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GRAND CHALLENGE CASE STUDIES IN A SIMULATION CURRICULUM

Michael Spiegel
Paul F. Reynolds Jr.
David C. Brogan

Modeling and Simulation Technology Research Initiative
151 Engineer's Way, P.O. Box 400740
Department of Computer Science University of Virginia
Charlottesville, VA 22904-4740, U.S.A

ABSTRACT

Students wishing to become experts in modeling and simulation (M&S) need to appreciate limitations of the technology. Our goal is to expose students to the current boundaries of simulation technology. To achieve this, we propose the incorporation of grand challenge case studies into a modeling and simulation curriculum. Grand challenge problems are defined as problems for which there does not exist a universally accepted solution (at present). We argue that grand challenge case studies are an excellent vehicle for discovering and appreciating current boundaries of M&S technology. We present three candidate case studies, one in detail - the ongoing U.S. Department of Energy analysis of Yucca Mountain as a location for nuclear waste storage - with supporting discussion about how these cases can enhance exploration of the challenges in M&S technology. We discuss the proposed Yucca Mountain storage facility, along with two other case studies, and examine their integration into M&S curricula.

1 INTRODUCTION

Our goal is to expose students to the current boundaries of simulation technology. To achieve this, we propose the incorporation of grand challenge case studies into a modeling and simulation curriculum. These case studies should feature complex applications that highlight the grand challenges in M&S, and they should lie on the threshold of what is possible with today's M&S technology. Case studies "[are] the vehicle by which a chunk of reality is brought into the classroom...A good case keeps the class discussion grounded upon some of the stubborn facts that must be faced in real life situation. It is the anchor on academic flights of speculation."(Lawrence 1953) We focus on a detailed case study related to the U.S. Department of Energy proposal for the Yucca Mountain nuclear waste storage facility. Yucca Mountain demonstrates the teaching of M&S grand challenge issues using real world case studies. Also, we briefly discuss two additional topics for case study analysis: weather forecasting and epidemic disease spread.

The analysis for Yucca Mountain requires the prediction of events up to one million years. The study requires "an analysis that couples atomic-scale processes, such as spent fuel and waste package corrosion, to crustal-scale processes, such as volcanic activity and climate change" (Ewing and Macfarlane 2002). The coupling of phenomena at disparate spatial or temporal resolutions is a hallmark of multiresolution modeling. The safety argument for Yucca Mountain involves a quantitative simulation that combines nuclear chemistry, corrosion chemistry, hydrology, geology, climatology, and ecology, among other fields. Combining these simulations presents a unique challenge for model validation. The challenges of multiresolution modeling and model validation will be explored in the Yucca Mountain case study.

The Dagstuhl report on Grand Challenges for Modeling and Simulation (Fujimoto et al. 2002) is an excellent overview of the current open research areas in M&S. Working groups at the workshop touched upon complexity, meta-modeling, uncertainty, abstraction, dynamic data-driven modeling, composability, reusability, multiresolution/multiperspective modeling, and cognitive modeling. The issue we find most urgent is the apparent weak preparation students receive for addressing M&S grand challenges. A survey of current M&S curricula at the college level reveals little emphasis upon relating known M&S grand challenges to science and technology modeling analysis. We believe a corpus of science and technology grand challenges which employ and/or depend on M&S solutions should be constructed. Accompanying this corpus should be the identification and analysis of the M&S grand challenges that cut across these application models. We argue there is no better material for exposing students to the critical issues, or for fostering cross-disciplinary studies for how to address them.

The next section discusses related work on simulation curricula and the uses of case studies. In Section 3 we provide background material on the Yucca Mountain storage facility. Section 4 outlines the grand challenge case study that focuses on coupling a series of models at different temporal and spatial scales. Section 5 describes the process of model validation for the Yucca Mountain project. Subsections 5.1.1 - 5.1.5 discuss each of the attributes that must be validated in order to meet the standards of environmental safety. Section 6 outlines the use of weather prediction and epidemic disease spread as topics for grand challenge case studies. The final section offers suggestions for selecting grand challenge case studies and incorporating them into existing course material. An appendix provides the recommended course readings for the Yucca Mountain case study.

2 RELATED WORK

We have surveyed the curricula of several institutions with a major M&S curriculum (Old Dominion University, California State University at Chico, Naval Post Graduate School, University of Hamburg, University of Arizona, Georgia Institute of Technology). Our goal was to discover how case studies are used in the classroom. We have found the use of small or moderately sized examples as teaching aids. The exercises instruct the students on successful methods for solving understood problems. The purpose of a grand challenge case study is not to show students how to employ known solutions and solution techniques. Grand challenge problems are defined as problems for which there does not exist a universally accepted solution (at present). The purpose of a grand challenge case study is to show students the possibility of design decisions in the face of great uncertainty.

Grand challenges reveal the state of the art for the hardest problems in M&S. Most curricula in modeling and simulation do not highlight the importance of these grand challenges. Rather they place emphasis on the tools and practices needed for becoming a simulationist (Szczerbicka et al. 2000, Altiok et al. 2001, Crosbie, Zenor, and Hilzer 2001). This is why most case studies in simulation appear in subject-specific courses where the focus is not on advancing M&S technology but rather on the case being studied.

We currently offer a graduate seminar that presents a critical analysis of the existing capabilities, challenges, and limitations of M&S technology (Reynolds 2006). Key topics in the course include multiresolution modeling, parallel and distributed simulation, dynamic data-driven application simulation, agent based simulation, model reuse, composability, and verification, validation, and accreditation. At present this course is taught as a literature survey. We have begun experimenting with the introduction of grand challenge case studies into this course. The Yucca Mountain project has been used in the discussion of multiresolution modeling and model validation. Recognition of the importance of this case study has led to our current argument that such case studies should be incorporated more deeply into M&S technology curricula.

3 BACKGROUND MATERIAL

The Yucca Mountain project calls for the storage of 70,000 metric tons of high-level nuclear waste in the Nevada desert. Ninety percent of the the waste will consist of spent nuclear fuel from commercial nuclear power plants in the United States. The facility will require between 1,150 to 2,500 acres of total underground storage area (Craig 1999).

Yucca Mountain is approximately 160 kilometers northwest of Las Vegas at the southwestern edge of the Nevada nuclear test site. The mountain is more accurately described as a series of ridges that extends 40 km in length. The water table is approximately 500 to 800 m underground at the proposed storage location. The proposed site would be located in the region of rock above the water table known as the unsaturated zone (Whipple 1996). Limited contact between nuclear waste and water is essential to minimize the environmental impact on the surrounding population.

Approximately 200 km of drifts (tunnels) will be dug into the mountain to store the waste in $\sim$ 10,000 metal canisters. The waste packages (metal canisters) consist of an outer wall of carbon-steel and an inner wall of a nickel-based alloy. A titanium enclosure known as a drip shield will be installed over the waste packages in order to divert moisture around the packages (Craig 1999).

A safety assessment that extends far into the future must address potentially disruptive events that occur on a geological scale. Specifically there is a possibility of either volcanic activity or seismic activity in the next million years that must be considered. Long-term climate change will likely induce periods of substantially increased precipitation. Other potentially disruptive events include accidental human intrusion into the repository (OCRWM 2002).

The storage facility has an allowable radiation dose to the residents of the nearby community of 15 millirems (mrem) per year for the first ten thousand years. The radiation dose is allowed to increase to 350 mrem/year for a period of 1 million years thereafter(Carter and Pigford 2005). These radiation limits can be compared to worldwide levels of background radiation which vary from 100 to 1000 mrem/year (Ojovan and Lee 2005).

4 YUCCA MOUNTAIN CASE STUDY

The Yucca Mountain case study is ideal for elucidating M&S issues such as multi-resolution modeling, model composition and validation. The Yucca Mountain study consists of the aggregation (composition) of multiple models of different parts of the studied system. In many cases the models incorporate or assume the same phenomena, but at different spatial or temporal resolutions (multi-resolution). Model composition and multi-resolution modeling are known to be extremely challenging problems in the M&S technology community. How well these issues are addressed has profound impact on model validity. The Yucca Mountain study offers an excellent opportunity for M&S students to study a socially relevant, technically challenging, high impact analysis that demonstrates the potential pitfalls associated with multi-resolution modeling, model composition and validation.

Copious government reports about the Yucca Mountain analysis are publicly available. Due to the potential environmental impact, the analysis of Yucca Mountain is available for public inspection. There is vigorous public debate regarding the accuracy of predictions on radionuclide containment. Neighboring Eureka County and the state of Nevada have conducted independent assessments of the site suitability.

The Department of Energy (DOE) is responsible for the assessment of Yucca Mountain, but the Environmental Protection Agency (EPA) is responsible for setting the environment standards of radionuclide containment. The Nuclear Regulatory Commission (NRC) is responsible for developing regulations based on the EPA standards and ensuring that the DOE is in compliance with these regulations. This legislative division of responsibilities ensures a healthy debate on the validation of the simulations that are used and has led to an abundance of available materials.

The Yucca Mountain case study should begin with background material on nuclear waste management. Students should use several readings to become familiar with the goals and parameters of the Yucca Mountain project. An abbreviated characterization of the proposed storage facility has been presented in Section 3. Students should be able to answer the following questions: Why is underground storage of high-level nuclear waste necessary? What are the spatial and temporal scales of waste repository site management? How do we predict the effectiveness of radionuclide isolation at the storage facility? How do we validate our predictions? How did we determine the standards against which we perform model validation? What is the margin of error of the model validation?

The best sources to answer these questions are available from the DOE. They have published the *Yucca Mountain Science and Engineering Report* (OCRWM 2002), which describes the scientific and engineering studies of the Yucca Mountain site, the nuclear waste to be disposed, the repository and waste storage designs, and the long-term performance of the proposed repository.

The safety case for the Yucca Mountain storage facility relies on a quantitative simulation known as the Total System Performance Assessment (TSPA). The TSPA attempts to predict annual radiation dosages to the nearby human community over a period of one million years. It is a system model built from a collection of coupled component models. The major components of the TSPA are presented in Section 5. These component models reveal the difficult issues that must be addressed in M&S composability.

The TSPA is explained in the DOE report *Total System Performance Assessment for the Site Recommendation* (OCRWM 2000g). Students should use this report as their primary source on simulations in the Yucca Mountain project. We recommend that the students focus on a subset of the TSPA model components. They should identify how these components fit into the larger total system performance assessment. What assumptions are made in the components? And how do these assumptions agree with the assumptions made by the larger system model?

The students should also read from the *Joint NEA-IAEA International Peer Review of the Yucca Mountain Site Characterisation Project's Total System Performance Assessment Supporting the Site Recommendation Process* (NEA-IAEA 2002). This international peer review was conducted by the International Atomic Energy Agency and the Nuclear Energy Agency. It contains an analysis of the Yucca Mountain performance assessment methodology with respect to international standards, recommendations, and practices. An external peer review, such as this one, offers another perspective on the difficulties of multiresolution modeling and model validation.

5 MODEL VALIDATION

Model validation for the Yucca Mountain project is a fascinating topic because it forces the recognition of all the challenges associated with multiresolution modeling and model composability. It is not sufficient to construct the total system performance assessment and then argue the relative safety of the storage facility based on this model. They must first be validated as a unit before they can be used in the safety case for Yucca Mountain. We must convince ourselves of the accuracy of the predictions that extend over a period of one million years. Model validation forces a careful investigation of the assumptions and decisions that were used for multiresolution modeling and model composability.

The Yucca Mountain total system performance assessment is required by federal law to perform the following obligations (10 CFR 63.2):

1. Identify the features, events and processes (except human intrusion) and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years af-

ter disposal [the Environmental Protection Agency has issued a proposal amending this section to 1,000,000 years (EPA 2005)];

2. Examine the effects of those features, events, and processes and sequence of events and processes upon the performance of the Yucca Mountain disposal system; and
3. Estimate the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, and processes, and sequences of events and processes weighted by their probability of occurrence.

5.1 Yucca Mountain Safety Case

The safety case for Yucca Mountain must involve a probabilistic assessment of the potential risks involved. The Department of Energy rests their proposed safety case on five key attributes: "(1) limited water entering waste emplacement drifts; (2) long-lived waste package and drip shield; (3) limited release of radionuclides from the engineered barriers; (4) delay and dilution of radionuclide concentration by the natural barriers; and (5) low mean annual dose considering potentially disruptive events." (OCRWM 2002) The component models that must be aggregated to address the safety case are illustrated in Figure 1.

5.1.1 Limited Water Entering Drifts

Limited water entering waste emplacement drifts is the first line of defense against radionuclide transport to the water table. The climate and geology of Yucca Mountain suggest that limited water will enter the emplacement drifts. The region experiences an average annual precipitation of 190 mm per year. And much of this precipitation either runs off the mountain or is lost to evaporation.

There is debate over how much water flows through fractures in the rock versus water flowing directly through the rock. Evidence from nuclear weapons tests suggest that water can flow long distances through rock fractures in short timespans. Fractures in the rock would lead to short transport times, but it is believed that the volume of water that takes this "fast path" is relatively small. We advise our students that while the volume of fast path water is an interesting debate (Metlay 2000), little of the evidence on either side relies on the validation of simulations.

5.1.2 Long-Lived Waste Packages

The metal canisters (waste packages) will be composed of an outer wall of a corrosion-resistant nickel-based alloy and an inner structural shell of stainless steel. The corrosion rates of the nickel-based alloy are on the order of 10 to 1,000 nm/year. Extensive modeling has been performed to simulate the physical and chemical conditions of the waste package repositories. These models need to accurately represent the temperature, relative humidity, rate of evaporation, composition of water and gas in the host rock, formation of salts and precipitates, effect of microbial activity on the chemical environment, etc. We must rely on simulations to measure the long-term performance of waste packages because the family of nickel-based alloys have only been used for a few decades at most.

5.1.3 Limited Release from Engineered Barriers

The engineered barriers consist of the waste packages, the drift invert (the platform for the waste packages), and the titanium drip shield. A one-dimensional transport model is used to represent advection and diffusion of radionuclides away from the engineered barriers. Advection is the process by which particles are carried along by moving water. Diffusion is the process of particle migration from zones of high concentration to low concentration within standing water. The transport model attempts to predict the interactions between the waste form particles, corrosion particles from the waste packages, and groundwater particles.

5.1.4 Limited Release from Natural Barriers

The natural barriers consist of the surface soils and topography, unsaturated rock layers above the repository, unsaturated rock layers below the repository, and volcanic tuff and alluvial deposits below the water table. Many of the same features that apply to limited water entering the waste emplacement drifts also apply to slowing the rate at which radionuclides travel through the natural barriers.

5.1.5 Potentially Disruptive Events

The low mean annual dose considering potentially disruptive events is most interesting because it attempts to quantitatively assess the probability and damage of potentially disruptive events. The Department of Energy developed an electronic database of over 1,700 potentially disruptive events. Next the events were screened on the basis of regulatory guidelines, probability of occurrence, and consequences to radionuclide containment. Any event with an estimated probability of occurrence less than 10^{-8} per year was excluded from further consideration. So for example an impact by a meteorite is not considered a potentially disruptive event because the estimated probability of occurrence is about 10^{-12} per year. The most high-profile potentially disruptive events that remain are seismic and volcanic activities.

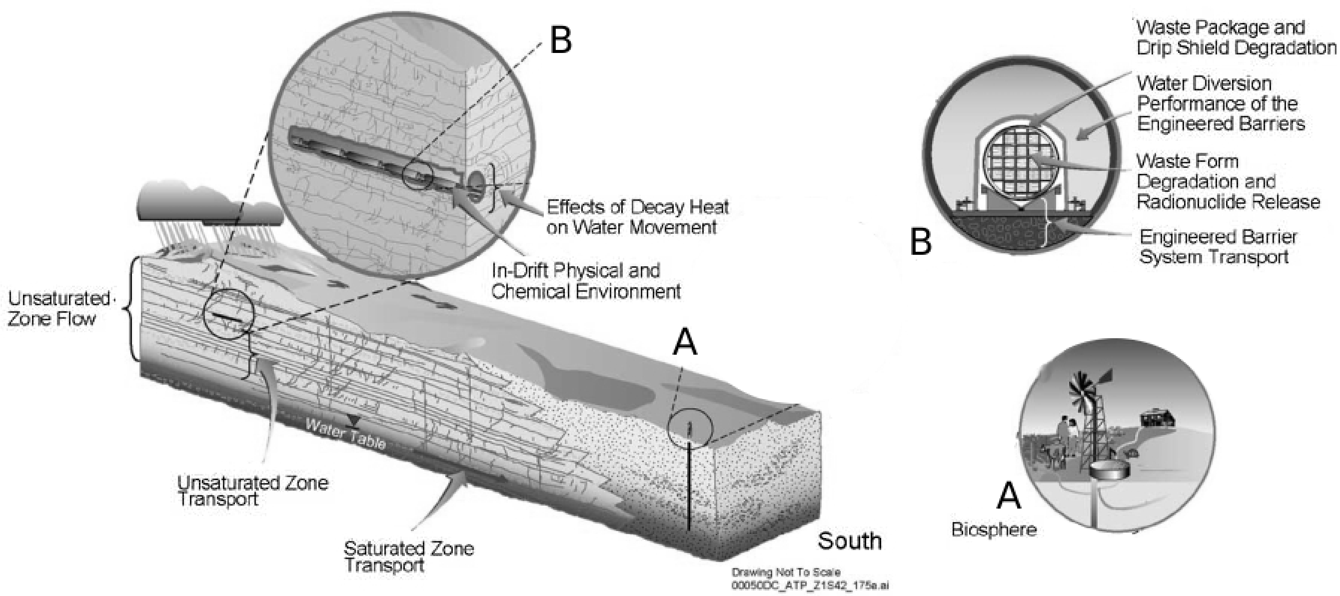

Figure 1: Component Models of the TSPA (Figure Courtesy of the U.S. Department of Energy: OCRWM 2002)

5.2 Component Models

Each component model of the total system performance assessment is individually documented:

- Integrated site model (OCRWM 2000d);
- Unsaturated zone flow and transport (OCRWM 2000h);
- Near-field environment (OCRWM 2000e);
- Engineered barrier system degradation, flow, and transport (OCRWM 2000c);
- Waste package degradation (OCRWM 2000j);
- Waste form degradation (OCRWM 2000i);
- Saturated zone flow and transport (OCRWM 2000f);
- Biosphere (OCRWM 2000a);
- Disruptive events (i.e., seismicity and volcanism) (OCRWM 2000b).

We recommend that the instructor select one of the five attributes of the safety case (presented in Section 5.1) and then use the matching component models to show a partial walkthrough of the model validation process. Alternatively the class can be split into smaller groups, and have each group responsible for learning and presenting one of the safety case arguments.

6 ADDITIONAL CASE STUDIES

We present two additional case studies as topics for a curriculum of grand challenge case studies. These two case studies are weather forecasting and the spread of epidemic diseases. Due to space limitations, these cases are described in brief. We have focused on the learning objectives for each of the two case studies as they relate to M&S technology challenges. Weather forecasting is an archetypal example of a chaotic system. Chaotic systems facilitate a discussion of model uncertainty and the various types of uncertainty. Epidemic disease spread is modeled in a bottom-up approach of interacting agents. We explore the advantages and disadvantages of using a bottom-up approach to modeling.

6.1 Weather Forecasting

The National Weather Service produces some 24,000 weather predictions per day or ten million predictions each year. Weather sensitive industrial sectors include agribusiness, ground-based transportation, homeowners insurance, aviation, and oil and gas production. It is estimated that $1 trillion of the nation's $7 trillion economy is weather sensitive (Hooke and Pielke 2000). The state of the art in weather forecasting has an effective limit of about 10 days in advance. This is because atmospheric dynamics is a chaotic system. Small changes in the initial conditions fed to a weather model will eventually lead to large changes in the simulation outputs (the butterfly effect).

The primary learning objective for this case study will be to focus on the properties of chaotic systems. Chaotic systems should be studied in the context of distinguishing between aleatory and epistemic uncertainty. Aleatory uncertainty is the uncertainty inherent in random phenomena. Epistemic uncertainty is the uncertainty attributable to incomplete knowledge about a phenomenon. Chaotic systems can appear to be random due to their sensitivity to initial conditions. A clear distinction should be made between uncertainty due to sensitive dependence on initial conditions and aleatory or epistemic uncertainty.

6.2 Epidemic Disease Spread

Infectious diseases have become an important issue facing both public health and homeland security communities. Threats of avian bird flu, SARS, or smallpox are receiving serious attention in the news media. One group of scientists at Los Alamos National Laboratory has created a simulation, Episims, to study this problem. Episims is an artificial population of 1.6 million residents in a virtual replica of Portland, Ore. Each individual has a prescribed daily routine that is statistically created using traveler activity surveys conducted by the Portland metropolitan planning office. The purpose of creating this artificial city is to study the effectiveness of various intervention techniques in response to the outbreak of a highly infectious disease (Barrett, Eubank, and Smith 2005).

Episims is novel for its application of massive data repositories to the design of a bottom-up, agent-based simulation. It is built on top of another Los Alamos simulation that is designed to study traffic planning in an urban environment. The traffic simulation contains a virtual map of the city of Portland, including rail lines, roads, signs, and traffic signals. When combined with data from the U.S. census bureau, a virtual city is created. Bottom-up modeling is characterized by the employment of simple local rules to generate complex behavior. The design philosophy argues that "certain sets of microspecifications are sufficient to generate the macrophenoma of interest" (Epstein and Axtell 1996). The challenge for model validation is to show that these microspecifications are also necessary conditions for the macrophenoma of interest. The objective for the Episims case study is to gain an appreciation for model validation of bottom-up models

7 DISCUSSION AND CONCLUSION

We have shown how the Yucca Mountain waste storage project can be used as a case study for some of the challenges in modeling and simulation. Specifically we have focused on multiresolution modeling and model validation. We propose that a set of these case studies be compiled and used in a M&S curriculum. Weather forecasting and epidemic disease spread explore the topics of model uncertainty and agent-based design. For each of the grand challenges in M&S, a suitable case study should be used to reinforce the desired learning objectives.

There are several characteristics that should be used when assessing a candidate case study. First, it should explore a non-trivial, complex application of modeling and simulation. There must be ample, relevant documentation that is both publicly accessible and easily comprehensible to the students. Second, the case study should have enough reading material that focuses on the simulation-based decision making process. We recommend that most of the case studies come from outside the primary disciplines of the students enrolled in the course. The students must understand that M&S challenges in their field are shared with disciplines outside their own.

Most curricula in modeling and simulation do not highlight the importance of grand challenges. A signature of a grand challenge problem is that (at present) there does not exist a universally accepted solution. Challenging, relevant case studies offer an opportunity for students to observe critical cross-cutting M&S technology issues in a wide array of disciplines, to appreciate the complexity of addressing the issues, to interact with experts in fields other than their own, and to become better prepared for current and future uses of simulation in significant decision-making processes.

APPENDIX A: RECOMMENDED YUCCA MOUNTAIN READINGS

We recommend that students read Whipple (1996), Craig (1999), Ewing and Macfarlane (2002), and Carter and Pigford (2005) as background material on the Yucca Mountain storage repository. Ojovan and Lee (2005) and Savage (1995) should be used as reference textbooks if necessary. The students should then read the following sections from these U.S. Department of Energy reports:

- *Yucca Mountain Science and Engineering Report* (OCRWM 2002) : Executive Summary, Sections 1.1 through 1.4, Section 4.1.
- *Total System Performance Assessment for the Site Recommendation* (OCRWM 2000g) : Sections 2.2 and 4.1.
- *Joint NEA-IAEA International Peer Review of the Yucca Mountain Site Characterisation Project's Total System Performance Assessment Supporting the Site Recommendation Process* (NEA-IAEA 2002) : Sections 1, 2, 4, and 5.

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AUTHOR BIOGRAPHIES

MICHAEL SPIEGEL is a Ph.D. Candidate in Computer Science and a member of the Modeling and Simulation Technology Research Initiative (MaSTRI) at the University of Virginia. Michael earned his B.A. in Computer Science at Swarthmore College. He has previously held the position of research associate at StreamSage, Inc. studying natural language processing for multimedia search engines. His email addresses is `<mspiegel@cs.virginia.edu>` and his web address is `<www.cs.virginia.edu/~ms6ep>`.

PAUL F. REYNOLDS, JR. is a Professor of Computer Science and a member of MaSTRI at the University of Virginia. He has conducted research in Modeling and Simulation for over 25 years, an has published on a variety of M&S topics, including parallel and distributed simulation, multiresolution modeling and coercible simulations. He has advised industrial and government agencies on matters relating to modeling and simulation. He is a plank holder in the DoD High Level Architecture. His email address is `<reynolds@virginia.edu>` and his web address is `<www.cs.virginia.edu/~pfr>`.

DAVID C. BROGAN earned his Ph.D. from Georgia Tech and is currently an Assistant Professor of Computer Science and a member of MaSTRI at the University of Virginia. For more than a decade, he has studied simulation, control, and computer graphics for the purpose of creating immersive environments, training simulators, and engineering tools. His research interests extend to artificial intelligence, optimization, and physical simulation. His email address is `<brogan@virginia.edu>`.