reuse by others if the producer (person or organization) chooses to and can afford to do so. So long as designing and documenting for reuse are not required and funded, these actions will be difficult to justify in the current contractual M&S culture.

In comparison to research on technical challenges, research in this area will require human experimentation, e.g., design of educational materials and testing of efficacy. Some challenges in this area may benefit from research into mental models of software users and developers in other communities including the open source community.

Programmatic

The lack of representation of non-DoD M&S domains in the ongoing conversation about reuse necessarily narrows the scope of knowledge and success that can be expected. Before addressing governance and ROI, it may be productive to survey other M&S domains concerning their status, needs, and challenges in the programmatic area.

Governance

The US federal government and especially the Department of Defense (DoD) are significant consumers of M&S, and commensurately stand to benefit the most from increased reuse. Federal procurement and acquisition policy currently rewards non-reuse behavior and, in some ways, punishes[1] design and implementation for reuse. While the resolution of these issues is outside the scope of technical research, recognition of them is key when considering mechanisms for improving social and behavioral aspects, especially for identifying the strict limits policy imposes on the efficacy of activities to shape behavior change. The CNA report (Shea & Graham, 2009) is a good source for understanding this issue. This barrier may not exist or be considerably lower outside the federal government market place.

Return on Investment (ROI) / Cost Benefit Analysis

Decision makers often ask about a new endeavor, "What's the ROI?" Answering this question in a manufacturing context where there are clear metrics of increased cost for process changes and (presumably) reduced unit costs is straightforward. The answer is considerably less clear in a

[1] Title 31 U.S. Code § 1301 restricts the use of current funds to fund future anticipated, but not yet realized, requirements.

context of cost avoidance, and where the precise cost of producing a model or simulation without reuse might be unknowable. The research challenges in this area include:

1. Defining a broadly acceptable framework for performing cost benefit analysis for reuse that does not rely on unknowable metrics.

2. Recognizing that different domains may have different mechanisms of practice, i.e. different protocols for reuse. These differences might lead to differing measures of effectiveness and / or methods for assessing effectiveness.

Risk and Liability

The risks and liabilities of reusing M&S developed by other organizations and / or for other domains and intended uses are too numerous to cite here. The challenge in this area is to determine where existing legal precedent applies and where new law must be established, an enterprise that can only be undertaken in collaboration with legal professionals, not by technical experts alone. Technical experts may contribute to this undertaking by providing and developing appropriate mechanisms for assessing the technical aspects of risk and failure. A notable example of extant work in this area is the Risk Based Methodology for VV&A (The Johns Hopkins Applied Physics Laboratory, April 2011). Intellectual property (IP) rights are also a consideration in this area. A user may discover the need to modify a reusable asset for their specific intended use. Without acquiring appropriate IP rights prior to reusing the asset, the user will have (unintentionally) accepted a risk or liability that is costly to mitigate. The CNA report (Shea & Graham, 2009) covers this topic in some detail.

Social and Behavioral

Motivating Behavior Change

Recognizing the constraints imposed by governance, reuse can only succeed through shaping changes in stakeholder behavior and decision making regarding reuse.

Specific research challenges associated with the social behaviors of producers, consumers, integrators, and decision makers necessary to build and sustain a viable community of reuse include:

1. Design for reuse

    a. What reward structures and / or response costs encourage this behavior? Could approaches such as gamification create a positive feedback loop between individual and group behavior?

    b. What skills and / or techniques are necessary to achieve reusable designs?

    c. What infrastructure and mechanisms are necessary to provide constructive feedback to designers of reusable assets?

2. Documentation for reuse

    a. Even when an asset is designed for reuse, failure to provide sufficient documentation, especially discovery and composition metadata, limits its reusability. It is not uncommon for software developers to resist producing sufficiently detailed and informative documentation once the code is working. The lack of documentation impedes verification and validation (V&V), and subsequently, reuse. The challenges in this area are similar to those in design for reuse, but require separate consideration.

3. Reusing / adoption of reusable resources
    a. What reward structures / incentives encourage this behavior in the absence of governance constraints?
4. Implied threat of reuse to potential stakeholders
    a. Reward structures and incentives represent the positive side of encouraging reuse, but reuse can also represent an implied threat to potential stakeholders, e.g. loss of funding, control, and / or perceived status. Research in this area needs to identify implied threats, and assess whether rewards and incentives can counteract them.
    b. While trust may not directly counteract perceived threats, it may ameliorate them. In this context, trust applies to individuals, organizations, accuracy of metadata, and quality of reusable assets.
5. Different levels / types of motivation and concerns
    a. Research in the preceding areas must account for the fact that different stakeholders will have different levels and types of motivations and concerns.

Education and Outreach

Finally, the results of the research described in the preceding subsection must be delivered to the target audience(s) and measured for efficacy. This research should address the varying challenges of identifying target students, delivering effective education, and measuring its efficacy based on the students' roles within a community of reuse:

- Producers
- Consumers
- Integrators
- Decision makers / policy makers

The education and evaluation process should investigate various outreach mechanisms including expert endorsements, and social media and networking. The LVCAR Asset Reuse report (APL, 2010) describes several such mechanisms.

Impact

Addressing the research challenges identified in this subsection has the potential to achieve the following positive impacts:

- Creating a verifiable body of knowledge and standardized processes for calculating the benefits of reuse
- Motivating a culture of reuse and rewarding stakeholders who engage constructively
- Providing stakeholders with constructive methods for overcoming resistance

The cultural norms resistant to reuse are entrenched and unlikely to change without arming individuals motivated to change it with concrete tools.

7 Concluding Remarks

Long established as a critical technology in the design and evaluation of systems, modeling and simulation is now at a critical crossroads. M&S technologies face increasing challenges resulting from the scale and complexity of the modern engineered systems that need to be designed, understood, and evaluated. At the same time, technological advances offer the potential for M&S technologies to not only meet these challenges, but also to provide even greater value in new areas such as the management of operational systems than is offered today.

As articulated in this document, advances in *conceptual modeling* are needed to provide a common language for experts in different disciplines to come together to create, analyze, and manage the complex systems that arise now, as well as those that will be created in the future. Means to transform these specifications into computer models and in many cases, operational components are needed. Advances in *computational methods and algorithms* are essential to handle the scale and complexity of modern systems as well as to exploit new technologies now arising from big data, the Internet of Things, and cloud computing to provide pathways for M&S to provide even greater benefits and value afforded by these other emerging technologies alone. Methods to better *understand and manage uncertainty*, backed with rigorous underlying theories are sorely needed to enable effective utilization of the capabilities provided by M&S. Finally, advances in the *reuse of models and simulations* can dramatically reduce the costs and timelines necessary to exploit M&S, especially in its application to engineering complex systems. Advances in these four areas will have far-reaching impacts in critically important areas such as the growth and development of cities, the realization of effective health care systems, the development and establishment of new approaches to manufacturing, the development of advanced aerospace systems, and development and acquisition of more cost effective defense systems.

While this report has focused primarily on key research challenges, it is clear that there are other essential ingredients necessary for advances in M&S to result in new value and impact in society. A highly trained workforce is essential to both develop technological advances and transform them into practice. Education programs are broadly needed that address both advances in M&S technologies as well as their practical usage and application. Mechanisms are needed to provide the means and incentives to transform technological innovations into economic growth and development through the creation of new businesses and infusion of technology advances into existing ones. While the M&S industry is substantial today, it will become even more important and critical to economic development in the future.

It is clear that through the Internet, social networks and other advances, the world is rapidly becoming more interconnected and complex, and the pace of change is quickening. While M&S has served society well in the past, new innovations and advances are now required to enable it to continue to be an indispensable tool to enable deep understandings and effective design of new and emerging complex engineered systems.

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Appendix 1. Workshop Participants and Group Leads

Conceptual Models (Leads: Conrad Bock, Leon McGinnis, Janos Sztipanovits)

Conrad Bock	Leon McGinnis
Steven Cornford	Rick McKenzie
Fatma Dandashi	Chris Paredis
Frederica Darema	Janos Sztipanovits
Paul Fishwick	Irem Tumer
Sanford Friedenthal	Adelinde Uhrmacher
Drew Hamilton	Hans Vangheluwe
Nathalie Harrison	Eric Weisel
Steven Jenkins	Lin Zhang
Traore Mamadou Kaba	

Computation (Leads: Richard Fujimoto, Charles Macal, David Nicol)

Chris Carothers	Madhav Marathe
Alois Ferscha	Pieter J. Mosterman
Richard Fujimoto	David Nicol
Teruo Higashino	Simon J E Taylor
David Jefferson	Chuck Turnitsa
Margaret Loper	Hamid Vakilzadian
Charles Macal	

Fidelity and Uncertainty (Leads: Wei Chen, Jitesh Panchal, Marty Wortman)

Sez Atamturktur	Tina Morrison
Osman Balci	John Tinsley Oden
Wei Chen	Jitesh Panchal
C. Donald Combs	Michael Pennock
George A. Hazelrigg	John Shortle
George Kesidis	Gabriel Terejanu
Zhongming Lu	Martin Wortman
Natesh Manikoth	Michael Yukish

Reuse (Leads: Ernie Page, Al Jones, Andreas Tolk)

George L. Ball	Mikel Petty
Randall Garrett	John Rice
Al Jones	William Rouse
Edward Kraft	Andreas Tolk
Roman Lysecky	Sandy Veautour
Imran Mahmood	Marjorie A. Zielke
Simon Miller	Philomena Zimmerman
Katherine L. Morse	Ty Znati
Ernie Page	

Applications (Leads: William Rouse and Philomena Zimmerman)

Appendix 2. Workshop Program

Wednesday, January 13: Generating and Organizing Ideas

7:30	Registration / breakfast
8:30	Welcome / Introduction, Chris Paredis, National Science Foundation and Richard Fujimoto, Georgia Institute of Technology
9:00	"Gigatechnology: Developing Sustainable Urban Infrastructure to Solve Gigaton Problems," John Crittenden, Georgia Institute of Technology
9:30	"Increasing the Impact of M&S on Health and Healthcare: Formidable Challenges and Realisable Opportunities," Donald Combs, Eastern Virginia Medical School
10:00	break
10:30	Break Out 1 (Conceptual Models; Computation; Uncertainty/Fidelity; Reuse) *Goal: Generate M&S research challenges related to the break out group. Intended to be a brainstorming session, the goal is to generate many ideas.*
12:00	lunch
1:00	"Some Lessons Learned from DARPA's Adaptive Vehicle Make Program" Michael Yukish, Penn State University
1:30	"Three Viewpoints for Analysis and Synthesis in Systems Engineering," Steven Jenkins, Jet Propulsion Laboratory
2:00	"Modeling of Complex Systems in the Complex Defense Enterprise" (Edward Kraft, U.S. Air Force)
2:30	break
3:00	Break Out 2 (Conceptual Models; Computation; Uncertainty/Fidelity; Reuse) *Goal: Continue generation of research challenges, cluster and consolidate these challenges into four or five major research challenges*
4:30	Day 1 wrap up
5:00	Mixer / Reception (Front Page Restaurant)

Thursday, January 14: Building Consensus Around a Common Research Agenda

7:30	breakfast
8:30	Reports from Day 1 break out sessions: summarize major research challenges (15 minutes per break out group); discussion
10:00	break
10:30	Break Out 3: (Conceptual Models; Computation; Uncertainty/Fidelity; Reuse) *Goal: Complete discussions from the first day; develop descriptions of sub-challenges within each major challenge, develop recommendations to be included in the workshop report.*
12:00	lunch
1:00	Break Out 4: (Conceptual Models; Computation; Uncertainty/Fidelity; Reuse) *Goal: Wrap Up discussions. Each break out session should develop an outline for one chapter of the workshop report and develop writing assignments as needed to complete the report after the workshop. Discuss next steps (e.g., sessions in conferences or other meeting or other ways to further disseminate workshop results).*
2:30	break
3:00	Reports from Day 2 break out sessions (10 minutes each); discussion
4:00	Adjourn, except workshop steering committee and writing leads
4:00	Planning meeting (steering committee and group leads only)
4:30	End of workshop

Appendix 3: Research Challenge Proposals

The following are research challenges suggested by participants prior to the workshop as areas meriting further discussion at the workshop.

Conceptual Models

The research opportunities and challenges should lead to improvements in how we do the following:

- specify, design, implement, verify, validate, execute, interpret, maintain, reuse, integrate, and manage models, model inputs, and execution results;
- that support characterization, prediction, and other analysis;
- of increasingly complex systems, processes, phenomena, within diverse domains of interest.

The proposed research challenge is to improve our ability to evolve models so they become part of an expanding body of knowledge, rather than creating standalone models with little connection to other knowledge sources. This requires connecting models with other models in a broader context, and to evolve models with increased fidelity. The following are two specific challenges in support of this general challenge:

- Formalize the approach to conceptual modeling that includes modeling methods, languages, and standards. A well-defined conceptual model based on standards provides the foundation to specify, validate, integrate, and evolve the knowledge that is encoded in simulation software. For example, the conceptual model can specify the properties, interfaces, and behaviors of entities being simulated before committing to detailed software design and implementation. This conceptual model can be integrated with other conceptual models in a broader context, or be elaborated to develop higher fidelity models as the need arises.
- Develop model management approaches including methods and standards to manage the conceptual models, simulation software, and simulation results across highly distributed and heterogeneous development and execution environments. The approach must clarify how to manage change due to version and variants with complex interdependencies across the models and knowledge sources.

Thoughts on critical M&S research challenges

My research is focused on simulation in the domain of discrete-event logistics systems (DELS), such as warehouses, factories, supply chains—systems through which discrete units of "product" flow and are transformed by "processes" which are executed by "resources". In this domain, simulation is essential to support distributed, multi-disciplinary decision making at all scales, from real-time, to tactical, to strategic, to system design, but it is not used nearly as much as it should be, due to the time, cost, and reliability of contemporary simulation practice. Some of the most critical research challenges include:

1. In contemporary practice, even when the system simulation requires no "new knowledge", the simulation model itself is still largely hand-built and *ad hoc*, with all the negatives implied, including excessive time and cost for the simulation results, inconsistency in application, and difficulty of re-use. The challenge is: "How can we make the use of simulation for analyzing well-understood DELS as cheap and fast as FEA analyses of solid models?"
2. In the DELS research literature, there is a giant void in terms of theoretical model interoperability, whether in terms of integrating analyses across scales of granularity (either physical or temporal) or in terms of integrating different types of analyses (e.g., simulation, queuing analysis, and optimization). The challenge is: "How can we achieve interoperability across different analytical models of the same DELS instance?"
3. The prevailing paradigm in discrete event simulation languages is the queue, with control exercised as a release decision using only local information. Intelligent control of DELS requires a much richer fundamental semantic model, which today can only be realized through *ad hoc* programming in the simulation language's underlying implementation language. This essentially guarantees there will be no long term learning, and certainly no sharing across the community of users. The challenge is: "How can we architect a simulation modeling language that provides native support for the kinds of complex decision making necessary in contemporary DELS?"

Model Engineering for SoS

Model Engineering is the general term of theories, methods, technologies, standards and tools relevant to a systematic, standardized, quantifiable engineering methodology that guarantee the credibility of the whole lifecycle of a model with the minimum cost.

Challenges in development and management of SoS models:

Although importance of the engineering idea is gradually recognized in applications of the full model lifecycle, currently no complete theory and technology system and philosophy is available. So there are still lots of challenges in the lifecycle of the model of SoS.

(1) High complexity of the referent SoS

(2) The long life cycle of a SoS

(3) Model heterogeneity

(4) Complicated evolution of models

(5) Difficult model reuse

(6) Massive processing data

(7) The multidisciplinary collaborative model development

(8) Higher requirements for system performance

A systematic methodology is needed to cope with challenges in model lifecycle management of a SoS. The model development and management activities change from a spontaneous and random behavior to conscious, systematic, standardized and manageable behavior by constructing a model engineering theory and methodology system in order to guarantee credibility of different model phases.

There are two key challenges for modeling dynamic systems conceptually: model engineering and personalization. Model engineering is figuring out how to proceed, in incremental phases, within a modeling process. How do we begin and how do we gradually form models? Given that verification and validation will always feedback into the model design activity, this leaves open how models are designed. Modelers hypothesize the structure of their models in some form. For example, a model may be defined as linear or it may be a directed graph of concepts. Many model types that we use in M&S are described in a complete syntactical form rather than as a model engineering activity indicating temporal progression. Forrester's System Dynamics (SD) is unusual since not only are there specific model types in SD, but these types are defined as incremental structures, evolving from one form to the other. Can this same model engineering approach be used for other M&S model designs? Would we begin with concepts and generate a concept map, semantic network, or an ontology? The second modeling challenge centers on personalization. News is routinely made personal either through viewer profiling, or by the viewer making topic selections. Can this personalization be made to happen in model design? Some models would be "soft" or conceptual, often with different media. So, the personalization challenge will intersect with user experience (UX) design. How will model and UX designers work together? If M&S is to obtain broader impact, we need to spend time considering many ways of experiencing models, as well as their simulations.

We believe that the single most important change to achieve correct-by-construction design is the introduction and systematic use of *cross-domain modeling*. However, creating design tool chains that cover all potentially relevant modeling abstractions in complex systems and satisfy the needs of all application domains is unrealistic. In addition, tool chains that are highly configurable to specific application domains are not available. Consequently, a more realistic objective is to develop horizontal integration platforms that allow the rapid construction of end- to-end modeling and simulation tool suites in domain-specific configurations. The OpenMETA integration platforms in DARPA's Adaptive Vehicle Make program are shown in Figure 1.

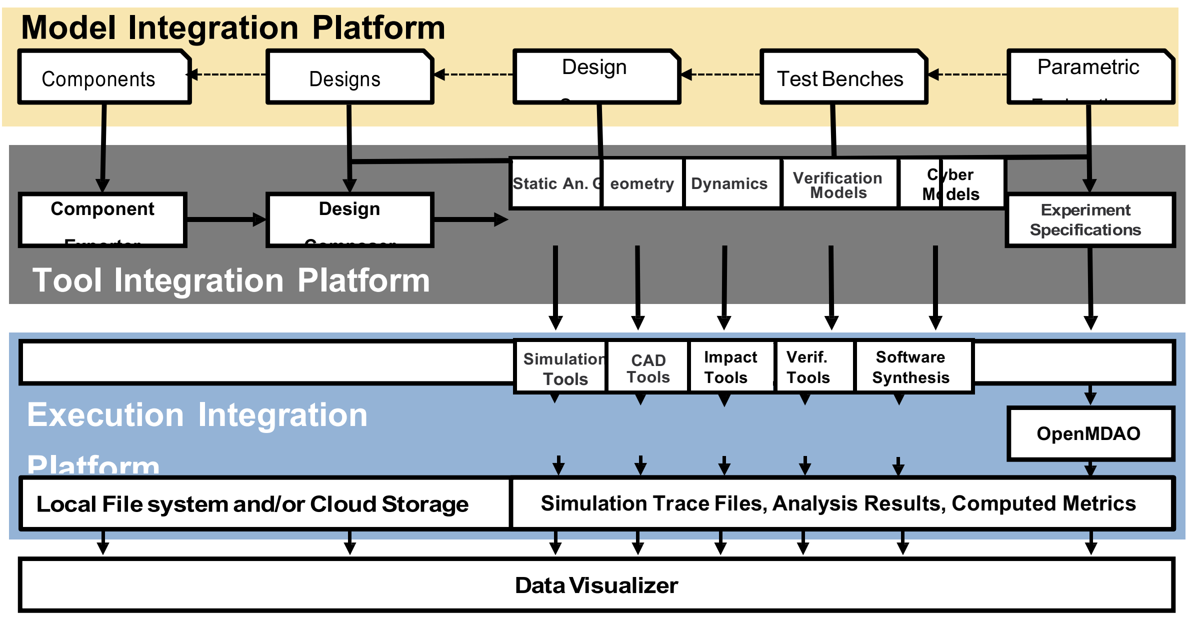

Figure 1: OpenMETA Horizontal Integration

While significant progress has been achieved during the development of a prototype system, some of the challenges requiring further research are the following:

1. Extension of the mathematical foundation of Model Integration Languages used in the Model Integration Platform.
2. Improved adaptivity in the Model and Tool Integration Platforms including support for goal- directed model composition tool reconfiguration.
3. New architectures, deployment methods and resource management for Execution Integration Platforms

(1) Common Virtual Proving Ground

Understanding complex systems requires large-scale distributed and seamless transdisciplinary integration of knowledge components into a common, shared, composable, extensible, persistent modelling and simulation enterprise.

How can the international community launch a common conceptual modelling enterprise? How can a conceptual model be opened, shared and advertised? How can it be augmented with knowledge contributed from everyone (like Wikipedia)? What guidance and education must be provided to the contributors? How does it need to be managed? What parts need to be secured and how can it be open and secure (e.g. forge.mil)? What structure should the conceptual modelling framework adopt (ref. https://www.cso.nato.int/pubs/rdp.asp?RDP=RTO-TR-MSG-058)? What base ontologies are required (ontology of physics, etc.)? How can the conceptual model components become executable model repositories and be plug and play into simulation architectures? How can the simulation conceptual model transcend seamlessly with reality to enable Live-Virtual-Constructive simulation applications, augmented reality, augmented virtuality, crystal ball applications, etc.?

(2) Transdisciplinary Simulation Architecture

Complex systems simulation requires seamless cross-domain interaction in order to observe emerging effects (e.g. Critical infrastructure protection requires connecting: country, power grid, internet, economy and military command and control; Combat vehicle survivability requires connecting: bones (human), metal, optics, electromagnetics, acoustics, cyber, etc.)

How can simulation architectures connect models that respond to different sets of laws? What mechanisms are required to efficiently interact between different sets of laws (e.g. layered architectures)? What algorithms can model these systems accurately in a non-chaotic and realistic way? What level of detail is enough to see emerging behaviours when integrated? How emerging behaviour revealed by simulation insert in the global scientific method for validation?

(3) New Simulation Computational Paradigms

Complex systems simulation pushes computational load, interactivity and distribution above current limits.

How challenges (1) and (2) could be better served with novel simulation computational paradigms (e.g. GPU computing, quantum computing and cloud computing)?

One challenge in modeling and simulation is make modeling accessible to engineering domain experts at the same time the resulting models are formal enough for automatic simulation. Engineers are typically not trained in formal verification and often prefer modeling terminology and concepts that seem far removed from formal methods. A key hurdle in addressing this is to link engineering concepts and terminology with formalizations in a way that does not require engineers to learn all about these formalisms. This requires modeling languages to be developed in layers that expose engineering-friendly concepts, with mathematical formalisms underpinning them to support automatic verification.

Conceptual Modeling - On the one hand, conceptual modeling is typically considered as the step before a certain formalism is chosen to represent the model formally, as one of its purposes is to lay the foundation to select a suitable formalism. On the other hand conceptual modeling refers to the concepts of the system to be modeled, like the basic entities, causal constraints etc. The conceptual model is also the subject of discussing and clarifying the concepts and constraints underlying the model to be built and thus asks for some means of representation. This leads some authors to consider, e.g., DEVS or Petri Nets, as a means for developing the conceptual model blurring the distinction between conceptual and formal model.
Domain specific modeling languages map central concepts of a particular application area to modeling constructs and combine those with a formal semantics. Thus, their increasing use might threaten the distinction between conceptual and formal model even more so. Thus, it appears timely to clarify what we expect from a conceptual modeling phase and how supporting this conceptual modeling could look like.

Model Reuse **-** Reuse of models by a third party is connected with specific requirements: an essential one is that the meaning of a model needs to be clear. Therefore, information about the semantics of a model (by means of mathematics or by a formal modeling language), its parameters (and their sources) and initial conditions, but also about algorithms used to execute the model, and further information how the model has been validated are central.

To facilitate model reuse the modeling and simulation publishing culture needs to change (at least in some areas), i.e., to include all information needed to reuse the model. Unambiguous means for annotating models with this kind of information would in addition allow exploiting computational support for reusing models which is highly desirable.
Therefore, description standards and ontologies are important, similarly as automatic means to generate, read and evaluate these annotations.

Some application areas appear more advanced when it comes to supporting the reuse of models, e.g., in terms of the information about models that need to be included in a paper to be publishable, and also in terms of curated model repositories, standards for describing models, and for describing experiments. Can those developments serve as blueprints for other application domains and how far are we referring to an automatic reuse of models?

What is the scope of M&S?

The open questions that M&S, as a discipline, is to address require a form other than "build a model of" – this is all of science. At the core, we need to differentiate between the science of modeling and the science of simulation and develop theory that enables the "build a model of" activity for the scientists who are doing so using M&S in their fields. So, along the simulation theory axis, we need to develop simulation science vice science that uses simulation; and likewise for modeling theory.

Develop a unified theory for simulation formalisms

In the strictest sense, formalism means the application of formal logic and proof theory to the objects studied by a particular science. In practice, however, most scientists rigorously apply a more informal logic in their proofs. Peer review confirms the results, or not. Likewise, within simulation science, formalism, or a formalism, usually means a mathematically rigorous approach to studying the simulation object. Several structures have been studied as formalisms, however, there is little consensus on the best approach. In the same way that the various models of computation provide a basis for theory within computer science, considering the various formalisms as models of simulation will further the development of a robust theory of simulation.

Develop a theory for model-based decision-making

Although recent work in validation theory is looking hard at the implication of risk on the simulation use decision and propagation of error in simulation is getting well-deserved attention, more basic research is needed to develop a robust model-based decision theory. Accuracy is well-understood, particularly in the context of physics-based models, but use is not well-defined. Within the context of the decision whether or not to use a simulation to inform a decision, acceptability criteria are often subjective and little theory exists to objectify the decision analysis. A well-developed model-based decision theory will place the validation concept in the language of decision theory, define use in a rigorous way, clearly differentiate objective from subjective elements of the use decision, and provide a defensible basis for using models and simulations to inform decision-making.

Computation

Topic 1: Use of Petascale and Exascale computing to simulate massive socially-coupled network of networks.

Socially coupled systems are usually composed of network of networks. Furthermore these networks vary in time, are highly unstructured and co-evolve Thus traditional methods for scaling motivated by simulations of physical systems are unlikely to work well. These networks lack typical notions of symmetry.

Q1: How does one load balance such systems?
Q2: How can one incorporate interactivity?

Topic 2: Calibration, UQ, SA, Validation and Verification of models to study massive socially-coupled networked systems

V&V continues to be an important question. Traditional methods for V&V that are based on physical laws are often not applicable when studying such systems as they are governed by human behavior, law and norms.

Q3: How does one build simulations for such systems that allows decision makers to have confidence in the outcomes.
Q4: Collecting more data is not the answer. What sort of theories can be developed here. Social sciences has worked on this problem but the a computationally motivated social theory might prove very useful.

Topic 3: How can one synthesize realistic socially coupled networked systems

Developing such network representation is challenging as data is sparse, time lagged and system is constantly evolving.

Q5: Availability of new emerging data sets is very promising but poses new challenges on integrating them meaningfully
Q6: Role of privacy and security are paramount for such systems and need to be further addressed.

Autonomous car is becoming realistic in the near future. It needs to be utilized in not only motorways but also in urban areas such as New York where many people and vehicles come and go. In the world, we need to consider more heavy traffic environments with much higher pedestrian and vehicular density (e.g. Beijing and Tokyo). Not only sensing information obtained from cameras and sensors installed under urban environments, those monitoring city traffic environments from moving vehicles, bicycles and pedestrians need to be used for constructing more secure and efficient traffic environments. Advanced simulation technology for building such an intellectual urban traffic environment in real time should be studied (challenge 1).

In the real world, sensing information might be able to be obtained for several hundred meters' areas (micro areas) and they can be used for modeling urban environments in the micro areas. On the other hand, sensing information from such micro areas might be combined and used for building much wider areas' urban models (macro areas). We need to study methods for hierarchically urban modeling from micro areas to macro areas, and vise verse (challenge 2).

In the above urban traffic environments, we also need to study modeling and simulation techniques to support socially vulnerable people with handicap and elderly people (challenge 3).

1. **Challenges Related to PDES**

PDES has been used to simulate complex systems, and turns out to be a very powerful tool. However there are still notable challenges in runtime efficiency and ease of use in applying PDES to engineering complex systems. We think the following questions should be addressed primarily.

(1) Emerging hybrid architecture, e.g. multi-core CPU + MIC, multi-core CPU + GPU, even multi-core CPU + DSP, has been used to construct the underlying platform for PDES. What is the best general structure and parallel mode when using PDES on these platforms? How to make best use of the capability of these hybrid platforms, how to exploit parallelism as much as possible with adherence to the local causality constraint, and how to accomplish automatic parallel execution on these platforms?

a) How to accomplish automatic decomposition, distribution, data preparation and parallel execution of computation missions in MIC, GPU and DSP-based accelerators.

b) Mechanism and algorithm that manage the collaboration between CPU and accelerators, and balance the communication and computation load between CPU and accelerators.

c) How to adapt existed synchronization algorithms to these new platforms? Are there some new and more efficient algorithms？

d) Does present event scheduling and management mechanism need to be changed a lot?

(2) To advance PDES applications, is it possible to propose a PDES programing specification that can be widely accepted by PDES community? The specification is to hide the details of underling hardware and software, and provide a standard for developers to construct PDES applications by models which are in library format.

(3) To support reuse and rapid-composition of models, a widely-accepted model specification which specifies the implementation restraints and external interfaces is needed, so that models can be independently developed, packed, fast assembled and platform-independently reused.

(4) Is it possible to specify a standard validation process (including prospectus, methods and criterion) for various types of conceptions and functions of conceptual model? A model is considered as credible(high fidelity) only if it passed the specified validation process.

2. **Challenges Related to Cloud Simulation**

How do models exist in cloud environment if MasS (Model as a Service) is intended? A descriptive specification of models is needed for searching and understanding models in cloud environment. How to implement a cloud-based simulation platform, which makes it easy to construct large scale simulation applications (e.g. PDES applications) by models and run efficiently in cloud environment? How to achieve efficient interaction and synchronization among models in cloud environment?

3. **Simulation and Big Data**

Is it possible to classify Big-Data-based modeling and achieve automatic modeling from big data? How to accomplish model checking and validation for these kinds of models?

A key observation in the "**post digital revolution society**" is that information and communication technologies (ICT) has become interwoven with human behavior, the "fabric of everyday life" and social structures to such an extent, that the separating view of a "physical world" being connected with a "digital world" is ceasing. Today we talk about **one** "cyber-physical" world (Cyber-Physical Systems, an NSF program developed by Helen Gill in 2007), referring to a tight entanglements of real world physical objects (things, appliances) and processes (services), with their digital data representation and computations in communication networks (the "cyber"). Embedded, wirelessly connected tiny compute plattforms equipped with a multitude of miniaturized sensors collect data about phenomena, analyze and interpret that data in real time, reason about the recognized context, make decisions, and influence or control their environment via a multitude of actuators. Sensing, reasoning and control, thus, are tightly interconnecting the physical and digital domains of the world, with feedback loops coupling one domain to the other. They implement notions of **autonomous adaptive behavior**.

Taking the plenty-hood of today's ICT platforms with their computational, sensory, reasoning, learning, actuation and wireless communication capacities (smart phones, autonomous vehicles, digital signage networks, stock exchange broker bots, wearable computers, etc.), it is not just considered possible, but already a reality that these are programmed to operate **cooperatively** as **planet scale ensembles of collective adaptive computing system (CAS)**. CAS research asks questions on the potential and opportunities of turning massively deployed computing systems to a globe-spanning super-organism, i.e. compute ensembles exhibiting properties of living organisms, like e.g. "collective intelligence" on their own. Essential aspects of CAS are that they often exhibit properties typically observed in **complex systems**, like (i) spontaneous, dynamic network configuration, with (ii) individual nodes acting in parallel, (iii) constantly acting and reacting to what the other agents are doing, and (iv) where the control tends to be highly dispersed and decentralized. If there is to be any coherent behavior in the system, it (v) has to arise from competition and cooperation among the individual nodes, so that the overall behavior of the system is the result of a huge number of decisions made every moment by many individual entities.

In order to develop a deep scientific understanding of the foundational principles by which CAS operate (see the EU research priority FoCAS, www.focas.eu) we need to address evident **foundational research concerns** like:

i. Understanding the trade-offs between the potentials of top-down (by design) adaptation means and bottom-up (by emergence) ones, and possibly contributing to smoothing the tension between the two approaches.
ii. Understanding the "power of the masses" principle as far as participatory ICT processes are concerned. We need to understand how and to what extent even very simple collective phenomena and algorithms – when involving billions of components – can express forms of intelligence superior than that of traditional AI.
iii. Understanding properties concerning the evolutionary nature of CASs, e.g. open-ended (unbounded) evolutionary systems, the trade-off and interaction between learning and evolution, and the effect of evolution on operating and design principles.
iv. Understanding the issue of pluralism and diversity increase in complex systems as a foundational principle of self-organization, self-regulation, resilience and collective intelligence.
v. Laying down new foundations for novel CAS theories for complex adaptive systems modeling large-scale socio-technical super-organisms (including lessons learned from applied

psychology, sociology, and social anthropology, other than from systemic biology, ecology and complexity science).

In order to develop principles and methods for the design, implementation and operation of globe-spanning CAS we identify **systems research concerns** like:

i. Opportunistic Information Collection: Systems need to be able to function in complex, dynamic environments where they have to deal with unpredictable changes in available infrastructures and learn to cooperate with other systems and human beings in complex self-organized ensembles.
ii. Living Earth Simulation: The provision of a decentralized planetary-scale simulation infrastructure strongly connected to the worlds online-data sources (search engines, power grids, traffic flow networks, trade centers, digital market places, climate observatories, etc.) is needed as a means to enable a model-based scenario exploration in real time - at different degrees of detail, varying time-scales, integrating heterogeneous data and models.
iii. Collaborative Reasoning and Emergent Effects: Reasoning methods and system models are needed that combine machine learning methods with complexity theory to account for global emergent effects resulting from feedback loops between collaborative, interconnected devices and their users.
iv. Awareness: Whereas today's context-aware systems are able to make sense of the activity of single users and their immediate environment, future systems should be able to analyze, understand and predict complex social phenomena on a broad range of spatial and temporal scales. Examples of the derived information could be: shifts in collective opinions and social attitudes, changes in consumer behavior, the emergence of tensions in communities, demographics, migration, mobility patterns, or health trends.
v. Cases: Look at the specifics of design, implementation and operational principles rooted in the very nature of application domains of societal relevancy: e-health eco-systems, fleets of self-driving vehicles, reindustrialization (Industry 4.0), physical internet (intelligent logistics), digital economy, energy management and environmental care, citizen science, combinatorial innovation, liquid democracy, etc.

1) Unification of discrete and continuous M&S: A key challenge in my view is the unification of methods for continuous and discrete simulation. Historically they have been very different, with different software paradigms and different expertise required. Yet more and more we find that the models we have to create for problems of national importance are mixed discrete and continuous. Too often these models are created by *ad hoc* problem-specific techniques that do not generalize and may have a weak theoretical underpinnings.

We really need a unification both at the mathematical level and at the software engineering level. At the mathematical level we need to be able to discretize differential equations into event-driven rather than time-stepped simulations, while maintaining stability, accuracy, and conservation (if necessary). We must allow arbitrary discontinuous state changes to be acceptable as events in otherwise continuous simulations. And at the software engineering level, we need to be able to combine in one parallel framework (a) time-stepped methods, (b) conservative event-driven methods, and (c) optimistic event-driven methods.

2) Ensemble studies: Serious simulation studies require running a particular model many times in an ensemble with different parameters, different inputs, different boundary and/or initial conditions, and different random seeds. The ensemble may be designed for various different purposes, e.g. parameter exploration, parameter sensitivity studies, parameter optimization, probability distribution parameter estimation, uncertainty quantification, etc. The outputs of the ensemble runs will generally be input to some post processing system for validation, statistical analysis, visualization, etc.

Hence, the proper unit of a simulation study is not the individual run, but the ensemble. And the ensemble is ideal for parallel execution since each simulation run in the ensemble is almost always independent of the others.

The challenge, then, is that we need a way to construct a single job that runs an entire ensemble of simulations, and any post processing required as well. The ensemble runtime system needs to be able to allocate file system directories (or database tables) for the inputs and outputs to the individual runs, allocate processors to the various simulations, decide what order they are to be run in, estimate their resource needs, launch them, and handle their normal and abnormal terminations without terminating the whole job. It amounts to building a special purpose parallel runtime system devoted to the support of simulation studies.

M&S Grand Challenges

- Simulation Everywhere
  Despite simulation being successfully practiced across many commercial sectors, it is by no means pervasive. Arguably this might be because it is not "embedded" into school's curricula or lifelong learning in industry. The challenges are therefore (1) can M&S be successfully introduced into schools (e.g. in a similar way to the successes of SCRATCH and similar languages) and (2) can professional development courses be made available to introduce and support M&S in lifelong learning (software vendors have good examples of these – can these be leveraged to develop online credit courses for M&S. In support of this are two parallel challenges – (3) how can M&S be disseminated into areas that do not typically use or fully exploit M&S (areas of healthcare and manufacturing, SMEs, etc.) and (4) how can successful academic/industrial collaboration be supported (e.g. how does a academia and industry understand how to get the best out of collaboration (knowledge transfer).

- What use is reuse?
  Reusability in M&S is arguably well understood in some areas (e.g. defense) but not in others. Is it actually possible to reuse M&S investment in areas such as manufacturing and healthcare? There are a very small number of examples (in manufacturing) where reusability has been very successful. These tend to be data-driven or use "template" models to create simulations. The challenges are therefore (1) where is reusability actually possible and desired from a stakeholder point of view (rather than just making assumptions from a "distance"), (2) what key reusability use cases and demonstrations can be created to best disseminate the "power" of reusability to a community, (3) what underlying technology should be used to create the most flexible approaches to reusability (especially bearing in mind that almost all commercial simulations are created using off-the-shelf simulation software!)

- Cyberinfrastructures for M&S
  As with Big Data there is a growing need for flexible, on-demand high performance computing (HPC) for M&S. There are instances where attempts have been made to provide cloud-based HPC for M&S. However, in Europe there has been significant investment in worldwide e-Infrastructures to provide common federated (single sign-on) high performance grid and cloud computing infrastructures. Several projects have successfully leveraged this investment to provide common HPC platforms for M&S. This work has a major overlap with DDDAS. There is still significant work to do and leads to the following challenges (1) how can US cyberinfrastructure (or indeed e-Infrastructures) be exploited to support M&S, (2) how can these infrastructures be used to support vast simulation experimentation, (3) how can these infrastructures be used to analyze huge amounts of simulation output data, (3) how can these infrastructures be efficiently connected to Internet of Things applications (e.g. Industry 4.0), (4) how can hybrid distributed simulations of reusable simulations be best supported, and (5) what are the key use cases across academia and industry that can best disseminate the impact of these infrastructures?

- *Large-scale simulations on emerging computing platforms*. Hardware performance improvements now arise almost entirely from increased parallelism rather than clock speed improvements. This has resulted in the creation of massively parallel supercomputers containing unprecedented numbers of processors or cores. Modern machines are increasingly heterogeneous architectures including specialized hardware, e.g., graphical processing units. Effective exploitation of platforms containing millions of cores for large-scale simulation applications remains a major challenge in the parallel simulation research community. Many applications that arise in practice are highly irregular, representing another area with major challenges. Cloud computing offers the ability to make parallel and distributed technologies broadly accessible to users without incurring the expense of purchasing and operating high performance computing platforms, but existing cloud platforms present new computational challenges, due to the shared nature of the computing platform and emphasis on high bandwidth communication rather than low latency. The difficulty of developing efficient parallel simulation codes remains a significant impediment to widespread adoption. Domain-specific programming languages designed for efficient parallel execution may help to address this issue.
- *Online decision-making using real-time distributed simulation*. Increasingly the operations of complex systems such as cities are continually being optimized and improved through a cycle that involves data collection, prediction, and action in real time. The emergence of ubiquitous computing, wireless sensor networks, and vast amounts of data enable simulations to be embedded into operational environments at unprecedented scales. Distributed simulation can play a large role in the online management and optimization of operational systems in areas such as transportation, energy, and law enforcement, however much additional research is required to explore these areas.
- *Energy and power efficient parallel and distributed simulation*. Embedded simulation applications such as those described above call for careful consideration of power and energy consumption. Energy consumption affects battery life in mobile computing platforms and power is a major expense in modern data centers. Yet power and energy consumption has received very little attention in parallel and distributed simulation to date. Little is known concerning the power and energy characteristics of parallel and distributed simulation algorithms, nor how to effectively manage these aspects of the program's execution.

Fidelity and Uncertainty

The problems of model calibration, validation, uncertainty quantification, model refinement and experimental design are closely related and they cannot be studied in isolation. The development of methodologies and algorithms for any of these problems needs to be informed by this natural relationship to fulfill the promise of modeling and simulation in accelerating scientific discoveries and decision making. In the following few guiding principles and opportunities are presented as well as the current challenges associated with them.

Model Calibration and Validation. In general, model calibration and validation are seen as an Afterthought to model development. The validation process focuses on characterizing the discrepancy between model predictions and observations usually approaching the model as a black box. While these discrepancies are due to various errors – modeling errors, measurement errors, discretization errors – the main contributor is the inadequacy of the model. Current strategies in calibrating black box models, such as Kennedy and O'Hagan framework based on the external discrepancy, fall short in providing a comprehensive uncertainty representation that can support reliable predictions of unobserved quantities of interest and usually yield biased estimates of physical parameters. The two processes should be developed around the following question: *What entitle us to trust model predictions?* Fortunately, for physics-based models the answer is simple – a set of highly reliable conservative laws (mass, momentum, energy) that shape the construction of the model. However, the final model needs to be augmented with less reliable constitutive models that are not based on first principles, leading to structural uncertainty. This presents an opportunity to develop calibration and validation methodologies based on an internal discrepancy formulation that exploits the source of the model error (see Reference). The internal discrepancy approach removes the constraints associated with the external discrepancy approach: (1) its stochastic solution satisfies physical constraints, (2) it reduces inference bias and under-estimation of uncertainty, and (3) it provides reliable extrapolated predictions for the QoI.

Fast Uncertainty Quantification Algorithms. Bayesian calibrations in the context of internal discrepancy formulation pose a number of computational challenges as it yields intractable likelihood functions. These types of problems are out of reach for Markov Chain Monte Carlo algorithms, as they either require an integration of the likelihood function at every step or to operate in high dimensional spaces. New algorithms are needed to address the problem of calibrating probabilistic models with intractable likelihood functions.

Model Refinement through Automatic Hypothesis Generation. While the location where uncertainty is introduced and should be modeled is clear at this point, the most appropriate form of probabilistic model for the internal discrepancy generally is not. New methodologies based on state-of-the-art machine learning algorithms need to be developed to automatically generate new internal discrepancy models as data becomes available. The correlation structures captured by the newly calibrated model discrepancies can guide future model refinements. This opens the opportunity to perform experimental design strategies to obtain informative measurements with the goal of discriminating alternative models, which brings us full circle back to model calibration.

1. Quantification of various sources of uncertainty that are beyond parameter uncertainty, such as those associated with the modeling and prediction, the design process itself, and the changing market.
2. Consideration of "unknown" uncertainty due to lack of knowledge, e.g., those associated with the emergent behavior of a complex system.
3. How can one trust the quality of data and the underlying model used to quantify the uncertainty, e.g., the use of Gaussian Random Process model to quantify the uncertainty due to lack of data?
4. Computational challenge associated with high dimensionality and high nonlinearity still remains. This challenge is particularly critical for problems that involve uncertainty in both the spatial and temporal domains such as in design of advanced materials systems.
5. Design can be viewed as an information seeking process, the complexity of a design problem will be escalated to designing both the design artifact and the information seeking activities. This is a very complex decision making problem due to its dynamic nature, i.e., decisions made in an early phase will have a direct impact on the subsequent phases. Methods are therefore needed to manage such complexity.

Advancing Regulatory Science In MEDICAL APPLICATIONS:

There is a great need to assess the credibility of models and simulations (M&S) for medical applications in order to expand their use in development, assessment and regulatory evaluation. Furthermore, if we want to foster good science for M&S, we must leverage the expertise in industry, academia and government, and develop a strategy to assess credibility from a sound scientific and engineering standpoint. Establishing credibility for M&S will give confidence to the medical community and enable the advancement and evolution of M&S tools.

There is a generic hierarchy to the development and implementation of M&S, which can be presented as follows:

I. system configuration (e.g., geometry of device, anatomy)
II. system properties (e.g., biological, chemical, physical properties of metals, polymers, tissue, cells)
III. constitutive laws and governing questions, (e.g., nonlinear plasticity, viscoelastic)
IV. system conditions (e.g., inflow wave form, environment)
V. numerical implementation (e.g., discretization, solvers)
VI. model & simulation output (e.g., velocity profile, strain distribution, toxicity)
VII. output validation, where comparators for medical applications could be
    - bench-top test data
    - animal study data
    - clinical data
VIII. determine credibility for predictions in the context of use (COU)

Establishing credibility (the trust in M&S results) follows a similar framework, which includes assessing the pedigree of input data, verifying the software, verifying calculations, validating the M&S outcomes with an appropriate comparator, quantifying uncertainty and performing sensitivity analyses to establish robustness (VVUQ), and assessing the level of VVUQ rigor needed to support the predictions in the COU. While many challenges remain for advancing M&S tools for medical product design and evaluation, developing a methodology for assessing credibility is an essential first step to expanding and increasing M&S efforts in regulatory science and submissions.

1. Often the motivation behind the use of simulation is to study situations for which we have no empirical data. Thus, the typical view of simulation validation as comparing simulation inputs and outputs to empirical data is insufficient. Structural validation is necessary. While this point has been acknowledged in the literature, there do not appear to be an accepted set of principles or standard approaches to guide structural validation of simulations.
2. When modeling and simulating complex socio-technical systems, it is usually necessary to consider multiple distinct viewpoints simultaneously. Examples include an economic view, an organizational view, a physical view, etc. The differences among these views are not wholly attributable to differences in scale. Consequently, the relationships between the different views are not always clear. This can make composing the different views into a single integrated simulation difficult or impossible. Thus, the challenge is how to make inferences about the system under these circumstances. While this has been accomplished on an ad hoc basis, there should be a more systematic approach to doing so.

Reuse

1. There is a critical need for dynamic, automated, and "smart" federated model component registration supported by model's and simulation's meta-data and a framework side (or agent based, self-forming, negotiated/ad-hoc) inferencing or ontologically driven mechanism. For example, a question that arises in section 2.4 of " How can one characterize the uncertainty of a model that is reused (possibly with some adaptations to a new context)?" Simple answer, it starts from developing simple meaningful mathematically based metrics that characterize the model. First syntactical metrics, then semantic, then pragmatic.

There are many branches to addressing this challenge. Another example for a deeper branch...Numerical methods for ordinary differential equations are methods used to find numerical approximations to the solutions of ordinary differential equations (ODEs). Their use is also known as "numerical integration", although this term is sometimes taken to mean the computation of integrals. Most of our models and simulations use some form of numerical methods for approximations, this leads to uncertainties in our solutions. The following questions around uncertainties exist: a.)What uncertainties affect our confidence in predicting outcomes? and b.)What are their impacts on System Level Outcomes? Can we ignore them? (what is their significance in the collective system)

When this thought process is applied at the System of System level additional uncertainties are introduced. As SoS missions often involve new intended uses that are seldom envisioned by the individual system and model developers, these incongruities from the disparate system developers can cause all sorts of various SoS level artifacts and uncertainties. Again, the key questions that eludes the community is "What are their impacts on the System of System Level Outcomes? Can we ignore them? How do we correctly characterize and/or assess SoS a.) additive, b.) compounding, or c.) internally propagated (no greater error but introduces similar size error elsewhere in the SoS) errors".

If this is the case, numerical approximations, high-run count simulations, and other "quicker" lower fidelity solutions have the potential to be leveraged to at least bound the problem space in a quicker fashion and allow more detailed simulations to focus on a very focused area of interest

We ultimately need decision quality data generated by our modeling and simulation systems and fundamental to that discussion what is "good enough" and how to quantify the uncertainty associated with any system representation

2. Model and Simulation and the Human Dimension. The Army has a need to optimize human performance to support the dynamic, asynchronous battlefield of the future. It is establishing a framework and processes to assess, integrate, and synchronize its training and education, science and technology, holistic health and fitness, medical and personnel policies, programs, and initiatives in support of the Army Profession. I believe that this core value applies to all industries and professions and model and simulation is a key enabler to success. This becomes even more critical for our industrial base when you consider the needs, wants, and desires of the "next-generation" of the workforce and the vastly different world view that that generation has compared to previous generations as a results of its data exposure. People are ever industry's most agile, adaptive, and valuable resource. Modeling and simulation technologies remain an essential enabler; however, there are few technological solutions that exist to provide leaders

with a significantly enhanced physical or cognitive edge on the battlefield (for the Army) or in any corporate setting. (from the US Army CAC White paper on The Human Dimension). The cognitive demands on a solider (or any leader) grow more important as strategic uncertainty grows. We need to actively and deliberately engage the modeling and simulation community to facilitate addressing this uncertainty and mitigating it for our Soldiers and leaders.

3. As complex system level behaviors become more dependent on the underlying components, more sophisticated models and simulations are required to gain a deeper understanding of the overall system behavior. As the simulations become more complex, more data is produced and more data analysis is required to draw valid, useable conclusions from the model and simulation runs. Traditional approaches to analyzing large quantities of data focused on data reduction techniques to provide one-dimensional answers, fail to explore all the interconnected behaviors that may exist in the systems. New "big data" technologies developed by industry shift the focus from data reduction to data management and data analytics. The classification and interconnected behavior analysis techniques leveraged by search engine companies, online sales, and other industries can have profound impacts on gaining a deeper understanding of our interconnected simulations and help us understand the additional emerging behaviors of our complex systems. The Defense Science Board report on Technology and Innovation Enablers for 2030, dated, October 2013 identifies big data analytics as one of its key R&D investment opportunities to support anticipation of surprise for the future defense of the Nation. Models and Simulations are key generators of decision quality data that can benefit significantly from the application and understand of big data methods.

1. Pragmatic Composition of Simulation models

Component based model development is quite successful because it favors reuse and simplifies the logical complexity of the modeling process. Model Composability has been studied in depth at syntactic and semantic levels [1] [2] [3] however pragmatic level of composability is still an open research challenge. *Pragmatic Composability* refers to a context based meaningful composition of the components. It evaluates the difference of actual effect of the messages with the intended effect during component interactions. It also evaluates the consistency of behavior of composed components under a specific context. The research of pragmatic level of composability involves in-depth study of computational linguistics, cognitive technologies and contextual computing [4]. An important issue at this level is pragmatic ambiguity. Pragmatic ambiguity arises when the message is not specific, and the context does not provide the information needed to clarify the intent, due to which the components do not interact according to the desired objectives. The pragmatic reuse of components is only valid when the composability is evaluated at the pragmatic level where the components are known to share correct contextual knowledge and resolve pragmatic ambiguities.

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1. Conceptual modeling - Composability is still our biggest simulation (vs modeling) challenge. But its roots are in conceptual modeling; we cannot compose what we cannot model. Rather than address the fundamental problem, individual projects that need this capability at some level are resorting to scope narrowing to be able to deliver the functionality they need when they need it. We must develop the authoritative atomic elements that will form the basis of conceptual models. This is predominantly an issue of funding, political will, and hard work.
2. Selected applications / security – For all the attention cyber security receives as a matter of individual and national security, it's still an isolated domain of modeling and simulation. Most cyber simulations are virtual simulations confined to cyber ranges. Progress is needed on multi-resolution models, constructive models, and interoperability solutions for integrating cyber ranges as assets in federated simulations.

For many modeling and simulation (M&S) developers, questions regarding the future interoperability and composability of their solution are not the main concern during design and development. They design their M&S system or application to solve a special problem and provide a solution. There is nothing wrong with this perception. However, there are many reasons why it is preferable to design interoperability and composability from the early phases on, e.g., by using open standards for the communication of information or by using standardized interfaces to common services. The main driving factor for this is the wish to enable the *reuse of existing solutions*. Why should we invest something into rewriting a solution that already exists? However, models are the purposeful simplification and abstraction of a perception of reality that is shaped by physical, cognitive, and often legal constraints, resulting in a conceptualization that becomes the basis for the implemented simulation. Implementation by itself is a series of choices, compromises, and heuristics. In addition, computer simulation is bounded by decidability and computational complexity. In order to reuse a simulation solution it is pivotal to unambiguously capture the assumptions and constraints on all these levels preferable in machine readable form. Ontologies have been identified to be specifications of conceptualization and are therefore promising candidates to support these endeavors.

The grand challenge to be solved is identifying a formal description that captures all required information to enable reuse of simulation solutions in a new context.

Data-Adaptable Models for Efficient Reuse, Composition, and System-level Optimization: Complex sensing and decision applications operate on vast data streams with dynamic characteristics with context dependent requirements. As the availability and quality of the sensed data changes, the underlying models, simulations, and decision algorithms should continually adapt in order to meet desired high-level requirements. Due to the complexity of such systems, traditional techniques are often incapable of producing a solution that remains optimal, or near optimal, in the presence of dynamically changing data, numerous algorithms exhibiting tradeoffs between computational efficiency and quality. New modeling approaches are needed to: capture available expected data types and data sources, define end-to-end application task flows, specify and discover alternative algorithms for tasks, associate quality metrics for data inputs and algorithmic outputs, specify an algorithm's data and quality requirements to support efficient composition of algorithms across for difference applications tasks, estimate the computational requirements given available computing resources, and

Runtime Optimization of Adaptable Systems: The performance and operation modalities of dynamic data-driven applications are largely dependent on the availability and, importantly, the quality of the incoming data. As these aspects of the data change at runtime, the underlying application should adapt its configuration by implementing more suitable data processing algorithms, or configuring data sensing devices in order to meet performance and quality constraints. Furthermore, the availability and capability of the underlying computational resources may change at runtime, requiring runtime methods to re-optimize the system implementation in response. Efficient runtime optimization methods are needed to ensure near optimal operation across all expected operation modalities. As runtime optimization will incur some overhead to execute the optimization algorithms and to reconfigure the system implementation, the runtime optimization process must be integrated within system-level modeling and design methodologies at the earliest design stages.

- Computationally integrating models at multiple levels of abstraction with differing representational ontologies.
- Assumption management for legacy models developed for one purpose but potentially relevant for new purposes.
- Assessing construct validity for models where predictive validity cannot be reasonably assessed.

Over the last 20 years, modeling and simulation has seen dramatic improvement in concurrent application and the use of HPC systems, but still in very specialized segments. My colleagues and I have been struggling with making M&S more usable across a wider range of disciplines. Our work has been directed at the development of new products in the defense and aerospace industries but is applicable across most industries.

Challenge: Language ambiguity

The major aspect in the use of models across domains is the inconsistent use of language. For instance, there is no truly agreed upon definition of what constitutes a model in such a manner that it is discoverable and easily used within a new environment. Much of this is due to a lack of consistent terminology regarding the description of the model and the inputs and outputs associated with it. Although everyone can agree on how a CFD model is used, each model there is no consistent definition of the inputs and outputs of the model to unequivocally declared the model to be of type "CFD." In addition, if the CFD model requires an input of an aerodynamic surface, how should it be described? A CAD model (what constitutes a CAD model for this purpose?).

Potential Solution: Ontological Representation

Position paper on M&S Research Challenges

Two M&S research challenges remain paramount, in my opinion, in spite of their long history of being designated as grand challenges. They are: reuse and composability (previously mentioned in [1]); and verification and validation (previously mentioned in [2]).

Reuse and composability. Reuse is "using a previously developed asset again, either for the purpose for which it was originally developed or for a new purpose or in a new context" [3]. Composability is "the capability to select and assemble simulation components in various combinations into valid simulation systems to satisfy specific user requirements" [4]. Despite substantial efforts, almost always well-intentioned and well-executed, such as those in [5], reuse and composability have not been fully achieved; indeed, the latter was recently described as "still our biggest simulation challenge" [1]. There are daunting engineering requirements, i.e., an effective and universal discovery mechanism and standardized content and format for software component metadata, identified more than a decade ago [6], that remain unrealized today [1]. There are also unavoidable theoretical obstacles; it has been formally proven that the composition of two valid models cannot be assumed to be valid [7] and the process of selecting components from a repository is NP-complete [8] [9].

Furthermore, we must acknowledge that not all the impediments to reuse and composability are technical. Developing reusable or composable software components is more costly than developing components without those requirements, and the benefits of the resulting reusability and composability often do not accrue to the organization that incurred the initial cost. Using reusable software developed earlier can reduce the cost of a subsequent project, which can counterintuitively be a disincentive to organizations seeking to maximize project size and thus funding level. Clearly, achieving reuse and composability depends in part on a compelling business case (or cases) to motivate them [6].

Verification and validation. Verification is "the process of determining that a model implementation and its associated data accurately represent the developer's conceptual description and specifications" [10]. Validation is "determining the degree to which a model or simulation and its associated data are an accurate representation of the real world from the perspective of the intended uses of the model" [10]. The credibility utility of a model depends on verification and validation [11]. The use of a model that has not been properly verified and validated entails potentially substantial risk. A wide variety of specific methods for verification and validation are available (see [11], [12], or [13] for surveys), but despite this range of methods, not all model validation situations are covered. Even when methods are available, not all simulation practitioners know which methods are suitable for a given model or a given application. This is especially problematic for statistical methods, which are too often applied in situations where the assumptions of the statistical methods are not met.

As with reuse and composability, proper verification and validation of a model are also often impeded by non-technical issues. Verification methods that are suitable and effective are frequently not applied because of time and cost limitations in a development project that has fallen behind schedule. Likewise, although independent verification and validation is recommended by experts, e.g., [2] and [13], too often they are not performed independently, but rather done by the model's developers who despite their best intentions are unconsciously motivated to confirm that their work is correct, and overseen by sponsors who despite their best intentions are unconsciously motivated to show that their investment in the model's development has been a good one.

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