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Grand Challenges for Modeling and Simulation

Dagstuhl Report

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Simulation and Agent-Oriented Software Engineering

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Preface

The identification and pursuit of Grand Challenges has been a hallmark of the high-performance computing arena for well over a decade. In recent years, many other technical communities, including the modeling and simulation (M&S) community, have begun defining Grand Challenge problems for their disciplines. While Grand Challenges themselves provide a useful focal point for research and development activities within a discipline, perhaps more important is the community dialogue that surrounds the formulation of Grand Challenge problems.

Within the M&S community, the dialogue surrounding the notion of Grand Challenges began with the First International Conference on Grand Challenges for Modeling and Simulation, which was held 27-31 January 2002 in San Antonio, TX, USA as part of Society for Computer Simulation (SCS) 2002 Western Multiconference. The conference program consisted of 15 papers and a panel.

The Dagstuhl seminar on Grand Challenges for M&S was dedicated to continuing this dialogue, with the goal of condensing ideas into a set of Grand Challenge problem statements that might serve to guide strategic research initiatives in modeling and simulation for the next decade.

The seminar was structured around various application and methodological areas of modeling and simulation:

- Simulation of cellular systems
- Simulation of air traffic
- Simulation large scale computer networks
- Simulation as part of agent-oriented software engineering
- Simulation in virtual manufacturing
- Simulation in military applications
- Parallel and distributed simulation
- Modeling and simulation methods

While the groups had unique perspectives derived from their particular application domain, they also shared a commonality derived from the modeling and simulation life cycle (i.e. understand a system, represent a system as a model, execute the model, analyze the results). Cognitive models of human actors, their decision processes, and their behavior are important in military applications, and in testing autonomous agent software. However, cognition processes are still little understood and "of the shelf" cognitive models that can be re-used in different settings do not exist. The same is true if we are looking at cellular, biological systems. The successful completion of the ambitious endeavor of the human genom project depends to a large degree on a better understanding of the behavior of cellular systems.

In dealing with complex systems, like cellular or cognitive systems, modeling and simulation has often played a role to support the development of theories and understanding of systems rather than predicting the systems' behavior. Efforts of the application area have to be combined with developing simulation systems that support an explorative approach to modeling and simulation more effectively. Whereas many techniques, e.g. hierarchical decomposition, object-oriented modeling and programming, graphical depiction of system behavior, visual modeling and programming, or agent-based modeling, have enhanced our ability to build and use complex models, despite efforts like HLA, still the challenge of re-usability of models seems largely unresolved, particularly if we are approaching the realm of multi-paradigm, multi-resolution modeling. Supporting multi-paradigm, multi-resolution modeling is arguably a central prerequisite to significantly advancing modeling and simulation in such diverse application areas like manufacturing, military, air traffic, biology, software development, and networks.

Complex systems, e.g. the world wide web, do not only require new techniques for a more effective representation of systems. The efficient execution of these models poses unsolved problems as well. New parallel distributed simulation methods are needed not only to support an efficient simulation but to adapt themselves flexibly to the changing demands of a multi-resolution and multi-paradigm modeling.

During the seminar, a set of Grand Challenge problems statements from each of the application areas was formulated, and in some cases, possibilities for research agendas were sketched. While the results of the seminar offer a good starting point, and illustrate a number of intersections of interest across M&S application domains, more thought and effort is required to develop concrete research agendas in the multi-disciplinary arena of modeling and simulation.

Organization

Dagstuhl is dedicated to working groups. In contrast to traditional conference settings, the schedule offered plenty of time for working groups, discussions, and spontaneous activities. The week was divided into two parts (1-4, and 5-8 respectively) and allowed everybody to participate in two working groups during the seminar. To give an overview about the different areas, state-of-the-art plenary talks were given. Short presentations provided the opportunity for each participant to present his or her work, and ideas on Grand Challenges for Modeling and Simulation before the parallel working groups started. In plenary sessions the results of the working groups were presented.

Intertwining working groups and plenary sessions helped to work on concrete challenges in the different groups and to support a cross fertilization among them. The seminar was a truly interdisciplinary event and all participants played an active role in driving the progress and content of the workshop.

As always, Schloss Dagstuhl and its ambiance, its unusual blend of the old with the new, the organization, and the very helpful staff contributed largely to the success of the seminar.

Collected Abstracts

Dealing with Complexity

by ***Paul Davis***

A criterion for a Grand Challenge should be: "Solving the problem would have the potential for substantially altering the field of modeling and simulation--e.g., by making possible a new and powerful style of modeling or by greatly enhancing the usefulness to analysis and decision support of existing types of modeling." In musing about this, it seems to me that one of the biggest challenges continues to be enhancing the ability of a person or team to comprehend and cope with massive complexity. Consider the following humbling questions:

- How often has it proven possible to transfer complex models successfully to new users?
- Even when we have built a complex model ourselves in the past, how long does it take for us to get back up to speed with it?
- And, even when we are up to speed, how many of us can thoroughly comprehend what we are dealing with?
- In distributed work, how well do the various collaborators truly understand what the "other" portions of the virtual model do, assume, etc?
- And, finally, how do the answers change if one is also faced with massive uncertainty about inputs (as in common in higher-level work)?

We already have many techniques that have enhanced our ability to build and use complex models. These include hierarchical decomposition, structured programming, object-oriented modeling and programming, graphical depiction of system behavior, visual modeling and programing, and agent-based modeling. Some of these are thought to be relatively mature; others are obviously still in the research stage. Thinking of my own work, I like to believe that multiresolution, multiperspective modeling (MRMPM) and exploratory analysis have great potential. I will summarize those briefly, but part of the purpose of discussion should be to understand better what all is needed in order to deal well with complexity.

Air Transportation is a Complex Adaptive System: Not an Aircraft Design - Comments on Modeling and Simulation

by George L. Donohue

The World Wide Air Transportation Network System has become indispensable to domestic and international trade. It has been known for some time that the US balance of trade is heavily dependent on the export of civil aircraft parts and services. The recent events of terrorism against the United States and the subsequent severe reduction in US air transportation services gave us a vivid example of the economic dependency of both regional economic activity and the entire world on these services. The growth in air transportation over the last 40 years has been an important ingredient in US economic growth. The rapid migration of the airlines to a hub-and-spoke system after deregulation in 1978 led to a significant rise in service frequency and price competition. The inherent efficiencies of this new regulatory environment resulted in a rapid rise in the utilization of the air transportation mode. Today, we are at the cross-roads of inefficient utilization of national airport infrastructure and an outdated air traffic control paradigm. These factors will severely limit the continued growth of air transportation unless modern technology and a new regulatory environment are put in place.

At the beginning of the 21st century, there are approximately 60 major airports in the United States owned and operated by local municipal governments with a maximum capacity of about 32 million operations per year. Current forecasts predict that the future demand for air travel will significantly exceed supply and delays will increase over the foreseeable future. In general, the National Airspace System (NAS) modernization and runway improvement programs that are being fielded are indicating substantially less than predicted performance increase. It is becoming increasingly clear that several important non-linear effects are complicating the NAS modernization program.

We could increase the NAS capacity in the USA to over 70 million operations per year by migrating from the use of radar surveillance to the use of aircraft broadcast Global Positioning System (GPS) satellite navigation fixes over a wireless digital data link. This important transition would also utilize the significant computer-based flight management systems that have been incorporated into virtually all of the commercial aircraft over the last 20 years. Over the last 7 years, we have observed a rapid growth in the use of small (e.g. less than 50 passenger) regional jets and privately operated business jets in the NAS. A co-dependent two tier air transportation system may be required to take maximum advantage of the different flight characteristics and operational profiles that these aircraft present the NAS. A new regulatory scheme including airport slot auctions will need to be implemented to take advantage of these technology advancements and encourage optimal safe use of the nation's airport infrastructure.

Just as the Alaska Capstone Operational Evaluation has led to a significant advancement in our understanding of the safe use of some of these new technologies and operational procedures, a bold step must now be taken in concert with the Cargo Airlines to integrate the new equipment and procedures into the mainstream of the nation's air transportation management system.

Human-Model Interaction

by ***Paul Fishwick***

Science fiction has long been a field responsible for foretelling how science may look in the future. Consider rockets and robots. Jules Verne crafted a marvelous look at the future of spaceflight with "From the Earth to the Moon." We finally reached the moon in 1969 but not with a cannon ball, but instead with chemical energy within Apollo 11. Fritz Lang introduces us to robots in 1927 with the film Metropolis. Books and films such as these not only introduced the general populous to strange mechanical creations, but also inspired generations of scientists and engineers to see whether something could be done about it. The science fiction authors were, and continue to be, progenitors of grand challenges. If we are to look modeling and simulation in the face and ask what its new face may look like in 5, 10 or 20 years in an attempt to embark upon grand challenge quests, then we should sift through today's science fiction for clues. There are several notable simulation environments of the future, including the Holodeck from Star Trek. The question we must ask ourselves is "How will we create, analyze, and execute models on the Holodeck?" We must ask this question because our technology advances to where the Holodeck, or its equivalent, will become a reality. We propose a study linked to novel interaction mechanisms between the human and the computer-based model, to the point where humans are capable of using a wide variety of sensory cues and devices in their model making. As a community, we have the potential to radically redefine how models are made and how they are formally specified, while building on existing state of the art approaches for complex system construction. I will present some of the work we have done in:

- model specification for the web, and
- alternate presentations for those specifications, which assume advanced audio-visual environments.

The reference web page for this discussion can be found at

http://www.cise.ufl.edu/~fishwick/rube.

This work, by no means, captures the Holodeck environment, but it might suggest some ideas and directions for our future model crafting. I would like to work closely with other methodology and applications attendees, to see what we can collectively invent.

Modeling and Analysis of Semiconductor Manufacturing

by ***John W. Fowler***

The electronics industry recently surpassed the automotive industry to become the largest basic industry in the world after agriculture. At the heart of this industry is the manufacture of semiconductor devices. The semiconductor market is expected to be about $150 billion in the year 2002 and has maintained an average annual growth rate of 15% over the last 15 years. However, costs continue to escalate; current wafer fabrication facilities cost $3 billion. Traditional productivity gains that have allowed the cost per transistor to continue to decrease have come primarily from:

1) wafer size changes;

2) devices shrinks;

3) yield improvements; and

4) factory and equipment efficiency improvements.

While some gains will continue to come from 1), 2) and 3), the fourth category offers the most potential for future gains. Operational modelling and simulation offer a way to determine areas that will lead to significant enterprise, factory and equipment efficiency improvements.

Modelling and simulation of semiconductor manufacturing operations is quite challenging. Models are necessary from the machine level all the way up to the enterprise level. Some of the key issues associated with modelling and simulating the manufacturing equipment, workcells, factories, and the entire semiconductor manufacturing supply chain are discussed in this paper.

Parallel and Distributed Simulation in the 21th Century

by ***Richard Fujimoto***

The origins of the parallel discrete event simulation field date back to the 1970?s and 1980?s with seminal work in synchronization algorithms by researchers in the high performance computing community. A separate track of research flourished in the defense community beginning in the 1980?s focusing on networking simulators to create distributed virtual worlds for training. Since then, distributed execution has been successfully employed time and time again to realize large-scale simulation environments. While important research problems remain, the parallel / distributed simulation field has matured over the last twenty years and basic premises concerning the feasibility and practicality of distributing the execution of simulations over multiple computer systems have become widely accepted. The 21st century brings new challenges to the parallel/distributed simulation research community. As processor speeds and memory capacities continue to increase at an exponential rate, simulations that previously required high performance computing platforms can now be executed on inexpensive personal computers. At the same time, ubiquitous computing and communications are beginning to appear, affording new opportunities and challenges for parallel and distributed execution. In this talk I will give an overview describing the evolution of the parallel / distributed simulation field over the last two decades, and speculate on grand challenges that can drive research in the field in the years ahead.

Simulating Synthetic Autonomous Behaviors in Augmented Reality

*by **Erol Gelenbe***

Integrating autonomous behaviors into augmented reality is one of the most challenging and innovative trends in modern simulation techniques. Applications include games as well as simulation systems for professional applications such as system design and military applications in training and situational awareness and operations planning. This presentation describes our COTERIE (Cooperating Teams of Realistic Robotic Entities) which combines goal based autonomous behaviors within a realistic augmented reality setting.

The Promise of Agent-Based Modelling and Simulation in Micro-Biology

by ***Catholijn M. Jonker***

The NetherlandsExisting chemical models of bacteria are complicated, due to the thousands of interacting chemical reactions within the cell. To gain a higher level of understanding, more transparent and abstract models are needed. In this paper an intentional dynamic modelling approach is introduced and used to simulate the behaviour of Escherichia coli. A model of the entire cell is presented that covers E. coli's behaviour, including its intracellular processes and their control. The intentional properties used in the model are in a one-to-one correspondence to chemical properties: concentrations of specific substances within the cell. Via these correspondences the dynamic relationships between intentional properties are justified by chemical laws. A software environment has been developed for simulation and automated analysis of such a model.

The presentation is based on the article:

Jonker, C.M., Snoep, J.L., Treur, J., Westerhoff, H.V., and **Wijngaards, W.C.A.**, *BDI-Modelling of Intracellular Dynamics.* In: A.B. Williams and K. Decker (eds.), Proceedings of the First International Workshop on Bioinformatics and Multi-Agent Systems, BIXMAS'02, 2002, pp. 15-23. Extended abstract in: C. Castelfranchi and W.L. Johnson (eds.), Proceedings of the First International Joint Conference on Autonomous Agents and Multi-Agent Systems, AAMAS'02. ACM Press, 2002, pp. 465-466

Agent-Based Analysis of Dynamics in Biological, Cognitive and Organisational Domains

by ***Catholijn M. Jonker***

To understand how an organisational or societal structure relates to dynamics is an interesting fundamental challenge in the area of organisational and social modelling. Specifications of organisational structure usually have a diagrammatic form that abstracts from more detailed dynamics. Dynamic properties of agent systems, on the other hand, are often specified in the form of a set of logical formulae in some temporal language. This paper addresses the question how these two perspectives can be combined in one framework. It is shown how for different types of elements within an organisation structure different sets of dynamic properties can be specified. Organisational structure provides a structure of mutual logical relationships between these multiple sets of dynamic properties. Thus specification of organisational structure relates to specification of dynamics. As an illustration, for Ferber and Gutknecht's AGR organisation modelling approach it is shown how a foundation can be obtained for integrated specification of both structure and dynamic properties of an organisation.

The presentation is based on the article:

Jonker, C.M., and **Treur, J.**,
Relating Structure and Dynamics in an Organisation Model.
In: J.S. Sichman, F. Bousquet, and P. Davidson (eds.), Proceedings of the Third International Workshop on Multi-Agent Based Simulation, MABS'02, 2002, pp. 71-80. To be published by Springer Verlag.

Understanding Biomolecular Systems and Processes Based on First-Principle Simulations

by ***Bogdan Lesyng***

Complex biomolecular processes occur in different spatial and temporal scales - ranging from microscopic (subatomic and atomic), through mesoscopic (macromolecular), up to macroscopic (subcellular and cellular). In order to overcome the current limitations in the formal description and understanding of complex structures and functioning of biomolecular systems and processes, an interdisciplinary approach is being developed. It accounts for:

- microscopic, quantum and quantum-classical models
- mesoscopic, potential of the "mean-force",
- Poisson-Boltzmann and generalized Born models, as well as effective models of hydrophobic interactions,
- macroscopic models utilizing the free-energy density approach,
- models describing kinetics of metabolic pathways, as well as
- genomics and proteomics techniques, including enhanced homology analysis

Such methods allow, in particular, to describe basic enzymatic processes, more complex enzymatic phosphorylation and/or ATP dependent structure formation, molecular recognition processes, as well as the kinetics of metabolic pathways. For a brief overview of selected methods see [1]. First-principle theories and simulations play an important role in theoretical studies of basic biomolecular systems and processes. They belong to the first, microscopic class. One should note, however, that for example "ab initio - type" protein folding models and dynamical processes which occur on a free energy surface (potential of the mean-force) belong to the second class. Once the free energy surface is determined, or computable "on the fly", the dynamics itself can be assigned to the first-principle simulations. Selected examples of microscopic quantum and quantum-classical simulations of the dynamics of model molecular systems as well as enzymatic reactions, including phospholipase A2 [2] and HIV-1 protease [3], as well as mesoscopic Lagrangian and quaternion simulations of conformational transitions in nucleic acids [4] will be presented. Complexity and mutual relations of microscopic and mesoscopic models related to proton exchange phenomena [5] will be indicated. The role of advanced, first-principle modelling tools and simulation results for understanding complex biomolecular systems and processes will be discussed.

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On Multi-Paradigm Modeling

by ***Pieter J. Mosterman, Hans Vangheluwe***

The use of models has found widespread application in systems engineering as a (semi-)formal method to manage the complexity and heterogeneity of large scale systems and their design teams and tools because they are amenable to analysis and synthesis tasks. For example, models are used for knowledge representation, requirements engineering, structured analysis, to manage complexity and achieve high quality of engineered systems, to handle the heterogeneous nature of embedded systems, as a high level programming method, and to bridge conceptual differences between domains. With the advent of ubiquitous computing, model-based applications, e.g., in control, diagnosis, and maintenance, will become pervasive and ultimately become as proliferated as embedded computing power. To avoid overspecification and attain optimal performance, new design paradigms based on holistic views (e.g., mechatronics) are a necessity to analyze subtle interaction between information processing components and the physical environment as well as between the different design tasks. This requires tight integration of the separate individual design activities. However, each of the engineering disciplines involved in system design and operation have developed domain and problem specific (often proprietary) formalisms that match their needs optimally but complicate the integration process. A challenging research topic is to develop and prototype a core of next generation multi-paradigm modeling methods and technologies that address this incompatibility and enable the development of novel applications. This is a powerful approach that allows the generation (instantiation) of domain and problem specific methods, formalisms, and tools and because of a common meta language, these different instances can be integrated by combination, layering, heterogeneous refinement, and multiple views. This breaks down into two types of activities: (i) heterogeneous modeling and formalism and tool coupling, and (ii) behavior generation. The first is mainly concerned with the symbiotics (symbols, syntax, and static semantics) of modeling formalisms, whereas the second addresses analysis and behavior generation using the dynamic semantics of such heterogeneous models, in general this behavior is of a mixed continuous/discrete, i.e., hybrid, nature. Three orthogonal dimensions of multi-paradigm modeling are

- multi-abstraction modeling, concerned with the relationship between models at different levels of abstraction, possibly described in different formalisms,
- multi-formalism modeling, concerned with the coupling of and transformation between models described in different formalisms, and
- meta-modeling, concerned with the description of model representations and instantiation of domain specific formalisms.

When extended with sophisticated model transformation facilities, the multi-paradigm modeling notions can be exploited to facilitate a suite of technologies and applications that manipulate a model into a different representation, possibly changing the abstraction, partitioning, and hierarchical structure to render it suitable for particular tasks, i.e., it is operated on the model rather than its generated information. Though some model transformation schemes exist within and between formalisms, there is still a prevalent need to manually design models in different representations for analyses, consistency checks, and execution. The model transformations that are available and current development efforts tend to focus on the goal of system realization from design (e.g., automatic code synthesis) while models embody knowledge, and as such they also form the core of intelligent applications (e.g., model-predictive control, model-based diagnosis, and self maintenance). When extended with sophisticated model transformation facilities, the multi-paradigm modeling notions can thus be exploited further to facilitate a suite of technologies and applications that implement a form of higher intelligence: Where present intelligent applications utilize a formal representation of some form of a process or system to derive information about its state and predict future behavior, higher intelligence manipulates this model into a different representation, possibly changing the abstraction, partitioning, and hierarchical structure to render it suitable for required tasks, i.e., it operates on the model rather than its generated information.

See also

http://www.op.dlr.de/FF-DR-ER/staff/pjm/papers/hai01/p.html

and

http://moncs.cs.mcgill.ca/people/mosterman/campam/.

Structure and Cognition in Complex Computational Organisations: A Meta-Network Approach in Organisational Analysis

by ***Pietro Panzarasa***

Recent advances in distributed artificial intelligence, social networks, cognitive sciences and organisation theory have led to a new perspective on organisations that takes into account both their computational nature and their underlying network complexity. Building on this perspective, I use a meta-network approach to modelling organisations in terms of agents, tasks and resources. Formalising dyadic dependencies between these domain elements at various levels provides a rich grammar for theorising about organisations. Using this framework, I show that structure places critical constraints on performance and, in turn, these constraints are mediated by the agents' cognition. The hallmark of this meta-network perspective is the idea that cognition occurs at multiple levels, not only within the individual agent, but also as an emergent phenomenon from the interaction among multiple agents. The new insight is that if relationships connecting bits of cognition can extend among agents, then the ways in which agents interact with one another are likely to impact upon the emergent global cognitive phenomena. This is a topic that is directly relevant to the social sciences: the role of social structure in generating global dynamical features. This talk offers a more specific way to cast the issue at hand. Firstly, I identify a set of structural parameters that can significantly affect the cognitive dynamics of organisations. Secondly, I analyse to what extent organisational structure and cognition generate combined effects upon performance. I show that the predictive power of structure depends on the generation of group mind-like forms of mental models (e.g. culture, mutual beliefs, transactive memory) emerging from a network of socially and cognitively integrated agents. Finally, I explore how and to what extent admixtures of randomness to an otherwise ordered social network can have a significant impact upon performance. This impact is mediated by the agents' cognition. When the agents are endowed with basic cognitive abilities, network complexity is detrimental to performance. However, when the agents' cognition become more sophisticated, network complexity can be exploited and performance improves. In this talk, an attempt is made to refine thinking on these matters by proposing the idea that organisations are complex, computational and adaptive systems in which action, knowledge and learning are distributed and where ecologies of skills and strategies synthetically emerge over time. Organisations learn and adapt to their environment by altering their underlying structural and cognitive networks. Drawing on this perspective, I show how it is possible to take some steps towards a new account of the structural foundations of organisational dynamics and cognition.

An Agents' Approach Towards New Fidelity and Scenarios in Airtraffic Simulation

by ***Amy Pritchett***

Simulation of air traffic systems will be increasingly important as we strive to implement revolutionary changes to air transportation in general (and air traffic management in particular) that increase both safety and efficiency. Such revolutionary changes may require evaluating centralized systems characterized by their size and complexity, or distributed methods of coordination potentially characterized as emergent behaviors generated by heterogeneous interacting agents. At this time, many models of system and agent behavior have been developed, but several challenges face the application of these models being used in analysis and design. First, these models have historically been developed as stand-alone applications with their own (often conflicting) methods of data-passing, time advance, etc. Second, simulation architectures too-frequently restrict the types of models they can support, limiting the range of applications they can be applied to and requiring a prohibitive amount of development to reconfigure the simulation to new levels of fidelity and new scenarios. Third, methods of verifying and validating simulations -- especially agent-based simulations -- need to be developed. Finally, better understanding of the types of models applicable to each stage of the design process should be established and a pattern of developing increasingly-high fidelity simulations in concert with designs demonstrated.

Simulating the Internet. How Big is Big Enough?

by ***George Riley***

Simulation has become the evaluation method of choice for many areas of computer networking research. However, most existing network simulation packages have severe limitations on the size and complexity of the network being modeled. Simulated networks of just a few thousand network elements and a few thousand data flows will quickly exhaust the computing resources in any reasonably sized computer workstation. Thus the researcher is faced with the dilemma of proving concepts designed to work efficiently on networks of tens of millions of elements, using a simulation of only a few thousand elements. The grand challenge we discuss in this paper is that of using simulation to reach credible conclusions about Internet--scale network performance. We present data that demonstrates that simulation of Internet--scale networks is not presently feasible, nor is it likely to be feasible in the near future. We present a summary of current research in the field of large scale network simulations. These recent advances, while not enabling Internet--scale simulations, do offer the tools with which one can begin to tackle the problem. We sketch one possible approach and describe the issues that need to be resolved in order to realize it.

Reference/benchmark Simulation Models for Complex Fabrication Facilities

by ***Oliver Rose***

One of the main purposes of simulation in virtual manufacturing is to emulate the real world / the real fabrication facility in order to develop, implement and evaluate complex factory planning and control tools. Today's factories have reached a level of complexity that makes it practically impossible to design efficient and accurate planning and control software without having factory simulation models with an adequate level of detail. Even for experienced engineers it is hard to figure out all possible scenarios that might be faced by planning and control tools and which might be critical for the factory performance. Thus, it is difficult to design and implement such tools in a way that they provide the correct answers because a lot of factory states were not considered during the design phase. In particular, this problem becomes apparent in industries with a complex flow of materials in their production facilities. For instance, the semiconductor industry where chips are made in several hundred process steps on several hundred machines of different types. In most cases, it is a mass production with a cyclic flow of material in a job-shop-like environment. The complexity is increased by batch machines, sequence-dependent setups, time-bound sequences, long machine downtimes, operator grouping, etc. In this area, it is almost impossible to develop planning and control tools without the help of detailed factory simulation models that mimic the material flow of a real semiconductor fabrication facility. Several problems or research questions arise in this area:

- Which degree of complexity of the simulation model is required to support the design of planning and control tools?

  Complex models represent the real factory behavior in a better way but need a lot of time and effort to be built and maintained. In addition, the run time of the simulation experiments become an issue. Simple models are easier to be built but might be too coarse to provide enough information for the planning and control tools. For a lot of academic questions simple models are accurate enough but as soon as the performance of prototype implementations of real planning and control tools have to be assessed, detailed simulation models are required.

- What are potential weaknesses of this approach?

  Two situations may have to be considered. On one hand, the simulation model does not provide enough information for the planning and control tool. On the other hand, the tool developer uses pieces of information from the simulation model that are not available in a real factory.

- Under which conditions is it possible to generalize the results?

  Due to time and cost constraints, it is only possible to test one or at most a few models operating under the regime of a certain planning and control tool. Thus, we have to develop reference/benchmark simulation models that offer a high level of confidence that the findings for this model also hold for other models and as a consequence for most or even all of the real production facilities it was designed for.

In conclusion, we need more research on reference/benchmark simulation models for complex fabrication facilities. We have to determine how we can build models of minimal complexity that help us to answer most of the questions for the design of factory planning and control mechanisms.

HLA-based Distributed Simulation as an Enabling Technology for the Digital Factory

by ***Steffen Strassburger***

Interoperability and reusability of simulation models are concerns which are addressed by the IEEE standard HLA. In the military simulation domain HLA is accepted since it is a mandatory standard in many cases. In the civilian simulation community HLA is only slowly becoming of interest. Many simulation tool developers (e.g., German market leaders Delmia with QUEST and IGRIP, Tecnomatix with eM-Plant and eM-Workplace) have a somewhat reluctant position toward introducing HLA interfaces into their systems. One reason might be that an HLA interface would enable their customers to let their models talk to models developed in tools from a competitor. Thus the customer is no longer bound to use simulation tools of one vendor. To force vendors to integrate HLA interfaces into their systems a strong pressure from large industrial customers is needed. On the other hand, industrial customers often fail to recognize the value of a standard like HLA. The advantage of HLA as a base technology for the digital factory and virtual manufacturing has not been discovered by most of the potential clients. This is an important problem, although not necessarily constituting a "grand challenge". It is therefore necessary to develop practical applications ('killer-applications') which demonstrate the potential of HLA in the daily business. It is not sufficient to have academic examples, since they are often considered as coming from the ivory tower. In summary, the algorithms and technologies in the area of parallel and distributed simulation have reached a very mature level and have led to an state-of-the-art standard for distributed simulation, namely HLA. Yet, this standard fails to have the deserved impact in many manufacturing applications and industrial applications in general. One party working on the communication and demonstration of the advantages of HLA is the DaimlerChrysler Research Center in Ulm, Germany.

Creating Human-Oriented Simulation: the Challenge of the Holodeck

by ***Bill Swartout***

The TV series Startrek created the notion of a holodeck--- a place on board a starship where a crew member may experience life-like simulations of real or imagined worlds populated by intelligent, interactive virtual characters. The holodeck can be used for education, training or entertainment. While the capabilities of Startrek's holodeck are well beyond what technology can achieve now (or may ever achieve) the vision is still inspiring and for us at USC's Institute for Creative Technology a challenge has been to create a simulator that would provide some of the holodeck's capabilities. While most military simulations involve simulating a vehicle such as a tank, an airplane or a helicopter, our simulation put trainees into human-oriented simulations, where they interact with real and virtual (computer-generated) humans. The behaviors of the virtual humans are not scripted in advance, but instead they use artificial intelligence to communicate with the trainee in natural language and to reason about the events as they unfold and react both rationally and emotionally. While the virtual humans do not strictly follow a script, there is an overarching interactive scenario that provides high-level structure for the training experience. The scenario is structured according to the pedagogical goals we have for the trainee and it contains plot twists and turns that present the trainee with dilemmas and problems to solve. The need for this kind of simulation has arisen because since the end of the cold war, the kinds of operations that the US military is involved with has expanded greatly. The need for peacekeeping and nation-building operations has grown, and humanitarian efforts such as disaster relief are common. A hallmark of these operations is that they frequently involve close ineractions between the military and the local civilian populace. To function effectively and avoid misunderstandings that could have unintended consequences, it is important that soldiers understand the customs, norms, habits and taboos of the local population and they need to be exposed to the thorny dilemmas that may await them. Our virtual human simulator is designed to address that need. In building a simulator such as this, there are many challenges. I will list a few of the major ones here.

- The first challenge is providing the virtual characters with human-like behavior and communication capabilities. We need to deal with the whole range of natural language processing, ranging from speech recognition, to natural language understanding, to generation, to speech synthesis. In addition, to seem human-like, the characters need to be able to engage in non-verbal communication such as gestures and those need to be coordinated with verbal commuication. In addition, to be engaging and natural, the virtual humans need to be able to model and exhibit emotions. This is a new area for AI research, which in the past has been more concerned with creating very rational systems, but not much concerned with trying to create systems that model human emotions.

- A second major challenge concerns the interactive story structure. We need a way of structuring the simulation so that the trainee goes through certain experiences that have training value, yet at the same time we want the trainee to have the perception that he has freewill --- he can do whatever he wants. How can we achieve these two seemingly contradictory goals? The answer seems to lie in directing the behaviors of the virtual humans and controlling the environment so that the trainee is forced into the pedagogical situations we want him to experience. Open issues include first, how to notice when the simulation seems to be getting off track and it is necessary to intervene by directing the behaviors of the virtual humans or environment, and second how to intervene in a way that is not obvious or heavy handed.

While building such a simulation is a major challenge, we have found that now is a good time to start because many of the required component technologies are reaching sufficient maturity. Our experiences in building an initial prototype are outlined in the references below.

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Online Modeling and the Body of Knowledge: Two Challenges for Simulation Methodology

by ***Helena Szczerbicka***

On-line simulation

On-line simulation is a new technology for on-line planning and controlling of systems, which needs further research. An on-line simulation is employed to predict the future performance of the system as it continues to operate under the current control policy. This simulation is also performed for other control strategies that could potentially be applied, IF their performance would exceed that of the control policy, that is currently being applied. A bunch of problems which has not been already crucial for an off-line situation emerge from this situation:

- auto-validation of a model based on actual measurements from the system
- experiment generation at a rate that is faster than real time
- statistical estimators for the future performance of the real system, based on transient behavior
- on-line analysis of a choice of a control policy
- speed-up of the execution of a simulation run

Body of Knowledge

In our efforts to establish Modeling & Simulation as a profession and a scientific discipline we urgently need an unambiguous and widely accepted definition of a notion of Simulation and a description of its Body of Knowledge. The aim of a work in the Workshop in this area could be to survey the recent advances in that field.

Some Ways to Think About Grand Challenges in M&S, and a Couple of Ideas Relevant to Miltary Applications

by ***Greg Tackett***

There are several ways to approach the definition of Grand Challenges, each with their own benefits and pitfalls. This paper discusses several of these approaches, recommends one, and looks at a few military applications.

One Grand Challenge approach is to follow the "Science Fiction" model, where we observe futuristic fictional capabilities such as the *holodeck* and set those capabilities as goals. Visionary science fiction writers such as Verne, Clark, and Roddenberry might tempt us along that path, but for every "20,000 Leagues Under the Sea" there is probably at least one "A Journey to the Center of the Earth", so we need to choose our fantasies carefully, and at least differentiate between Grand Challenges to M&S technology and Grand Challenges to the laws of physics.

A second approach is to look back at computer technology and computer science and correlate great breakthroughs in M&S capabilities to great breakthroughs in the computer industry at large, then use that trend to predict what kind of M&S we might be able to expect by anticipating the next few breakthroughs. This evolutionary approach is conservative in the sense that we don't know what we don't know about the next great invention, but can at least project future capabilities by Moore's Law and today's research projects. The problem with this approach, especially for military applications, is that the systems we are required to simulate are also becoming more complex and high speed, so that every breakthrough in computer technology puts us further behind rather than catching us up.

Perhaps our Grandest Challenge would be to simply catch up with our current requirements! This leads to a third, and most conservative, approach, the "Requirements" model. This approach lists all the things we need to simulate and all the M&S improvements that would need to occur to accomplish them, rank orders them in terms of cost/benefit, and projects that onto current research and development. This approach is near-sighted by design, and perhaps is more likely to generate Great challenges rather than Grand ones.

Integrating these three approaches together, it should be possible to identify some "Grand Challenge Vectors" that pass through current requirements on the way to meeting future ones, and could supply some of the key M&S technologies that could be used for truly futuristic M&S. Three such vectors with application to military systems as well as broader application, are proposed as follows:

Vector 1: Unattended Simulation. This concept is referred to by Dr. Richard Fujimoto of Ga Tech as "Human-out-of-the-Loop". Creating M&S that behave like internet servers, allowing passive execution on demand from remote locations, can meet the immediate requirements of "low overhead simulation drivers" and "client-server" simulations, while positioning us for future requirements through the drastic reduction of manpower and cost associated with M&S, tending towards the goal of "Ubiquitous Simulation", or "Simulation on Demand".

Vector 2: Component Level Interactions. Simulation of military systems and their interactions at the platform level has reached a relative state of maturity, but is very immature at the subsystem and component level. Representations at this level, including vulnerability and reliability of components, are critical to design of systems and logistics on future battlefields. The need to represent this fidelity in battlefield-sized simulations is an immediate requirement for the US Army in the Future Combat Systems (FCS) context, and is fundamentally required for longer-term substitution of simulation for testing.

Vector 3: Distributed Virtual Physical Interactions. Breakthroughs in simulation capability and cost reduction could be seen through the use of distributed, passive simulation objects that interact with one another through the virtual equivalent of Newtonian physics. Virtual environments populated with these models could grow in complexity and content at internet-style rates. This vector has immediate application through the immersion of virtual prototype controls into virtual space, and through interoperability of distributed simulations using advanced state vectors. A more complete discussion of this vector was presented at the Grand Challenges forum of the 2002 Western Computer Simulation Multiconference in San Antonio, TX.

Fast-time Simulations - to Improve the Airspace Structure and Procedures at Airports

by ***Wolfgang Theeck and Michael Moor***

Growth in air traffic has been tremendous over the past 10 years, and is going to rise in the future. Since 1990 the traffic has been growing with a rate of 6.1 %, in fact, passenger traffic doubled in this period. Due to the economic crisis, and the terror attack in New York, in the last two years we have a stagnation of the traffic growth but the forecast for the next year's shows again a growth of about 4%. Faced with the unprecedented growth, airports and air traffic services are being challenged to make even more effective use of their airspace and facilities. Fast- time simulation is a highly cost and time effective way of optimizing our operation to cope with growth, increase the quality of service to customers and provide that service as efficiently as possible.

In this regard, it is important to plan ahead of time and in the right way. Acting too late or in the wrong way can easily lead to enormous costs as a result of delays. The German air navigation services provider DFS Deutsche Flugsicherung GmbH has already mastered many of these challenges with great success.

The DFS Simulation team offers a comprehensive range of services. The team conducts airspace and airport studies in order to:

- Determine capacities and workload of air traffic control sectors
- Design and examine new sectors and ATS- routes
- Optimise arrival and departure routes (STAR/SID)
- Determine capacities of airports
- Optimise taxi procedures
- Optimise the allocation of gates
- Test new taxiways, runways, gates, terminals, de-icing areas

In the future we plan to expand our performance. We see the necessity to solve capacity problems already in the preplanning phase. In nowadays there is still a gap between the preplanned traffic situation and the existing capacity. So the planned traffic situation very often exceeds the existing capacity. It would be helpful to use fast- time simulations already in the preplanning phase to analyze the planned traffic situation and then to correct the planned daily flight plan.

Another field for further improvement is the enhancement of the traffic forecast. In nearly all countries of the world we see a deficit of resources and ATC-controllers. That's why we need the right number of controllers at the right time at the right place. Therefore a new quality of the medium and short term traffic forecast is necessary. A better situation could be reached by a continuous simulation process. A simulation based on the actual radar and planed flight plan information could provide the supervisor with a precise traffic forecast for the next 30-60 minutes.

We obviously see a wide spectrum for fast time simulations in the future. The currently used mechanical simulation tools enable us to solve current problems. In the future we need powerful, enhanced tools, which give us the possibility to model even more complex procedures. That's why the creation of a new model for aviation simulation, which can be used for the rebuilding of the entire airspace structure and procedures is necessary and really a Grand Challenge for Modelling and Simulation.

Technological Challenges for Large-Scale Distributed Simulation

by ***Stephen J. Turner***

Distributed simulation has become increasingly important in recent years as a strategic technology for linking simulation components (or federates) of various types at multiple geographical locations into an overall simulation (or federation). While the High Level Architecture (HLA) [4] has had some success in promoting interoperability and reuse of simulation components, there are still a number of technological challenges to be solved in order for distributed simulation to become more widely accepted. A distributed simulation may involve the integration of simulation components from various organizations and the sharing of disparate and heterogeneous resources. Issues that need to be addressed in order to provide a secure and robust distributed simulation include location of simulation models, access to and management of resources, remote activation of federates, selective information sharing/hiding, security of data, fault tolerance, etc. In addition, in order to provide an effective simulation tool in a distributed environment, new mechanisms may be required, such as cloning [3] for alternative scenario analysis. In many cases, extensions to the current facilities offered by the HLA Runtime Infrastructure (RTI) are required, but these must be implemented in such a way as to preserve the benefits of interoperability and reusability. Many of these technological challenges are similar to those that arise in the emerging field of grid computing [2], in providing flexible, secure and coordinated resource sharing among dynamic collections of individuals and institutions over large-scale networks. The aim of this position paper is to define these challenges and present possible solutions in the wider context of grid computing. A case study from the area of virtual manufacturing is used. Distributed supply chain simulation [5] covers the planning and management of material and information flow through multiple stages of manufacturing, from raw materials through to the customer. With the globalization of markets, a supply chain has evolved from a single enterprise with multiple facilities to one that comprises of companies from various enterprises, dispersed across many different countries. Each of these factories may already have its own simulation model to perform "what-if" analysis of its daily operation and ideally a supply chain simulation can be constructed by reusing these existing models. However, there is a requirement for selective information sharing/hiding in that certain sensitive information should only be available to the factories that belong to the same company or group of companies. This is difficult to achieve with a flat federation and requires an extension to the RTI to support the more general structure of a federation community [1].

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Integrating Simulation inti AOSE - a Multi-Facetted Endeavor

*by **Adelinde M. Uhrmacher***

A gap exists between the current state of the art of simulation methods and the current "modi operandi" in designing agents. Closer cooperations between software engineers, agent developers, and simulationists are called for. Testing of agents requires not only to bring best practice of modeling and simulation to the attendance of agent developers but also to tailor methods and technologies to the specific needs of this challenging application domain. Simulation being an inherent phase in designing agents seems still far away and the path towards this goal provides many challenges.

- Flexibility and "Easy to Use"

  We envision modeling and simulation methods and tools which support a flexible and comfortable composition of test environments for multi-agent systems by re-using models of different languages and by an interoperation with other simulation systems that takes into consideration the semantics of the exchanged information.

- Dynamic Structures

  Agents are characterized by interaction pattern or spheres of influence that vary over time. The ability to adapt their own interaction, composition and behavior pattern challenges the expressiveness of formalisms, and efficiency of tools likewise.

- Efficient Execution

  Methods have to be developed that support the efficient execution of combined, continuous, discrete models that exhibit dynamical interaction and composition structures. As no single strategy will yield the optimal solution independently of the concrete test scenario, flexible simulation tools are required that allow to replace and refine execution methods on demand.

- Models and the "Real Thing"

  The testing of agents would be facilitated if we could switch arbitrarily between an execution in the real environment and an execution in the virtual test environment. In addition simulation means also modeling of agents, and the experimenting with these models. Thus, tools are required that support a graceful transformation from simulation to emulation.

From Simulation to Emulation

by ***Brian Unger***

The simulation of communication traffic and associated network performance is of great economic importance and presents substantial technical problems. The design and provisioning of networks depends on such modeling and analysis, and there are a number of real-time decision support applications that require Internet emulation and simulation at the packet level and above. As wavelength switching becomes practical, there will be a need for very fast performance prediction and network optimization and repair based on these predictions. Both autonomic and direct manual user control will be required. The technical challenges include fast efficient execution; varying levels of abstraction, possibly including flow models; large network and traffic model specification and instantiation; varying the focus of instrumentation, data collection and reporting; dynamic network and traffic parameters and model reconfiguration; real-time decision support through embedded simulation - emulation; and validation at all levels.

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Supporting the Entire Analysis and Design Process

*by **Hans Vangheluwe, Pieter J. Mosterman***

Based on collaboration with bio-engineers to build the WEST modelling and simulation environment (http://www.hemmis.com), a tool to study (build new models) and design (build optimal systems using models) bioactivated sludge waste water treatment plants, I find the two items below most challenging. Though a specific bio-molecular application, bioactivated sludge waste water treatment does exhibit typical characteristics of complexity found in bio-systems which are not found in traditional (electrical, mechanical, hydraulical, ...) engineered systems.

Modelling and Simulation support at different levels of abstraction, in different formalisms.

It should be possible to use custom formalisms (with accompanying techniques and tools) to investigate domain/abstraction-specific sub-problems by domain-experts. These experts should not be burdened with non-essential (to their goal) distractions. Existing modelling formalisms should be chosen and new formalisms should be designed to be as close as possible to the problem domain. Formalism choice should be exclusively driven by the requirement that modellers must be able to reason compositionally in terms of principles relevant in their problem domain. For example, a modeller should be able to think in terms of conservation of energy rather than in terms of numerical solutions to underlying differential equations. This challenge is closely related to the Multi-Paradigm and Unification challenges described in the position statements of Pieter Mosterman and myself in the Modelling and Simulation Methods section.

Modelling and Simulation support for Experimentation.

Not only Modelling and Simulation environments, but rather complete Experimentation Environments must be built to support the whole spectrum of tasks a bio-molecular researcher is faced with. In particular, (statistical) data analysis, model calibration/parameter estimation, optimization, ... must be designed into an Experimentation environment and should not be an afterthought. Identified gaps in model bases must lead in a natural way to meaningful experimental setups (e.g., by means of optimal experimental design based on sensitivity analysis of models). Results of experiments should lead naturally to new information to be added to model bases. This iterative, combined inductive/deductive process must be studied, modelled, and designed into Experimentation Environments.

A Model-based , Unifying Framework for Inter-disciplinary Design

*by **Hans Vangheluwe, Pieter J. Mosterman***

The complexity of systems we study and design, in particular those of an inter-disciplinary nature, has increased dramatically over the last few decades. This complexity is due to a number of factors:

- the number of components of the system;
- the diversity of these components, in particular the presence of hardware, software, and cognitive parts. More formally, this implies the use of a plethora of formalisms, some of which are highly domain-specific (e.g., in hydraulics);
- the different levels of abstraction at which systems are studied;
- the abundant presence of feedback;
- dynamic, structural changes;
- adaptivity, often combined with reflection of systems upon themselves;
- the spanning of multiple applications domains.

Research in different application domains, on different formalisms, as well as on different techniques and tools has hitherto been mostly isolated (with the notable exception of Zeigler's Theory of Modelling and Simulation). There is a need to unify and integrate the above to address the analysis and design of truly multi-disciplinary, complex prolems. In particular, there is a need for a unifying framework for multi-disciplinary problem solving, with a focus on design. The focus on design is pragmatic. Focusing on analysis will require the inclusion of inductive methods. The need for a framework must be addressed at the level of a unifying theory and should be supported by methods, techniques, tools, and above all standards to be adopted. The modelling and simulation viewpoint provides a general and intuitively appealing paradigm for unification. In my opinion, the starting point for this should be existing work in multi-formalism modelling and simulation, meta-modelling for software design, hybrid systems design, and solutions in particular inter-disciplinary application domains such as the automotive industry. The above really boils down to the need for Multi-paradigm modelling as described in Pieter Mosterman's position statement. The Grand Unification challenge is not an unattainable goal. I will demonstrate a first attempt which combines meta-modelling (to describe formalism syntax) with Graph Grammar models of transformation (to describe formalism operational and denotational semantics, code synthesis, model simplification, ...). The demonstration will use the AToM3 multi-paradigm modelling tool

http://moncs.cs.mcgill.ca/MSDL/research/projects/AToM3.

Aviation Modeling and Simulation: The Agony and the Ecstasy

by ***Fred Wieland***

An air traffic control (ATC) system is an example of a complex, nonlinear, adaptive system whose modeling requirements span the gamut detailed interagent interactions through system-wide queueing abstractions. As an example of ATC complexity, consider a scenario in the summer of 2000, where five extra arrivals at Newark airport in the northeastern United States caused over 250 delays throughout the northeast, through the propagation of delays from one air traffic center to another. This situation has become increasingly more common in the last few years.

The events of September 11 2001 have ameliorated this condition somewhat, but only temporarily. Models of ATC complexity can be classified into three categories. First, there are mechanical models that move aircraft through well-defined procedures. Secondly, there are economic models that determine the behavior of the institutions involved in air transportation, such as airlines, regulatory authorities, and passengers. Finally, there are information models that compute the flow of information among the various agents. Any comprehensive study of air transportation must consider all these dimensions to provide valid and useful recommendations for evaluation ATC changes.

Simulating What Cannot Be Simulated

by ***Olaf Wolkenhauer***

The background to these notes is the expectation that mathematical modelling and simulation is going to play increasingly important role in the understanding of the organization and control of genetic-, metabolic-, and signalling pathways. I am going to argue that for modelling and simulation to help our understanding of cellular dynamics, the current practice of experimental design has to change - away from a `mining' approach towards a signal- and systems-oriented methodologies. The emergence of systems biology has therefore as much to do with the development of new techniques as it is relying on a new `way of thinking' about cellular systems. This argument leads us to the fact that there exist a principal limit (or uncertainty principle) to what we can achieve in simulation and with the machine metaphor in particular. Amongst the many modelling paradigms suggested for cellular systems, it is clear that none is accurate and yet general. I am therefore to discuss a conceptual framework that generalizes a number of models (including Bayes nets, state-space models, Boolean networks) and should allow us to discuss the previous issues in a formal framework. From my discussion of the fundamental questions of the life sciences, the following key research challenges arise for modelling and simulation:

- Dynamic regulation and spatial organization: the need to capture both, spatial as well as temporal aspects simultaneously (spatio-temporal modelling).
- Intra- and inter-cellular actions and interactions: the need for large-scale and hybrid-systems modelling and simulation.
- Crossing organizational levels: from cells, to colonies, tissues, organs and organisms, ...
- Integrating experimental levels: genome, transcriptome, proteome, metabolome and the physiome.
- Combining data analysis and data management: The need to combine computational tools, developed for specific tasks and different organizational and descriptional levels.
- Relating formal representations (mathematical models, e.g. Boolean networks and rate-equations). Providing a conceptual framework and theoretical foundations for the previous five points.

Simulation and Agent-Oriented Software Engineering

*by **Franco Zambonelli***

Agent-oriented software engineering promotes modeling software systems in terms of autonomous components interacting with each other and with the environment in which they are situated. Indeed, it appears like most of modern software systems exhibits characteristics of autonomy, interactivity, and situatedness that can make them assimilate to multiagent systems. These include pervasive computing systems, mobile computing systems, and Internet applications. By broadening the perspective beyond computational systems, almost all types of complex systems with which science has to deal with are made up of autonomous, interactive, and situated systems. These include ecological and biological systems, social systems, and economical systems. Starting from the above perspective -- and after having introduced the basic concepts underlying agent-oriented software engineering -- the talk will analyze how agent-oriented software engineering has the potential to emerge as a general-purpose approach to deal with the complexities of today's systems -- whether computational or natural. In particular, by specifically focusing on simulation issues, the talk will try to show that:

- multi-agent systems may be effectively used to simulate the behavior of several complex systems, with a greater accuracy than it is achieved by other computational methods (e.g., cellular automata), typically failing in taking into account characteristics such as situatedness, autonomy, and/or interactivity.

- the isomorphism between natural systems and multiagent systems, and the fact that natural systems may exhibits very complex emergent behaviors, let us envisions that similar sort of emergent behaviors will characterize multiagent systems as soon as they will start populating our computational and physical environments. To be ready for that time, and given that the irreducibility of such complex behaviors make traditional analytical methods fall short, simulation methods and tools appears the only way to promote and engineered and reliable approach to multiagent systems development.

Working Groups Results

Molecular & Cellular Systems Working Group

Summary of the Dagstuhl Working Group, Tusday, 27 August 2002

LIST OF PARTICIPANTS

Catholijn Jonker, Bogdan Lesyng, Dieter Lorenz, Alke Martens, C. Michael Overstreet, Mathias Röhl, Hans Vangheluwe, Olaf Wolkenhauer

INTRODUCTION

Mathematical modeling and simulation of molecular and cellular dynamics is widely perceived as a bottleneck for a better understanding of gene expression and regulation, genetic-, metabolic-, and signaling pathways. With the availability of new experimental technologies to observe cellular systems, life scientists are considering "their" particular systems no longer in isolation or at only one particular descriptional level but instead consider a wide range of techniques, providing information from the genome, transcriptome, proteome, metabolome, cellome, and physiome. A number of challenges arise from this new approach that characterizes the post-genome era of the life sciences.

In the following the discussion of the working group is summarized. The aim was to discuss challenges for modeling and simulation in the post-genome era of the life sciences and to devise a "grand challenge"/"competition" as a vehicle to stimulate research and help bring together interdisciplinary research groups to tackle some of the hurdles that have been identified.

The composition of the working group and the relatively short time that was available, necessarily restricts the scope of this report to sketch only some of the issues that are relevant to this vast emerging area of research.

CHALLENGES AND HURDLES

Despite decades of research into systems theory, modeling and simulation of dynamic systems, the **complexity** of molecular and cellular systems is striking. Even for what life scientists would consider a 'simple' system, the number of interacting components or subsystems is 'large' compared to the systems successfully dealt with, for example, in the physical and engineering sciences. The systems are further connected, building **networks** that are again integrated in **hierarchies** or multi-layered architectures. The complexity of the systems considered does therefore highlight the importance for a study of the way in which we approach such biological systems. Ontological questions, posed by biologists, generate interesting epistemological questions related to the way of thinking that is chosen.

In other words, not only the type of mathematical model used (e.g. differential equations vs. automata) is important but also the modeling process itself, the strategy to identify the appropriate mathematical formalism is relevant. The need for such **meta-modelling** becomes clear when we look at the purpose or use of the final model. The purpose of mathematical modeling and simulation of molecular or cellular systems is usually not to provide accurate, quantitative predictions of variables in a system. Instead, the aim is to elucidate the principles that generate an observed phenomenon. For instance, in time series analysis and forecasting the quality or "usefulness" of a model is determined by a measure such as the mean square error. The nature of the model (e.g. stochastic, deterministic, rule-based, ...), the order, structure etc. does not matter too much. In molecular and cell biology however, the mathematical model is required to have not just predictive power (can be validated through experiments) but also explanatory power. The semantics or interpretation of models is playing a bigger role in generating and testing hypotheses. For alternative formalisms, the transformation of those models from one conceptual framework into another poses a number of methodological as well as technological challenges.

The task of modeling and predicting processes within a cell may provide a challenge that reminds us of weather forecasting. Despite the ever more increasing computer power which allows us to simulate increasingly complex (and thus more accurate) models, our conclusions from it can only be expressed with some **(un)certainty**. Ideally, any formal approach should therefore be capable of producing some measure of uncertainty associated with inferences and predications. Our analogy of "cellular weather forecasting" highlights another challenge for modeling and simulation in the post-genome era: **spatio-temporal modeling**. To study **intra- and inter-cellular dynamics** it will be important to not only consider temporal aspects but also to account for the topology of these systems. The function or behavior of a biological pathway is determined by space *and* time. For a simulation of such systems that takes us from particle systems to the physiology of an organism, a very large range of time scales has to be dealt with in simulations.

GRAND CHALLENGE ON CELLULAR SYSTEMS

In this section we outline a "grand challenge"/"competition" as a vehicle to stimulate research and help bring together interdisciplinary research groups to tackle some of the hurdles that have been identified. One outcome of such grand challenge are 'test bed', 'benchmark' problems which are going to allow computer scientist, physicists, mathematicians and engineers with little or no experience in the bio-sciences to enter this interdisciplinary field. In honour of Alan Turing, the first computer scientist and of those the first to take an interest in mathematical biology, such a competition could be referred to as the "TURING CELL PROJECT". The development of cell models in numero, in silico will provide a platform to test bioinformatics algorithms but may also generate useful educational tools.

- Tests: input / output behavior
- Models: explanatory vs. predicitive
  testing (bioinformatic) algorithms
- Competition
  - Free style simulation: biologists (students) identifying biological systems (education, value for)
  - Abilities
    - Abstraction / generalization
    - Testing hypothesis
    - Generating hypothesis
    - Allowing genetic modification
    - Allowing experimental modification of variables & structure
  - Leagues / teams
    - e.g. E. coli league
    - Organisms / cells ?
  - E-environment (computer(s) - plugged into a wall)
  - SBML (System Biology Markup Lanuguage), SBWB (System Biology WorkBench) compliant
- Types of users:
  - Life scientists
  - Non-biologists with an interest in math & computing
  - 'Physical sciences'
- Winning by votes:
  - Innovation, 'beauty' of the approach
  - "Usefulness"
    - Educational
    - Industrial / Sociable
    - Scientific practice
- System / parameter identification from numerical data
  - Model validation

Report of the Aviation Grand Challenge Working Group

The aviation group consisted of: Fred Wieland, George Donohue, Amy Pritchett, Wolfgang Theeck, Michael Morr.

The goal of civil aviation agencies worldwide is to simultaneously maximize throughput and safety in the air transportation system, subject to a variety of environmental, regulatory, and economic constraints. In both Europe and North America, the growth in the air transportation system is limited by its capacity: in Europe, there is limited capacity in the airspace, while in the United States the capacity constraint is airports. However both regions are experiencing growth such that future capacity constraints are likely to be in both airspace and airports. Creating a common platform for modeling future visions of air transportation systems - from small changes like congestion-based pricing to large changes such as bidding for arrivial time slots - is the Grand Challenge that must be met by the modeling and simulation community. To provide a common environment for future vision analysis requires cooperation among various institutions, international standards (probably mediated by an international board), and commitment to explore changes in a virtual environment.

Such a "system of systems" approach requires that each institution create models and simulations in specific, focused areas of air transportation that they know best. For example, airlines might create realistic models of scheduling dynamics in the face of traffic restrictions; civil aviation authorities might create realistic models of decision making for flow control; airframe manufacturers might contribute realistic models of aircraft performance. A "system of systems" simulation environment would allow each institution to contribute without revealing proprietary algorithms of decision making policies. A study of the current or future air transportation system would involve identifying a study question, selecting a situable set of models, integrating them in a common environment, running distributed experiments, and analyzing results.

The Grand Challenge is to create an environment in which this paradigm can be realized. Such an environment requires technical advances, inter-institutional coordination, an overarching design and vision, and the incentives necessary to motivate organizations to contribute. The combination of all these areas - technical, institutional, and economic - constitutes a Grand Challenge for the aviation community.

Parallel/Distributed Simulation Working Group

Summary of the Dagstuhl Working Group, Tuesday, 27 August 2002

LIST OF PARTICIPANTS

Rassul Ayani, John Fowler, Richard Fujimoto, Pieter Mosterman, George Riley, Oliver Rose, Steffen Strassburger, Helena Szczerbicka, Steve Turner, Adelinde M. Uhrmacher, Brian Unger, Franco Zambonelli.

INTRODUCTION

The field of parallel/distributed simulation has matured over the last twenty years and its feasibility and practicality have become widely accepted. The focus of this working group was on parallel/distributed *discrete event* simulation. Parallel simulation refers to the execution of a simulation on a tightly coupled architecture, such as a shared memory multiprocessor, where the main objective is to reduce the execution time. Distributed simulation refers to the execution of a simulation on a loosely coupled system, such as a set of computers connected by a LAN or WAN. Here the main objectives are the linking of distributed resources and/or people and the reusability and interoperability of simulation components.

The group recognized that the consequences of Moore's Law meant that sequential computing speeds are fast enough for many simulation applications. Although there are some large-scale simulation applications that do require parallel computing, these are relatively few in number. For a simulation that is synchronized with the physical system, "faster-than-real-time" forecasting can require the use of parallel simulation techniques. Also, Moore's Law does not help when the problem size is growing at the same or a faster rate than the speed of sequential computers. An example is simulating the internet, where the router link traffic doubles every six months. However, the widespread use of parallel simulation techniques seems unlikely in the near future.

The group agreed that ubiquitous computing and communications offered new opportunities and challenges for parallel and distributed execution. The discussion therefore focused on a new paradigm for discrete event simulation that involves interaction with the physical system in a mutually beneficial way. It was decided that the name "Symbiotic Simulation System" best describes such simulations. The following sections address the questions: What are Symbiotic Simulation Systems? What are the Grand Challenge Applications? What are the Grand Challenges or milestones for parallel/distributed simulation?

SYMBIOTIC SIMULATION SYSTEMS

A Symbiotic Simulation System is defined as one that interacts with the physical system in a mutually beneficial way. It is highly adaptive, in that the simulation system not only performs "what-if" experiments that are used to control the physical system, but also accepts and responds to data from the physical system. The physical system benefits from the optimized performance that is obtained from the analysis of simulation experiments. The simulation system benefits from the continuous supply of the latest data and the automatic validation of its simulation outputs. Such a definition implies continuous execution of the simulation and real time interaction with the physical system.

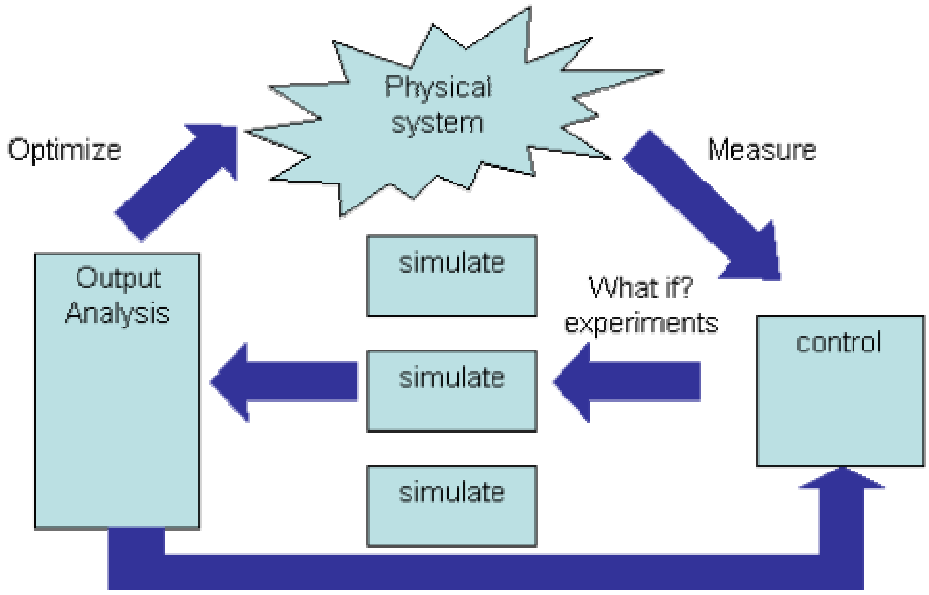

Figure 1. Symbiotic Simulation System

The structure of a symbiotic simulation system is shown in figure 1. Measurements are taken from the physical system in order to obtain the latest data. A control or decision support function conducts "what if" experiments to investigate alternative scenarios based on these measurements. From an analysis of the output results, the physical system is optimized so that its performance is improved. The results are also fed back to the control function for automatic validation and subsequent decision making. Such an approach provides a new paradigm for discrete event simulation, allowing the construction of applications with greatly enhanced capabilities.

GRAND CHALLENGE APPLICATIONS

Symbiotic simulation systems have the potential to provide near optimal management and control of physical systems in many diverse areas including transportation, communication, manufacturing, commerce, etc. Some Grand Challenge application areas for symbiotic simulation systems are:

- *Urban Transportation Systems.* A large-scale distributed simulation, executing on an ad hoc network of vehicles, could provide personalized information services and a predictive capability that would avoid congestion and crashes. Major benefits would be improved safety, economic savings and a reduction in environmental pollution.
- *Internet or Military Communication Networks.* Online network simulation could be used to provide self optimizing communication networks. Measurements of the physical network could be used by the simulation system to optimize and reconfigure the physical network in order to improve its performance and avoid bottlenecks.
- *Manufacturing.* There is a need for quick "what-if" analysis in order to respond to abrupt changes in the status of a factory. An online simulation of a factory that is continuously updated with manufacturing system data can provide such analysis on demand, thereby improving the performance of the factory and the competitiveness of the company.

Other potential application areas include simulation of computational grids, large-scale transportation systems, air traffic, multi-agent systems, etc.

GRAND CHALLENGES FOR PARALLEL/DISTRIBUTED SIMULATION

In addition to the Grand Challenges presented by the above application areas, constructing such a large-scale symbiotic simulation system provides a number of Grand Challenges for parallel/distributed simulation:

- *Compact Representation of System State.* A large-scale symbiotic simulation system may have up to a million elements in its system state. How should we represent these so that they can be sampled as often as is necessary for output analysis and optimization of the physical system?
- *Fault Tolerant, Robust Systems.* Components of a distributed simulation are liable to failure. How can we ensure that the overall system remains operational, despite some percentage of failed components and/or links?
- *Multi-Resolution Modeling.* How can we integrate different levels of abstraction dynamically as new simulation component models are embedded into the distributed simulation?
- *Model Execution.* How can we obtain fast model execution for self adaptive simulations of complex systems that must meet real time constraints (typically with a speed of 10 × real time)? For some applications of symbiotic simulation systems, the system size/complexity is increasing faster than Moore?s Law (circuit simulation, internet).
- *Interoperability.* How do we achieve true "plug-and-play" interoperability where we are able to create a simulation "widget" and embed it into distributed simulation in less than 1 minute?

- *Large-Scale Time Synchronization.* How can we provide time synchronization across such large-scale distributed simulations? Existing algorithms do not scale well and new algorithms and methods are needed.
- *Automatic Validation.* How can we automatically validate the output from the simulation system against the physical system? Some self adaptive validation mechanism is required to improve the accuracy of the simulation.

CONCLUSIONS

This working group summary describes a new paradigm for simulation applications: symbiotic simulation systems. Such a simulation system can dynamically accept and respond to online data from the physical system in order to improve the accuracy of the model. Analysis of the simulation output can be used to control and optimize the physical system. A number of potential Grand Challenge application areas are identified where such as approach can greatly enhance the simulation capabilities and provide major benefits. This summary also presents a number of technological Grand Challenges for parallel/distributed simulation that need to be addressed to enable such symbiotic simulation systems to be constructed. Associated with the idea of symbiotic simulation systems are "everlasting" (or "immortal") simulations, where the simulation is running all the time and is fed with a continuous supply of data from the physical system. Another related topic is "simulation on demand", where an online simulation that is continuously updated with real time data can provide instant "what-if" analysis.

Summary of the Findings from the Military Working Group of the Dagstuhl Seminar on Grand Challenges for Modeling and Simulation

Introduction

The military working group consisted of: Paul Davis, Paul Fishwick, Dell Lunceford, Ernie Page, Bill Swartout, Greg Tackett and Jayne Talbot. The group met from 10:20 - 4:00 on Tuesday 27 August 2002.

The group began by considering the points raised by Lunceford in his military keynote. The group attempted to cover the widest spectrum of the military modeling and simulation problem domain as feasible in the time allotted, and attempted to limit its focus to hard, but tractable, problems. The goal of the discussion was to characterize a hard problem (in a given area) and its possible solution, rather than all hard problems (in that area). In the end, the group suggested six areas from which Grand Challenge problems for military modeling and simulation might be formulated.

Military M&S Challenge 1: Training

Problem Statement: *Provide a simulation capability for the individual ground combatant, in an urban environment, executing a mission such as warfare, limited police action, or peacekeeping, that is equal or superior to current training*.

Motivation: The challenge for simulation-based training, in general, is to provide a cost-effective alternative to other training methods. That is, the benefit-to-cost ratio for simulation-based training must exceed the benefit-to-cost ratio for "live" training. Using the ratio as the metric, the benefits of simulation-based training might be less than the benefits of live training, so long as the costs are commensurately less also. The Grand Challenge for training (simulation-based or otherwise) is to provide an equal or superior surrogate to "real-world experience." That is, we would like to be able to provide a combat training environment within which the learning is equivalent (or superior) to actual combat experience.

Today: The military has used simulation-based training as effectively as any other institution in the world. Simulation is used to train individuals and groups at all levels of combat and across the widest range of missions. Beyond the opportunity to simply rehearse motor skills (e.g. manipulating the stick controls on a flight simulator) techniques for introducing the psychological factors of immersion and decision-making within "fog-of-war" are well-known in the military training community.

Thoughts on the Future: Could we develop a cost-effective, deployable, re-configurable MOUT-site capability (e.g. using technologies similar to Institute for Creative Technologies FlatWorld)? Could building interiors be configured for specific missions using data feeds from mobile robotic sensors?

Military M&S Challenge 2: Testing

Problem Statement: *Provide a simulation capability to enable acquisition of a future Army system, without the use of full-system physical prototypes, that is equal or superior to current developmental and operational testing practice*.

Motivation: The use of full system prototypes to support developmental and operational test can be a significant cost for major systems, since these prototypes are developed and subjected to destructive testing and therefore cannot be fielded. These tests are necessary to help validate that certain system characteristics are within predefined performance thresholds-or, in some cases, to help identify these performance thresholds. If these thresholds *could* be reliably determined using computer models of the system, thus eliminating the need to develop and destroy physical prototypes, a significant cost savings would result for many acquisition programs.

Today: A mathematics for quantifying and reasoning about uncertainties and error estimations in physical testing and simulation-based testing for arbitrary systems operating in arbitrary environments does not exist.

Thoughts on the Future: This problem is probably best attacked from both theoretical and practical perspectives. On the theoretical side, a statistics of small numbers must be matured such that better estimates can be derived from limited numbers of live fire events. A methodology (and more robust mathematics) for model validation must be defined such that we could say, for example, given model, M, of system S, x simulated live fire events are required to generate a 0.95 confidence interval for the value of a given random variable, which would require y actual live fire events on a full system prototype(s). Or, more likely, we'd like to say that a 0.95 confidence interval can be attained using a combination of x simulated live fires events and y actual live fire events- where we expect that x is much larger than y, and that y is small but, perhaps, never reaches zero. On the practical side, we could empirically evaluate the utility of simulation-based evaluation versus hardware-based evaluation in controlled experiments. For example, under the auspices of an ATD, or ACTD, conduct a controlled acquisition experiment within which two similar (unmanned) systems are manufactured and certified through DT/OT where one system is subject to traditional DT/OT practice and the other is conducted entirely in simulation.

Military M&S Challenge 3: Real-time Decision Support

Problem Statement: *Provide a simulation capability equivalent to a wargaming capability, deployable on portable handheld devices, usable by combatants in the field.*

Motivation: The individual combatant's need for situational awareness (SA) is well-known, and much of the focus in the development of next-generation warfighting equipment, e.g. Future Combat Systems (FCS), Objective Force Warrior (OFW), involves techniques to capture and disseminate SA. Beyond SA, however, we believe that an automated decision-support facility would also enhance warfighter effectiveness.

Today: Programs such as Land Warrior and Objective Force Warrior seek to equip the individual combatant with an advanced uniform coupled with integrated weapons and communications systems. Features of these systems include helmets with integrated information displays, weaponry equipped with laser-sighting, global positioning and video capabilities, integrated radios and computer subsystems. Some work ongoing includes the use of handheld devices with the capacity to sense threats such as mines.

Thoughts on the Future: What types of decision-support models could be utilized using the information being collected by the systems of OFW? Could these models be resident on the soldier's uniform-based computing subsystem (e.g. what is there memory and power footprints)? Or could they be remotely located on robotic followers? What is the nature of the user interfaces to these models, e.g. voice, eye-tracking?

Military M&S Challenge 4: Defining the Family of Abstractions for Military Simulation

Problem Statement: *Define a broadly applicable family of abstractions for modeling military systems. Formulate a mathematics that allows formal reasoning about these abstractions and their relationships to one another.*

Motivation: The need for, and benefits of, modeling systems at varying levels of abstraction is well known. The Laws of Newton and Kepler, for example, view the Universe at one level of abstraction while Quantum Mechanics views the Universe at a very different level of abstraction. In cases where we can formally relate varying abstractions of identical systems, our ability to reason about these systems is significantly enhanced. A good example of such a capability is within the integrated circuit design and manufacturing communities. These systems may be modeled at the physics level, or at any number of levels of logic (and/or gates, adders, etc.). The relationship between a representation at one level and a representation at another level is unambiguously defined by physics. In the military domain, we often align our abstractions with military echelon (e.g. individual combatant, platoon, company, battalion, etc.). However, the techniques that we use to reason about the relationships between these levels of abstraction are often ad hoc.

Today: The emergence of "interoperability" as a system objective as enabled by the High Level Architecture has resulted in a proliferation of couplings (federations) of disparate simulations. Resolving the differences in the underlying modeling objectives, assumptions, objects, attributes, spatial and temporal resolutions, and units of measurement (to name only a few) is a manually-intensive effort that is the heart of the FOM building and FEDEP processes. While these processes provide a potential systems engineering framework for the reconciliation effort, a mathematics that formally verifies and guides these activities is not well-defined. The independent efforts of Davis, Reynolds and of Deitz begin to provide (at least a form for) some of the needed mathematics in "multi-resolution modeling".

Thoughts on the Future: Continue the theoretical work. Support with focused experimental efforts within the context of such systems as the Joint Virtual Battlespace. Attempt to construct an environment within which highly detailed engineering-level models feed models at successively higher levels of aggregation up to, and including, models used for strategic (campaign-level) analysis. Evaluate the performance of such federations and their analytical robustness.

Military M&S Challenge 5: Interface Methodology

Problem Statement: *Create a more effective interface for model design and development since models in today's military M&S are treated purely at the level of code. Effective human interfaces to these models are lacking.*

Motivation: Models of theatre conflict and materiel often lie at a level above computer code, and need to have more substantial support in both their: (1) interfaces to the human, and (2) dissemination among organizations.

Today: Models are often referred to in terms of "code", but most models are more effective when specified and presented visually. These visual models are rapidly playing more significant roles in software development, and they can play a concomitant role in model development.

Thoughts on the Future: Ideally, models would be created and represented in ways that are engaging and immersive with respect to human analysts. This suggests more research in human interfaces to model components and their interconnections. Also, better interface languages, can foster interoperability of models at a level above code, in terms of model structure and model interaction. While the Holodeck presents a futuristic view of interfaces to models, today's technology in graphics, sound, and multimedia creates a pathway for future progress in making models as immersive as the military phenomena that they are modeling (i.e., materiel, missions and scenarios).

Military M&S Challenge 6: Analytical Effects of Assumptions

Problem Statement: *Create a methodology to explicitly and automatically associate assumptions with the validity and utility of analytical results.*

Motivation: The danger of using a model in contexts that violate the modeling assumptions is well known.

Today: Theoretically, the number of assumptions underlying any model is infinite. Practically, however, a manageable number of key assumptions could be identified. Most often, when these assumptions are identified, they are provided to a modeler in human-readable form, e.g. text. Little, to no, automated assistance is available to a modeler to determine if a model application is consistent with the model assumptions.

Thoughts on the Future: Develop a schema (e.g. using XML) to encode modeling assumptions in machine-readable form. Develop an analysis tool that examines the modeling assumptions and model source to advise of potential conflicts. We recognize that the Halting Problem implies that such a system cannot guarantee that all possible conflicts are determinable. It may also be useful to instrument the model to execute *within* the context of the analysis tool, thereby enabling the tool to determine if certain dynamic properties of model execution took it outside the bounds of the modeling assumptions (in a manner similar to running a program within a debugger to catch, for example, division-by-zero errors).

Modeling and Simulation Methods Group

Summary of the DagstuhlWorking Group, Thursday, 29 August, 2002

Introduction

The methods group consisted of: Paul Davis (chairman), Paul Fishwick, Erol Gelenbe, Catholijn Jonker, Alke Martens, Ernest Page, Pieter Mosterman, Helena Szererbricka, Olaf Wolkenhauer, and Hans Vangheluwe

The methods group discussed a wide range of subjects, but organized thinking around three dimensions: abstraction, formalism, and perspective. Models and model families need to cover the resulting space and there is need to be able to move around within that space (e.g., from a high-resolution model in a particular formalism and perspective to a different model with lower resolution and the same perspective, but a different formalism). Key elements of being able to do so will include multiresolution, multiperspective modeling (MRMPM); exploratory analysis and models enabling it; tools for dynamically adjusting and tailoring abstractions; tools for mapping among and making use of very heterogeneous model and data types; and improved human interface modalities afforded by viewing models from multiple perspectives.

The overarching goal is to have methods and tools that facilitate the semi-automated development and adaptation, for particular purposes, of mutually self-consistent models of various types. These should make use of all available information and should map consistently to each other so that users can tailor models to their specific needs while drawing upon pre-existing constructs in diverse forms, and while making use of context-specific information.

Taken together, this goal generates several grand challenges involving concepts, methods, and tools-including those making it possible to efficiently transfer model understanding to others (i.e., to enable rapid learning).

Grand Challenge 1: Develop environments facilitating multiresolution, multiperspective modeling (MRMPM) and subsequent adaptation.

Motivation: It is increasingly recognized that workers in many fields need models representing the subjects of their study at different levels of resolution and from different perspectives. Having such multiple representations is of limited value, however, unless the relationships among them are well understood, which leads to the desire for families of models and, ideally, integrated families. The goal here is to have model families that permit a user of models to apply the appropriate model for his very specific purpose, and to then move to higher or lower resolution, and from one to another perspective, as necessary to exploit or explain different classes of information, address different questions, or communicate with people having different backgrounds.

Today's Baseline : Although the idea of model families is hardly new, it continues to be quite difficult for most organizations to develop such families, much less to maintain them. Much of what has been done in the past has amounted to collecting independently developed models, declaring them to be a family, and working hard to understand how to move from one to another. Even in organizations that use model families (which may have as few as two members), the norm is to relate the models only occasionally, as in calibrating a low-resolution model.

Vision: The goals described under "motivation" appear to be at least plausible, but very challenging. It seems likely that an ideal environment facilitating development and use of MRMPM will allow for

- Built-in exploratory analysis to assist in developing local abstractions (i.e., abstractions suitable for a particular domain of the problem space) (see Figure 1)
- Dynamically created and adjusted abstraction hierarchies (i.e., the capability to generate local metamodels or appropriate disaggregations)
- Mutual calibration for consistency within a model family, using all available data, including heterogeneous
- Multiple modes of human interaction with the model, by altering the look and feel, using for example, 2D and 3D presentation styles which can be changed to suit the individual modeler.

Elaborating on the last point, the goal in building the environment should not be automated operations, but rather highly effective man-machine interactions. A user, for example, may have enough domain-specific knowledge to suggest the structural form of a metamodel, i.e., to guide the computer in "motivated metamodeling." Similarly, the user may be able readily to suggest assumptions to be used in disaggregation (e.g., equal splitting among components, or splitting weighted by one or another component attribute).

Grand Challenge 2: Develop tools for creating, transforming, and tailoring multiresolution, multiperspective model families, starting with models and data that may be quite heterogeneous in formalism and in other respects.

Motivation: Model families will often (and perhaps typically) have to be constructed by pulling together and adapting models that were developed independently. They may all be imperfect in various ways (either in concept or in the sense of their implementations having some errors). Similarly, the data available for calibration and validation will be imperfect. Both the models and the data will often be very different in character. Some may be mathematical in nature, but even there large differences may exist. One model, for example, may be developed in a formalism of continuous partial differential equations; another may be developed in a formalism of discrete-event simulation; yet another may be a closed-form analytical model. Still other models may not even be mathematical in nature: they may, for example, be in the form of data bases or iconic representations. All disciplines from Physics to Landscape Ecology exhibit these scales, and while there are approaches in each area, we still lack a science or domain-independent methodology for multiresolution, multiperspective modeling. What is needed, then, is the ability to begin with such a mixture and generate a respectable family of models that are mutually calibrated and consistent with all known information (suitably "weighted" according to its relevance and perceived validity) (Figure 1).

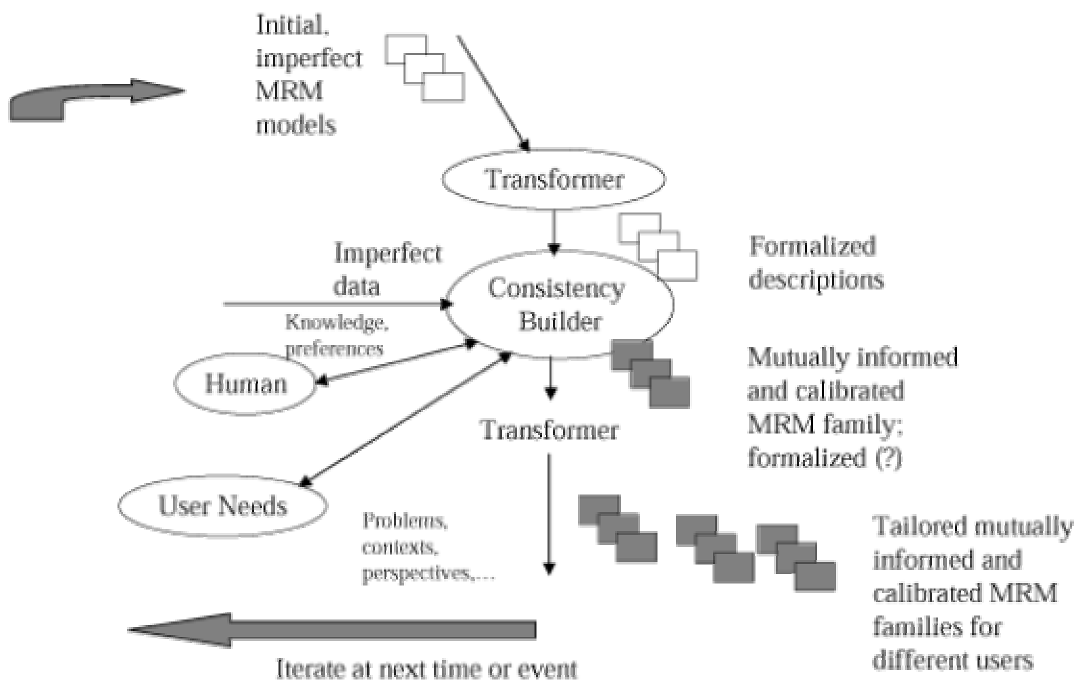

Figure 1: Capabilities for Creating, Transforming, and Tailoring MRMPM Familes from Diverse Starting Components

Grand Challenge 3: Understand theory for and propose "streams" for future multi-model frameworks over time, starting close to the implementation end of things, extending to broaden applicability, and moving farther into the realm of model character and content. What is desirable and feasible, building on HLA, XML, and other contemporarary items?

Motivation and Vision: Dealing with "heterogeneity" as discussed above means working in a "multimodel" construct that pulls together highly disparate forms of information.

The Baseline: Understanding how to do so is still in its infancy

Grand Challenge 4: Build, use, explain use of, and transfer effectively a large, complex simulation model (e.g., 100, 000 lines of code) with "order of magnitude" improvements in clarity and transferability.

Motivation: Increasingly, it is essential for geographically and even organizationally separate work groups to use models developed elsewhere. This is fundamental to distributed war gaming, for example, but also to simulation-based acquisition. It is not sufficient merely to take in an alien model and "run it;" instead, there is often need to understand it, and perhaps to adapt it or suggest changes in its operations consistent with one's own purposes.

The Baseline : Although large models have certainly been transferred, documented, and used, the time and trouble involved in doing so is notorious. It is probably not uncommon for such efforts to involve tens of man months with only partial success.

The Vision: It is plausible that dramatic improvements can be made in the efficiency and effectiveness of such transfers. This will surely require tools such as standardized beseline cases, tutorials, and the like, but dramatic improvements will likely also require fundamental changes in the methods used. In the learning of foreign languages, for example, "total immersion" has been found to be far more effective than lengthy classroom learning. In strategic planning, organizational learning is often much faster when brought about with techniques such as gaming, which capture attention and emotion as participants work problems. Virtual environments are proving effective for some kinds of learning, and also for military mission rehearsal. Tools may be feasible that could semi-automatically translate documentation and tutorials into a variety of languages, formats, and characters. It is plausible, then, that much can be accomplished (or attempted).

Simulation and Agent-Oriented Software Engineering: Working Group Report of the Grand Challenges Dagstuhl Seminar

Members of the Group: P. Ciancarini, G. Donohue, D. Lorenz, P.Panzarasa, A. Pritchett, W. Swartout, A.M. Uhrmacher, F.Zambonelli

Introduction

Modeling and Simulation are indeed important phases in the engineering of any complex system, and they are also fundamental for the understanding and control of existing systems. However, it appears like: on the one hand, current approaches to modeling and simulation still fall short in capturing essential properties and behaviors of several classes of complex systems (e.g., Internet traffic and air traffic control); on the other hand, the results achieved so far in the area of modeling and simulation are largely under-exploited, as there are areas in which modeling and simulation theories and tools -- although likely to be useful -- are not systematically used, e.g., agent-oriented software engineering.

The "simulation and agent-oriented software engineering" was one of the working groups at the Dagstuhl Seminar (02351) on Grand Challenges for Modeling and Simulation, and was composed by an inter-disciplinary group of researchers in different topical areas related to both agent-oriented software engineering and modeling and simulation. The main goal of the working group was to identify the "Grand Challenges" for researches in the area of simulation and agent-oriented software engineering, by trying to work and discuss along two different perspectives:

- *agent-oriented software engineering for simulation:* to which extent the research results recently achieved in the area of agent-oriented software engineering can be of use in improving current practice in the design of simulation systems?
- *simulation for agent-oriented software engineering:* to which extent modeling and simulation methods can be of use in improving current practices in agent-based computing and agent-based software engineering?

State of the Art in Agent-oriented Software Engineering

As in many working groups on agents, one of the first problems we tackled was to settle on a definition of agents, e.g., "is this an agent, or just a program"[4, 6]

When adopting a "weak" perspective on agency -- to which some of the working group members committed -- even concurrent objects with their own thread of control can be considered, to some extent, agents. However, the weak perspective on agency appears unsatisfactory when one is looking for higher-order functionality and characteristics that are more and more required in several applications areas. In particular, two of such characteristics, reflection and introspection, related to agents and multi-agent systems ability to change their own behavior for adaptability's sake, are currently sufficiently supported neither by conventional modeling and simulation methods nor by current agent-oriented software engineering approaches. Such characteristics are those that the "strong" perspective on agency -- to which some others of the working group members committed -- consider as those that definitely make agents and multi-agent systems different from other systems.

Whatever, weak or strong, perspective on agency is adopted, current software engineering practice is mostly experimental in nature. Wooldridge and Jennings[2] recently stated that agent development intrinsically leads to experimental endeavor, since no tried and trusted design methods are currently available and maybe never will be. In fact, the complexity of today's software systems, and specifically the complexity of agents' internal and of multiagent systems interactions, can make the development and the understanding of these systems very hard, challenging any engineered approach[1, 3] . For instance, concepts such as "emergent behaviours" and "self-organization" are becoming part of the everyday vocabulary of software engineers.

One flew east, And one flew west, And one flew over the cuckoo's nest.

Any discussion on applying simulation as a method for agent-oriented software engineering is difficult and prone for misunderstandings (as it was at the beginning of the Dagstuhl Seminar). On the one hand simulation is used for agents, on the other hands agents are used for simulation. W.r.t. the former case, most multiagent systems and applications are executed in simulated environments and often within a simulated network, with the main goal of illustrating the effectiveness of a systems and with the final results of producing nothing but a simple toy simulation, hardly representative of the potential behaviour of the real system. W.r.t. the latter case, agents or likes (e.g., simple active objects) are often used in the modeling of, e.g., sociological system, or to design simulation systems as communities of "weak" agents.

The relationship between agents and simulation makes them very closely interwoven and, although initially misleading, was successively exploited by the working group to clearly detail the commonalities between simulation and agent-oriented software engineering, and the mutual benefits that could possibly derive from *(i)* the application of agent-oriented software engineering concepts to simulation and, *vice versa* from *(ii)* the exploitation of simulation and modeling in the development of multiagent systems. In particular:

- Both agents and simulation have in common the concept of "environment", and both give importance to the representation of such environment. Agents, the same as those systems typically the subject of simulation, are embedded in complex environments about which they typically maintain an abstract representation, i.e., a model. Understanding how the two separated and hardly interacting communities of agent-oriented software engineering and simulation approach the same problem of modeling the environment may provide sources of inspiration and useful feedbacks to both.

- Agents and multi-agent systems are complex systems whose behavior -- in several cases -- cannot easily be predicted and engineered in a direct way [1, 3]. Modeling and simulation typically deal with predicting and understanding the behaviour of complex systems for which no engineering practice can guarantee a predictable behaviour. The consequence is, agent-oriented software engineering cannot abstract from the presence of agent-specific modeling and simulation tools, as the only means for understanding and evaluating the behaviour of complex multi-agent systems before their actual deployment.
- Simulation of complex systems often involves the presence of humans and of human organizations (both reflective and introspective by nature), requiring modeling the presence of such adaptive behaviors. The lessons of agent-oriented software engineering can be exploited to this purpose and to enable the definition of more accurate models and of more realistic simulations. On the other hand, knowledge and experiences in the area of modeling and simulation could contribute to more valid and more sophisticated user models for testing and evaluating multi-agent systems.

The above identified commonalities and the fact that there is room for mutual benefits, have been used as a starting point to identify Grand Challenges for research in the area.

A Grand Challenge: Valid Environmental Models

If we wish to experiment with multiagent systems, the modeling of the environment in which agent executes, typically open and dynamic, is central. A typical example for an agent system's environment is the Internet: Internet and Web agents have to execute by interacting with each other and with an environment made up of a variety of services, data sources, operating systems. So, one cannot think at properly simulating agent systems without being able to properly model and simulate such environment.

For instance, one very important reason calling for a proper modeling of the environment comes from the observation that the environment and its dynamics may dramatically impact on the global emergent behaviour of agent systems and, more generally, of any systems of autonomous components (there included biological and social systems).

However, defining proper modeling of an agent environment is definitely a grand challenge. For instance, with reference to Internet agents (i.e., agents executing and carrying on their activities in the Internet and/or in the Web), it turns out that simulating the Internet and the Web, due to their size and dynamics, is a Grand Challenge by its own (compare the working group on Grand Challenges on Simulating Computer Networks). Simulating the Internet and the Web for the sake of multiagent system simulation may be a bit more feasible: in this case, there is no need to simulate the level of single IP packets, and coarser modeling of interactions, e.g. between service providers and others, may be enough. Still, how such simplified modeling should be and how it should be tackled is an open uneasy question: *(i)* the same modeling can hardly apply to all of the agent systems (e.g., E-commerce agents may require a different modeling of the Internet than required by, say, network manager agents); *(ii)* most of today's agent-oriented software engineering methodology provides little or no attention to the problem of environment modeling, and sometimes also provides only ill-defined or partially specified environments. This makes it very hard to develop "plug and play" simulation environments to support the user and to facilitate a systematic simulation of agent-systems.

A Grand Challenge: Modeling Human Behavior

In the interplay between simulation and agents, valid models of human behavior play often an essential role. On the one hand, in the testing of multiagent systems, modeling the behaviour of human actors interacting with the system may be very important, e.g. the acceptance of many service agents will depend on a suitable, timely interaction with human actors. On the other hand, simulation systems that require simulating the presence of humans in the loop, may take advantage of the lessons of agent-oriented software engineering only if specific models and tools to effectively simulate human behaviour are available.

This interdisciplinary challenge requires the cooperation between the community of cognitive science and psychology, of modeling and simulation (e.g., to help fostering such valid models of human behavior and to enable their re-fining and re-using in different settings), and of agent-oriented software engineering (e.g., to produce usable agent-based software modules of human behavior), are necessary. Far from being easy, and calling us back to the very unanswered questions of artificial intelligence and cybernetics, the development of reasonably accurate and usable models of humans behaviour could provide notable advances in both agent-oriented software engineering and simulation.

Conclusions

Beside those deeply analyzed within the working group, a lot more challenges -- both small and large ones -- have been identified, e.g.[5]. All of these challenges have to be met before simulation will be established as a basic tool for the designing of agent systems. Designing engineered multiagent systems is a grand challenge by its own. Researches in agent-oriented software engineering are at the very beginning, and still mainly focused on a weak perspective on agency. All of the members of the working group agreed that it would be essential to establish simulation more firmly in the software engineering life cycle of agent systems and that this will happen eventually. Unfortunately, detailing roadmaps to fasten this process seemed too difficult to develop given the short time frame of the working groups and must be reserved to subsequent activities.

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Modeling and Simulation of Manufacturing Systems

Report of the Manufacturing Working Group

List of participants: John W.Fowler, Oliver Rose, Steffen Strasssburger, Steve Turner

Even though we have moved beyond the Industrial Age and into the Information Age, manufacturing remains an important part of the global economy. There have been numerous efforts to use modeling and simulation tools and techniques to improve manufacturing efficiency over the last four decades. While much progress has been made and more and more manufacturing decisions are being made based on the use of models, their use is still sporadic. We believe that there is a need for pervasive use of modeling and simulation for decision support in future manufacturing systems. There are several challenges that need to be addressed by the simulation community to realize this vision. First, we discuss the grandest of the challenges and then discuss three other grand challenges. We call the first challenge the "grandest" because the next three challenges are really subsets of the first. Finally, we discuss a challenge that is not truly a grand challenge, but it is challenging and is also important.

Grandest Challenge #1: An order of magnitude reduction in problem solving cycles

It currently takes too long to design, collect information/data, build, execute, and analyze simulation models to support manufacturing decision making. This leads to a smaller number of analysis cycles than is desirable. While there are opportunities for efficiency improvements in all phases of the simulation process, we particularly see opportunities to reduce the time needed to collect and synthesize the required information and data and opportunities to reduce the time to carry out the experimentation. The reduction in information/data collection and synthesis time can partially be achieved by proactive data analysis and by instilling better factory discipline in maintaining current information systems. The reduction in experimentation time can be approached from a number of different angles including exploring models of reduced complexity that still give high fidelity results, using variance reduction techniques, and possibly through distributed and parallel simulation.

Grand Challenge #2: Development of real-time simulation-based problem solving capability

The status of the factory is constantly changing and the changes often occur very abruptly. This leads to the need for quick what-if analysis at any time. Currently, the time needed to collect and synthesize the required information/data and the time required to do the experimentation are simply too long. Having a persistent model that is constantly updated with current manufacturing system data and therefore available on demand could potentially reduce the time spent dealing with the information/data.

<*Grand Challenge #3*: **True Plug-and-Play Interoperability of Simulations and Supporting Software within a Specific Application Domain**

If we begin to have persistent models of the manufacturing system, it is likely that there will actually be models of many different subsets of the factory. These models will need a seamless way to interact with each other. In addition, more and more of the information/data will be provided from other manufacturing support software such as the Manufacturing Execution System, Available To Promise systems, analysis software packages, etc. It will be increasingly more important for all of these systems to be able to quickly communicate with each other and the outside world in an unambiguous way. The High Level Architecture is a partial solution to this challenge.

Grand Challenge #4: **Efficient Hierarchical Simulations of Manufacturing Systems/Supply Chains**

Simulation models are currently being used to support decision making at the machine, factory, and enterprise/supply chain levels. For the most part models are used at just one of these levels and little information is shared between them. In the future, it will become increasing necessary for these models to used in conjunction with one another. In order to do this several key questions remain; what is the right level of abstraction for each model? Can parallel and distributed simulation capabilities be employed? What is the right way to share information between the levels?

Big Challenge #5: **Greater Acceptance of Modeling & Simulation within Industry**

Our group decided to label this challenge as a "Big" challenge instead of as a "Grand" challenge because it is not really a technical challenge but more of a social challenge. While the use of modeling and simulation in manufacturing is steadily gaining acceptance for certain applications (such as capacity planning), there is still a long way to go before it is commonly applied for a multitude of applications. Currently modeling people often spend much of their time convincing management of the need for these services. This has the potential to ultimately be successful, but we caution simulationists to resist the temptation to oversell the use of the model's results; this may be a good short term strategy, but it can have very negative long term consequences if the expectations of the users of the model results are not met.

Network Simulation Working Group

List of Participants: George Riley (chair), Rassul Ayani, Richard Fujimoto, Erol Gelenbe, Brian Unger

Introduction

Simulation has become the method of choice for a large part of computer networking research. Building simulation models of end protocols, routing protocols, queuing disciplines, and communications links (just to name a few) is in general easy and gives suitably accurate results for the research at hand. However, creating and executing simulation models for networks of moderate to large size is very resource intensive. Modeling a network of just a few thousand network elements will exhaust memory and CPU cycles quickly, unless care it taken in the design and deployment of the simulator.

Future uses for simulation in networking research will certainly require simulation models far exceeding the size and complexity of that presently achievable with existing simulation environments. The working group identified a number of emerging research areas that will require simulation models consisting of tens of thousands to millions of network elements in order to reach valid conclusions.

1. Predict the evolution of the Internet. Can we make reasonable predictions about the growth and demand on the Internet as a result of fundamental changes and advances in end-user behavior? What type of services will be needed and how will they perform in the presence of ubiquitous Internet access using portable hand-held access devices? Will present day routing protocols and end user protocols be sufficiently robust to handle another order-of-magnitude (or more) increase in end systems and end user data requests?
2. Evaluate the security of the Internet. Can we simulate the behavior of large–scale Denial–of–Service (DOS) attacks on Internet hosts and servers? Can we use such simulations to develop and evaluate counter-measures for these attacks. Can we use simulation to evaluate methods to strengthen the security of presently deployed systems, to subvert future attacks before they happen?
3. Evaluate the affects of new router design and switching methods. The fundamental packet–switched design of the present day Internet is not well suited for wavelength switching using optical networks. Can we design and simulate new router designs, and new routing methods that utilize emerging optical networks? What affect will these new switching methods have on the performance of the Internet as perceived by the end user?
4. The social and economic impact of using the Internet. Can simulation models of large–scale networks be used to predict the economic impact of Internet usage? Will the use of cheap advertising and “renting eyeballs” on popular web servers

result in a positive return on investment for the advertisers? Does large–scale e–mail spam achieve the desired customer response and return?

5. Using on–line simulation be used to optimize revenues at a large Internet Service Provider. ISP's derive revenue by receiving packets from their customers, and expend funds by delivering packets to their peers and their next–level providers. Can real–time, on–line simulation methods be used to dynamically adjust routing paths between providers to optimize revenue and minimize costs? Can we reduce load from end users during times of higher costs, and increase load from users during times of lower cost?

6. Predicting the affect of large socio–economic changes in third world countries. Can large–scale simulation of portions of the Internet predict the affect of the emerging social and economic changes in countries such as China and Korea? Can we use simulation to predict in advance the network demands due to these changes? Can the simulation drive the design and future deployment of the Internet based on simulation results?

7. Understanding the affect of the next *Killer Application*. Recently the end user load placed on the Internet has been dramatically affected by the emergence of peer–to–peer networks, such as Napsterand Gnutella. Before that, the emergence of the World–Wide–Web caused a shift in network usageand demands. Before the World–Wide–Web was email and file transfers. Each new killer application causes a fundamental shift in network usage and load. Can we use simulation to predict the affect on the network of the next killer app, such as:

   (a) Entertainment Content Distribution. Internet experts and researchers have long predicted the use of high–quality audio and video distribution (such as current television signals and emerging high–definition television) using the Internet infrastructure. While this type of network usage is not presently feasible, new and advanced methods for last–mile network access (such as fiber to the home) will enable these and other high–bandwidth data access methods from personal and home end systems. What fundamental changes need to be planned for, designed, and deployed in the Internet to enable such delivery mechanisms? What will be the expected demand on the network in the presence of high–demand items, such as World Cup soccer or first–run movies? What will be the social impact on the availability of all sorts of video entertainment in the home environment?

   (b) Tele-Presence. With the future availability of high-quality video and audio services in the network, can we predict the impact on network usage due to electronic meetings. What will be the overall economic impact on the transportation industry due to reduced travel requirements for face–to–face meetings. Will electronic job interviews reduce employer expenses or increase expenses due to possible poor hiring choices?

   (c) Distributed Immersive Environments. Will future advances in haptics and other sensory stimulus devices affect the demand and performance of the Internet? Can we simulate the data requirements and performance demands place on the Internet due to extensive use of these immersive environments?

In light of these future requirements for large–scale network simulation, the group identified three Grand Challenges to pose to the network simulation research community.

Grand Challenge 1. The ability to simulate efficiently and accurately the consequences of *fundamental changes* in end user demands and expectations on the Internet, to enable the design and deployment of a network infrastructure to support those changes **before** those changes are actually needed in the network. Can we determine *in advance* the equipment design requirements for things such as interior routers and high–speed backbone links? Can we design and recommend a reasonable and workable network topology to support the increased demands?

Grand Challenge 2. The use of simulation to improve the resilience of the existing communications infrastructure to deliberate electronic warfare (Cyber–attacks). Can we simulate the existing infrastructure in sufficient detail to find vulnerabilities **before** they are exploited? Can we test and evaluate proposed defensive measures? Can we perform sufficiently detailed and accurate post–incident analysis simulations to determine cause and affect of attacks? Can we determine the social and economic impact of these potential attacks, such as the inability to complete financial transactions on a timely basis?

Grand Challenge 3. The use of simulation for real–time network management and control. Can on–line and real–time simulation assist in disaster recovery activities, to help maintain critical communications in the presence of catastrophic disruptions, either deliberate or natural. Can on–line simulations be used to maximize profit, reliability, and quality of service at first and second tier Internet Service Providers?

Summary. The grand challenges are all loosely based on the requirement to provide a simulation environment for research in computer networks that can efficiently and accurately model and simulate networks consisting of hundreds of thousands of network elements. Further, these simulation models must be driven by and based on accurate predictions of end user behavior, and must be able to analyze the simulation results in terms of economic and social impact of the network behavior.

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