Grand Challenges on the Theory of Modeling and Simulation

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Abstract

Modeling & Simulation (M&S) is used in many different fields and has made many significant contributions. As a field in its own right, there have been many advances in methodologies and technologies. In 2002 a workshop was held in Dagstuhl, Germany, to reflect on the grand challenges facing M&S. Ten years on, a series of M& S Grand Challenge activities are marking a decade of progress and are providing an opportunity to reflect and plan for the future. This second Grand Challenge Panel brings together a new set of experts from both industry and academia to reflect on M&S Grand Challenges. Themes include big simulation, coordinated modeling, large scale systems modeling, human behavioral modelling, composability, funding availability, cloud-based M&S, engineering replicability into computational models, democratization of M&S, multi-domain design, executing and targeting hardware platforms and education. It is hoped that these activities will provide inspiration to those already working in or with M&S and those just beginning their career.

Keywords: Modeling, Simulation, Grand Challenges

1. INTRODUCTION

Modeling & Simulation (M&S) is used in many different fields and has made many significant contributions. As a field in its own right, there have been many advances in methodologies and technologies. In 2002 a workshop was held in Dagstuhl, Germany, to reflect on the grand challenges facing M&S. The report is still accessible (www.dagstuhl.de/02351) and it is interesting to reflect on the degree to which these challenges have been met and the degree to which these still present a challenge. Ten years on, a series of M& S Grand Challenge activities are marking a decade of progress and are providing an opportunity to reflect and plan for the future. The first of this new phase of activities was the M&S Grand Challenge Panel at the 2012 Winter Simulation Conference [Taylor, et al. 2012]. This discussed issues including interaction of models from different paradigms, parallel and distributed simulation, ubiquitous computing, supercomputing, grid computing, cloud computing, big data and complex adaptive systems, model abstraction, embedded simulation for real-time decision support, simulation on-demand, simulation-based acquisition, simulation interoperability, high speed optimization, web simulation science, spatial simulation, and ubiquitous simulation.

This second Grand Challenge Panel brings together a new set of experts from both industry and academia to reflect on M&S Grand Challenges. Themes presented here both complement and extend the first Panel and include big simulation, coordinated modeling, large scale systems modeling, human behavioral modelling, composability, funding availability, cloud-based M&S, engineering replicability into computational models, democratization of M&S, multi-domain design, executing and targeting hardware platforms and education. It is hoped that these activities will provide inspiration to those already working in or with M&S and those just beginning their career.

2. AZAM KHAN

2.1. Big Simulation

I introduce the term "big simulation" to describe a grand challenge for the modeling and simulation research community. This term describes issues of scale for big data input, very large sets of coupled simulation models, and the analysis of big data output from these simulations, all running on a highly distributed computing platform based on standard internet tools and protocols. Specifically, these scenarios call for integrated relational and non-relational database support for data modeling as well as data output, ontology-driven generation of models, and model development coordinated through standard model interfaces that may also be ontologically defined. Robust domain decomposition and dynamic model partitioning will also be needed. Finally, live simulations that are continuously running, controlling physical systems or informing decision making activities, will become more prevalent and will likely grow significantly in scale and complexity. Embedded in this challenge is the need for multidisciplinary integrated systems design, combining commercial and open source models, a challenge in its own right. Solutions to big simulation problems will need to consider their objects of concern as being essentially infinite and will likely focus on streaming paradigms to maximize processing throughput of their current window of visibility into the larger problem.

2.2. Coordinated Modeling

The improvement of user interfaces and information visualization for the entire modeling and simulation process is still needed [Vangheluwe and Vansteenkiste 1996]. For all but the simplest of simulations, this means that users must be able to easily access and manage high performance computing resources, databases of input and output, and visualizations for decision support. The construction of scalable cyber-infrastructures is a major undertaking but they can then support a multidisciplinary modeling community. But to promote the collaboration of the community, standard ontologies and data models must be adopted. This situation calls for overlapping models: data models, ontological models and simulation models which must be procedurally coordinated to ensure ongoing compatibility. Finally, if this can be achieved, the related empirical and deduced knowledge can be linked in-place resulting in an overall encoding of a scientific discipline.

2.3. Systems

Pursuing the development of large complex systems simulations will require scalable online solutions. Prime examples of big simulation applications include whole-cell simulation [Karr, et al. 2012], brain modeling of cognitive processes [Newell 1994], global system models of anthropogenically-caused environmental change [Sokolov, et al. 2005], and anatomical biomechanical simulation [Lloyd, et al. 2011]. Each of the systems mentioned could greatly benefit from big simulation solutions and by working within these domains, this grand challenge may be addressed.

3. KATHERINE L MORSE

3.1. Modeling vs. Simulation

In this context, the difference between modeling and simulation is critical. Model and simulation can be defined as [M&SCO 2011]

- Model - A physical, mathematical, or otherwise logical representation of a system, entity, phenomenon, or process.
- Simulation - A method for implementing a model over time.

By definition, a modeling grand challenge is one of representation while a simulation grand challenge is one of infrastructure and engineering.

3.2. Modeling Grand Challenge – Human Behavior

The most significant and unanswered modeling challenge, in my opinion is human behavior, both representation and prediction. Prediction is the harder problem because sociologists and psychologists have not arrived at reliable, much less repeatable, models. And they may never since human beings are notoriously chaotic and contrarian.

Better progress has been made on representation, but the models are not transitioning to simulation tools. They still require specialized knowledge to operate and interpret, and we have no basis for comparison of results. This is partially due to a lack of multiple, validated data sets on which to run them, but also because of a resistance by researchers to compare the results of their models to other models.

In our 2011 paper [Morse and Schloman 2011], John Schloman and I reported the results of our investigation into the feasibility of data interoperability for Human, Social, Cultural and Behavior (HSCB) models because data interoperability is the first necessary step for any level of model interoperability; data from one model must be usable by another model. We concluded with the following recommendations:

1. Establish a dataset and data format clearinghouse.
2. Develop business rules and social network graphs in standard formats analogous to military rules of engagement, but derived from applicable policy.
3. Develop standardized formats for the types of data required by HSCB tools:
   - Event coding
   - Keywords and taxonomies
   - Business rules
   - Time-coded term alias tables, e.g. aliases for individuals
   - Social network output

These recommendations were subsequently folded into an expert panel discussion at the 2012 Fall Simulation Interoperability Workshop [Morse, et al. 2012]. The final recommendations of that panel are provided in the paper. Areas identified as extremely challenging ("very complex domain; standards problematic") were considered to need more research focused on transitioning models to simulation tools including:

- Cognitive behaviors subdomain (the conscious structures of human cognition and their logical organization) in particular reasoning, and decision-making;
- Cognitive social psychological subdomain (conscious and subconscious determinants of individual behavior regarding the outside world including behavior within groups) in particular attentional behavior and values; and

Social Psychological subdomain (external pressures in society and culture on individuals and groups) in particular norms and culture.

3.3. Simulation Grand Challenge – Composability

Composability is still our biggest simulation challenge. Rather than address the fundamental problem, individual programs 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.

But that does not help when we need to federate. Then we are back to either depending on everyone to be using the same interoperability solutions already or we are undertaking a major engineering effort.

In our 2004 paper [Morse, et al. 2004], we made the following recommendation for a composability framework concept:

- Dynamic component registration & discovery via a directory of all registered components & repositories
- Virtual repository with version control
- Semantic query, search, & reasoning capabilities, supported by component specifications (i.e. meta-data)
- Distributed processing across multiple platforms, systems, services, and domains
- Support for intelligent and polymorphic proxies for components
- Automated composition procedures to combine components
- Ability to save useful compositions
- Support for and supported by standards
- Software authentication and information exchange services

Almost none of these recommendations have been achieved to a satisfactory extent

3.4. The Real Challenge

If you had asked me this same question 5-10 years ago, I probably would have given you the same answer. I conclude that we are not addressing the known problems. So, the real Grand Challenge is political will and funding.

4. ANDREAS TOLK

4.1. Cloud-based Modeling & Simulation

Cloud computing is a field of increasing importance. Using the idea of virtualizing hardware and software and offering those as services over a network did lead to the development of new concepts, such as data storage as a service, software as a service, special hardware as a service, infrastructures as a service, testing as a service, etc.

In other words, if a special hardware or software can be used to solve problems of a special community group, it may make sense to virtualize such services and offer them for potential customers. This idea is also for M&S services of interest, as many customers are using simulation for training, for optimization, or to provide an agile test environment. Although there are several papers that evaluate the use of M&S to evaluate the usefulness of cloud computing, such as Calheiros, et al. [2011], there is not much work published on cloud-based simulation. The question arises if M&S solutions, such as simulation systems or composable M&S services as e.g. specified in [Tolk, et al. 2006] can be treated like software as a service, or if M&S as a service (MSaaS) deserves an individual bullet in the enumeration above.

As current research shows, treating MSaaS as simply software is insufficient, and MSaaS can easily evolve into one of the new grand challenges.

The idea to web-enable simulations and simulation services is not new. The Extensible M&S Framework (XMSF) group looked at utilization of web technologies in support of better M&S nearly a decade ago [Brutzman, et al. 2002, Blais, et al. 2005]. Web services are used to provide common services to simulation systems, such as weather or even weapon effects [Neugebauer, et al. 2009]. Simulation systems are already provided as services [Wiedermann 2001], and academic discussions go back to Fishwick [1996]. So why is this still an issue?

The foundational reason lies in the observations summarized by Tolk et al. [2011] that simulation systems regard their conceptualization of the real world referent as their reality. Simulations implement conceptualizations. In particular when composing several services to build a new simulation system it must be ensured that in addition to making the simulation services interoperable, we also must make sure that the underlying models are composable. This is a unique requirement that only exist for model-based systems.

Hofmann, et al. [2011] observe that it is necessary to capture the conceptualization of the simulation in the referential domain (what do we model) as well as the implementation of the simulation in the methodological domain (how do we model). This concept of having to capture two categories of metadata to support the composability of domain conceptualization on the one hand as well as the interoperability of the implementation reflects the uniqueness. One possibility is the use of interoperability maturity models as recommended in Tolk, et al. [2012]. In any case, the metadata accompanying the services have to capture the modeling as well as the simulation aspects.

This requires that the domain of conceptual modeling supports the definition of metadata standards that allow to evaluate if two simulation services are integratable (i.e., they are executable on infrastructures that can be integrated), interoperable (i.e., the simulation systems support consistent interoperability protocols), and composable (i.e., the underlying models are conceptually not contradictive). Only if integratability, interoperability, and composability can be ensured, it makes sense to compose the simulation services into a common new system. If such a composition will result in an inconsistent representation of truth in participating subsystems it is still possible to apply the ideas of multi-modeling instead of federating to address the various facets when dealing with a problem.

5. LEVENT YILMAZ

5.1. Reproducible Modeling & Simulation Research: Engineering Replicability into Computational Models

Recent years have seen proliferation of the use of simulation models in computational science. Most of these models have never been independently replicated by anyone but the original developer. However, replication is critical to scientific transparency, and availability of *replicability-aware* model development infrastructures is imperative to enable the practice of reproducibility [Yilmaz, 2012].

Replicability refers to the ability to reproduce, and, if needed, independently recreate computational models associated with published work. Emergence of reproducibility as a critical issue is based on growing credibility gap due to wide spread presence of relax attitudes in communication of the context, experiments, and models used in computational science and engineering [Mesirov, 2010]. Furthermore, as indicated in [Fomel and Claerbout, 2009], a published article is not the scholarship itself; it is merely advertising of the scholarship. The actual scholarship involves the model, the simulation development environment, and the complete set of instructions, which generate the article. These observations, coupled with disputes such as Climate Gate [Economist, 2010], the microarray-based drug sensitivity clinical trials [Baggerly and Coombes, 2009], and article retractions due to unverified simulation code and data [Alberts, 2010] suggest a pressing need for greater transparency in Modeling & Simulation (M&S) research.

Replicability involves implementation of a conceptual model in a simulation study that is already implemented by a scientist or a group of scientists. Unlike reproducibility of results by (re)using the original author's implementation via executable papers and workflow systems and repositories [Anand et al., 2009], replication refers to creation of a new implementation. To facilitate replicability, provision of an extensible and platform neutral interchange language for the specification, distribution, and transformation of model, simulator, and experimental frame elements is critical. Support for independent replication of computational experiments could be highly beneficial, because such infrastructure and the associated methodology will allow cross-validation while demonstrating that observed results can be repeatedly generated and thus the original findings are not exceptional.

The challenge before the M&S community is to develop strategies for replicability by understanding the methodological developments contributing to reproducibility while developing the necessary technical infrastructure to support them. Table 1 outlines the three critical dimensions of reproducible M&S research.

Table 1: Dimensions of Reproducible M&S Research

Scholarly Communication	Legitimization, Dissemination, Access	
Process	*Roles*	Scientist, Journal/Publisher, Funding Agency
	Ownership	Citation, Licensing, Open Source
Infrastructure	*Content*	Model, Simulation code, Data, Publication, Experiment
	Service	Search/Discovery, Collaboration, Sharing
	Tools	Authoring, Version control, View/distribute/transform, Quality control

Among the challenges that need to be addressed include the following:

- What constitutes output of reproducible M&S research, and how can these components be packaged for dissemination and access?
- What are the main quality criteria pertaining to objectives such as legitimization, dissemination, and access?
- Achieving those quality objectives requires adherence to certain principles that characterize the process by which reproducibility is achieved. Therefore, what are the basic simulation software engineering principles that support these concrete objectives?
- Conformance to a process governed by those principles should result in research artifacts that possess attributes considered to be desired and beneficial for replication. Hence, what strategies and software technologies can facilitate enhancing the reproducibility by allowing the engineering of desired attributes into computational models?

A critical challenge will be in evaluating how replicability-aware scholarly communication, process, infrastructure, and tools impact the M&S research practice and attainment of the reproducibility criteria. Besides, science is a collective phenomenon. Progress in simulation-based science and engineering requires the ability of scientists to create new knowledge, elaborate and combine computational artifacts, and establish analogy and metaphor across models. The inability of others to independently reproduce and verify published results will slow down the adoption and the use of knowledge embedded within models. Therefore, reproducibility should become responsibility of the broader scientific community.

6. JUSTYNA ZANDER

Now it is the first time in history that a citizen scientist can acquire the skill and capitalize on the opportunity to contribute to new high-tech trends. Let alone building the collaborative technical platforms based on Content Management Systems, but more astonishingly, deploying engineering methodologies to design a mobile-phone application [AppInventor], build a customized robot [Aldebaran Robotics], or conceptualize an electronics board within an arbitrary device.

Reaching deeper, for example in the robotics sector, it is nowadays possible to work at different abstraction levels. The key component for each of these abstractions is *simulation*, mostly because it gives meaning to the models. Simulation environments for interactive humanoid behavior such as in NAO robots are enabled at a user-based functionality level (e.g., jumping, dancing, or singing) [Aldebaran Robotics]. Rapid prototyping using the electronics board within such a robot can be designed with MATLAB® and Simulink® and their support packages for the Arduino microcontroller. Reasoning about mathematical foundations of the robotic components becomes increasingly adopted because of MATLAB and Simulink interfaces to hardware targets (e.g., LEGO blocks).

In the next paragraphs, selected *challenges* have been distinguished to be explored in more detail.

6.1. Democratization of Modeling and Simulation

From the perspective of supporting collaborative effort the main challenges in Modeling and Simulation (M&S) are affected by the *democratization* of the Modeling and Simulation (M&S) technologies. Democratization, in turn, is influenced by adoption, a wide adoption across the disciplines. Here, the construction industry may serve as a guiding example with around thirty years ago Computer-Aided Design (CAD) disrupting the incremental industry progress [Gardiner 2007]. Similarly, M&S including *Model-Based Design* (MBD) constitute the concepts and technologies that have been disrupting the field of engineering for about ten years now. Seeing the development cost reduction of about 30% [Broy, et al. 2011] that MBD creates, it is valid to conclude that M&S have become the tools of choice in today's computation- focused system design.

Now, seeing how the adoption of cloud computing and web-based tools [Zander and Mosterman 2013] is progressing, how tablets are increasingly used as the communication and creativity evoking devices, but also how the industrial and digital information exchange [Gee 2012] is being transformed with the use of mobile devices, M&S may become an autocatalytic technology for enabling a predictive analysis of almost every physical and engineering phenomenon that is embedded in such an emerging technical infrastructure. A crucial factor here is the appropriate *delivery* to the user, including a designer, a technologist, a citizen, and in the future, a mass M&S user. Thus, another aspect of the *M&S collaboration challenge* is *investigating virtual platforms* and organizations dedicated to creating M&S with and for mass capabilities. *Measuring the benefits* for productivity and innovation purposes with such means constitutes a further element of the collaboration challenge.

Furthermore, some high-tech visionaries speculate that *prediction engines* will scale up and complement today's search engines in the mid-term future [Zander, et al. 2012] to raise consumer awareness, others call for teaching domain-based engineering that includes M&S as a primary education subject [Zander and Mosterman 2013].

6.2. Multi-Domain Design

From the mathematical and technical viewpoints, many breakthroughs in solving scientific problems have been enabled by advances in algorithms. Thus, computational methods are often taken for granted because of the past (isolated or shared) successes [NSF 2011]. However, there still exists a necessity to work on the *scalability* of the computational M&S methods. Petascale systems require advancing, in particular, when relating to modeling *heterogeneity* issues, *multi-physics couplings*, *multi-scale* and *multi-rate* behavior, *uncertainty*, dynamically evolving and *emergent* behavior, and so on. Thus, systematic research in those areas is imperative for developing the next-generation M&S methodologies and technologies.

Next, challenges such as *multi-domain design* and its corollary the definition of a *unified M&S semantics*, can be identified as critical enablers. The semantics for simulation (i.e., execution) must be defined in such a manner that it is understandable for the community but also for the end user, in particular because this end user may eventually become a part of this community.

A further implication of a multi-domain approach is the *interaction of approximations* in the various numerical algorithms. Such algorithms must be combined to solve differential equations, difference equations, algebraic equations, algebraic loops, root-finding inequalities, etc. [Mosterman, et al. 2012]. A precise formal semantics for such interactions, a common understanding of the notion of time, and its proper indexing in the solvers (cf., semantics domain) constitute specific items under this umbrella.

From a technical system perspective, *the verification and validation of models and of simulation in its own right* are still challenges that have not been solved, although distinct progress is being reported [Zander, et al. 2011].

M&S enable *high risk research*, holding the promise of potential breakthrough with high technological and societal impact. The *challenge* is to capitalize on the abundance of simulated realities to have impact on a *social good cause* [Zander and Mosterman 2013].

6.3. Execution and Targeting Hardware Platforms

Further, *execution and targeting hardware platforms* becomes increasingly important from the technical designer, but also a citizen viewpoint. Nowadays, rapid prototyping based on M&S that includes hardware components (e.g., the Arduino platform) is possible and easier than ever before. It is becoming increasingly cheaper and scales up in the educational classroom.

The next element to consider is the Internet of Things (IoT) that uses radio-frequency identification (RFID) technology to connect an increasingly broad range of various artifacts around us. In ever more areas companies depend on the Internet as a powerful, cost-effective medium for data transport. The *challenge* is to *interface IoT with M&S* and leverage this combination to build *Computation of Things* [Zander, et al. 2012], where the items are not only connected but actually process the data and come up with novel solutions. This will open up the space for services that organize and automate governmental, societal, and engineering systems and structures even more and to an as of yet unimaginable extent.

6.4. Education

Another challenge is the *education* in its *multi-domain cooperation* dimension. Collaboration on the level of scientific disciplines, but also from an organizational viewpoint is a necessity. Hence, creating sustainable programs that promote multi-cooperation is required for academics to pursue their career. Institutional transformative change is to come at the level of governments, educational units, and industry. Training to exploit careers in Computational Science and Engineering is required for M&S to maintain its pace of growth and keep up with its increasing demands. For example, European research on technology-enhanced learning investigates how information and communication technologies can be used to support learning and teaching, as well as more generally competence development throughout life [Bullinger, et al. 2009]. This is an opportunity for M&S to become part of such a learning initiative, in particular because M&S is the foundation for *interactive interfaces* that provide difficult to overstate value. Raising the interest in this context includes not only openness to industry consumers. It also calls for openness to the young people who should be offered *scientific and technical education* at the same time.

Education constitutes one of the keys for the success of M&S. In particular, broad application of M&S, including *technology democratization* is significant if not critical as the driving force for human progress over decades to come.

7. CONCLUSION

This panel has presented a wide range of views on M&S Grand Challenges. We hope that these will help both practitioners and researchers to reflect on their current practices and how they might change in the next decade.

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Biography

Simon J E Taylor is the convener of this new phase of Grand Challenge activities. He is the Founder and Chair of the COTS Simulation Package Interoperability Standards Group under SISO. He is the Editor-in-Chief of the UK Operational Research Society's (ORS) Journal of Simulation and the Simulation Workshop series. He was Chair of ACM's SIGSIM (2005-2008) and is a member of the SIGSIM Steering Committee. He is a Reader in the School of Information Systems, Computing and Mathematics at Brunel and leads the ICT Innovation Group. He has published over 100 articles in modelling and simulation. His recent work has focused on the development of standards for distributed simulation and grid- and cloud-based simulation in industry as well as the spread of the international Grid Infrastructure into Africa. His email address is <simon.taylor@brunel.ac.uk>

Azam Khan is the Head of the Environment & Ergonomics Research Group at Autodesk Research. He is the Founder of the Parametric Human Project Consortium, SimAUD: the Symposium on Simulation for Architecture and Urban Design, and the CHI Sustainability Community. He is also a Founding Member of the International Society for Human Simulation and is currently the Velux Guest Professor at The Royal Danish Academy of Fine Arts, School of Architecture, at the Center for IT and Architecture (CITA) in Copenhagen, Denmark. He received his B.Sc. and M.Sc. in Computer Science at the University of Toronto (1990, 2008) and is currently a Ph.D. candidate at the University of Copenhagen. He has published over 50 articles in simulation, human-computer interaction, architectural design, sensor networks, and sustainability. His team is currently developing a new experimental DEVS simulator called DesignDEVS to explore big simulation.

Katherine L. Morse is a member of the Principal Professional Staff at the Johns Hopkins University Applied Physics Laboratory. She received her B.S. in mathematics (1982), B.A. in Russian (1983), M.S. in computer science (1986) from the University of Arizona, and M.S. (1995) and Ph.D. (2000) in information & computer science from the University of California, Irvine. Dr. Morse has worked in the computer industry for over 30 years, specializing in the areas of simulation, computer security, compilers, operating systems, neural networks, speech recognition, image processing, and engineering process development. Her Ph.D. dissertation is on dynamic multicast grouping for data distribution management, a field in which she is widely recognized as a foremost expert. She is a member of Phi Beta Kappa, Dobro Slovo, ACM, and a senior member of IEEE. Dr. Morse was the 2007 winner of the IEEE Hans Karlsson Award.

Andreas Tolk is professor for engineering management and systems engineering at Old Dominion University in Norfolk, VA. He also holds a joint appointment with the Modeling Simulation and Visualization department and is affiliated with the Virginia Modeling Analysis and Simulation Center in Suffolk, VA. He received the Frank Batten Award for Excellence in Research (2008), the Technical Merit Award from SISO (2010), and the Outstanding Professional Contribution Award from SCS (2012).

Levent Yilmaz is Associate Professor of Computer Science and Software Engineering and holds a joint appointment with the Industrial and Systems Engineering department at Auburn University. He received M.S. and Ph.D. degrees from Virginia Tech and the B.S degree in Computer Science from Bilkent University, Turkey. His research interests are in Modeling & Simulation, Agent-directed Simulation, and Self-Organizing Complex Adaptive Systems with a focus in advancing the theory and methodology of Computational Modeling and Simulation. Dr. Yilmaz is a member of the Board of Directors of SCS and is currently serving as the Editor-in-Chief of Simulation: Transactions of the Society for Modeling & Simulation International. He also serves as the Associate Editor of International Journal of Simulation and Process Modeling, Springer Complex Adaptive Systems Modeling Journal, the International Journal of Engineering Education, and the Simulation & Gaming Journal. He is member of ACM, IEEE Computer Society, Society for Computer Simulation International (SCS), and Upsilon Pi Epsilon.

Justyna Zander (PhD at the Technical University Berlin, Germany) is Senior Technical Education Evangelist at MathWorks in Natick, MA, USA and Assistant Professor active in Computer Science and Engineering at Gdansk University of Technology in Poland.