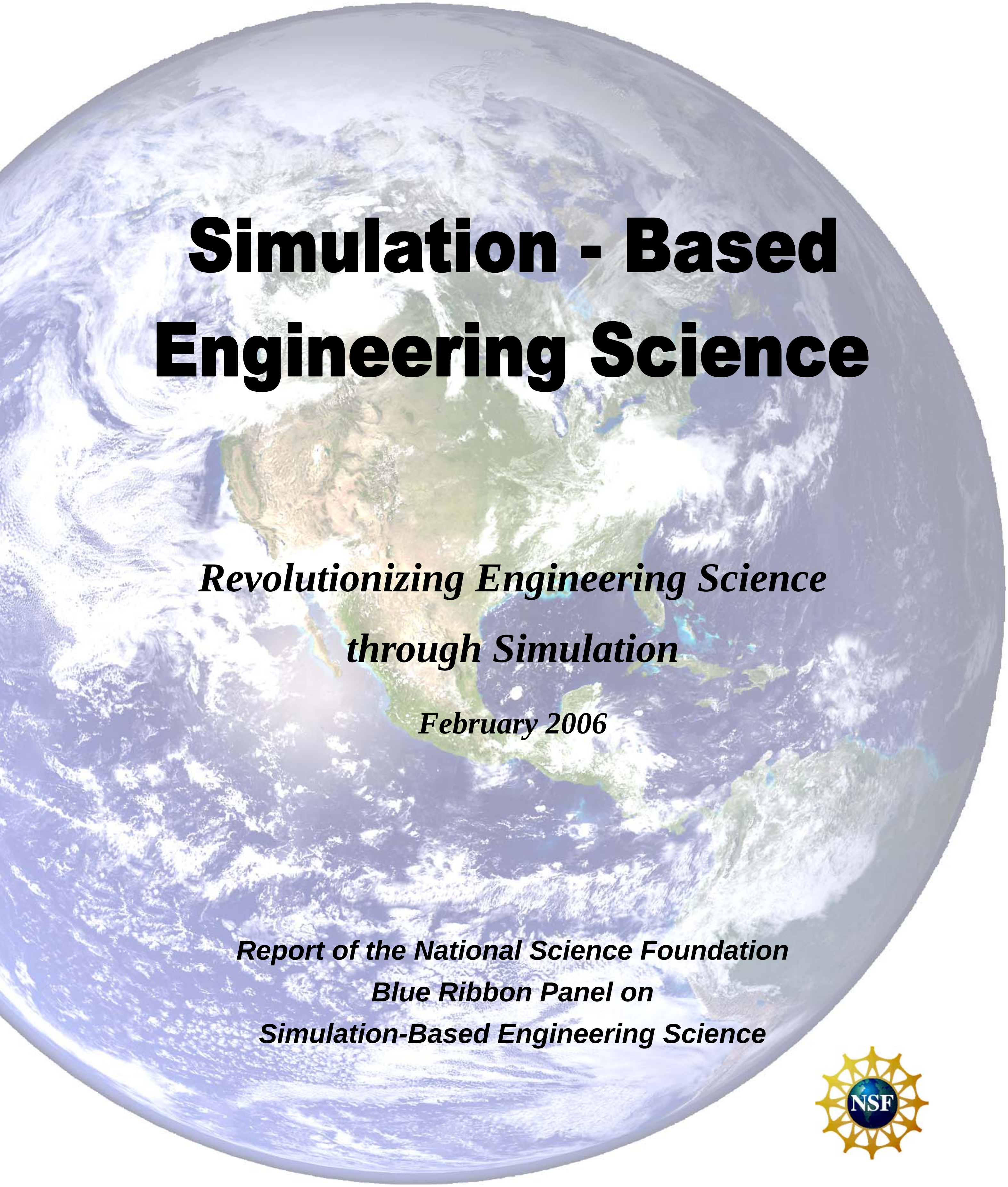

Simulation - Based Engineering Science

Revolutionizing Engineering Science through Simulation

February 2006

Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science

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THE NSF BLUE RIBBON PANEL ON SIMULATION-BASED ENGINEERING SCIENCE

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PREFACE

This document is the final report of the findings and recommendations of the Blue Ribbon Panel on Simulation-Based Engineering Science to the National Science Foundation (NSF). The report contains recommendations critical to the acceleration of advances in Simulation-Based Engineering Science (SBES), and it identifies several areas in which SBES can play a remarkable role in promoting developments vital to the health, security, and technological competitiveness of the nation.

For over a decade, the nation's engineering and science communities have become increasingly aware that computer simulation is an indispensable tool for resolving a multitude of scientific and technological problems facing our country. To define the field of computer simulation more precisely and to assess its potential impact on important areas of engineering science, in April 2004 the NSF organized a workshop on SBES. Encouraged by the widespread interest in the results of the workshop, the Foundation appointed a Blue Ribbon Panel on Simulation-Based Engineering Science. The purpose of the Panel was to explore the challenges and potential benefits of SBES, as well as the barriers to its development. Furthermore, the Panel was tasked with making recommendations on how the discipline could be nurtured within NSF and in academia, industry, national laboratories, and government agencies. A second workshop on SBES was held in September 2005, at which time the Panel received input on SBES from a broad constituency.

Acknowledgements: The Panel has benefited from the advice and council of many individuals. The enthusiastic support of Drs. Richard Buckius and Ken Chong of NSF and Dr. John Brighton, formerly of NSF, is gratefully acknowledged. Valuable advice from the over 100 workshop attendees has also been factored into the findings and recommendations. In addition, a large group of experts outside the workshops have provided valuable commentary on the early drafts of this report.

The Panel gratefully acknowledges the following individuals and institutions for providing the graphics that appear in this report: NASA's Earth Observatory (Cover Image); Charles Taylor, Stanford University (Figure 1); Y. Zhang and C. Bajaj, University of Texas and the New York University School of Medicine, respectively (Figure 2); SCI, University of Utah (Figure 3); SCI, University of Utah, and J. Bell and V. Beckner, Lawrence Berkeley National Laboratory (Figure 4); and the U.S. Department of Energy (Figure 5, a reproduction from the SCaLeS report). Particularly helpful in the preparation of this final report were the comments and advice of Drs. Chandrajit Bajaj, Larry Biegler, Mark Carpenter, Alok Chaturvedi, Weng Cho Chew, Frederica Darema, Omar Ghattas, George Hazelrigg, Craig Henriquez, Anthony Ingraffea, Kirk Jordan, Chandrika Kamath, Dimitri Kusnezov, Wing Kam Liu, Robert Moser, Habib Najm, Anthony Patera, Mark Rashid, Mark Shephard, Charles Taylor, Elizabeth Tornquist, Mary Wheeler, Daniel White, Jacob White, and David Young,.

Although this report was prepared by an officially appointed advisory panel to the National Science Foundation, all opinions, findings, and recommendations expressed here are those of the Panel and do not necessarily reflect the views of the National Science Foundation.

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EXECUTIVE SUMMARY

S*imulation* refers to the application of computational models to the study and prediction of physical events or the behavior of engineered systems. The development of computer simulation has drawn from a deep pool of scientific, mathematical, computational, and engineering knowledge and methodologies. With the depth of its intellectual development and its wide range of applications, computer simulation has emerged as a powerful tool, one that promises to revolutionize the way engineering and science are conducted in the twenty-first century.

Computer simulation represents an extension of theoretical science in that it is based on mathematical models. Such models attempt to characterize the physical predictions or consequences of scientific theories. Simulation can be much more, however. For example, it can be used to explore new theories and to design new experiments to test these theories. Simulation also provides a powerful alternative to the techniques of experimental science and observation when phenomena are not observable or when measurements are impractical or too expensive.

Simulation-Based Engineering Science (SBES) is defined as the discipline that provides the scientific and mathematical basis for the simulation of engineered systems. Such systems range from microelectronic devices to automobiles, aircraft, and even the infrastructures of oilfields and cities. In a word, SBES fuses the knowledge and techniques of the traditional engineering fields—electrical, mechanical, civil, chemical, aerospace, nuclear, biomedical, and materials science—with the knowledge and techniques of fields like computer science, mathematics, and the physical and social sciences. As a result, engineers are better able to predict and optimize systems affecting almost all aspects of our lives and work, including our environment, our security and safety, and the products we use and export.

Whereas the use of computer simulations in engineering science began over half a century ago, only in the past decade or so have simulation theory and technology made a dramatic impact across the engineering fields. That remarkable change has come about mainly because of developments in the computational and computer sciences and the rapid advances in computing equipment and systems. There are other reasons. For example, a host of technologies are on the horizon that we cannot hope to understand, develop, or utilize without simulation. Many of those technologies are critical to the nation's continued leadership in science and engineering. Clearly, research in SBES is quickly becoming indispensable to our country's security and well-being.

This report was prepared by a Blue Ribbon Panel on Simulation-Based Engineering Sciences, which was convened by the Assistant Director of the Engineering Directorate of the National Science Foundation (NSF). The Panel was directed to explore opportunities for and potential advances in SBES and to make strategic recommendations as to how NSF should structure its programs to foster SBES.

The Panel developed its findings and recommendations from several information sources. Among them, interactions with recognized leaders of the computational engineering and science communities played an essential role. Another important source of information was the work of previous panels and committees. The results of those earlier efforts, which have accumulated over the last decade, address major issues in the computational and computer sciences. The Panel also relied on input from leaders in the computer simulation community who participated in the NSF-supported workshops on SBES. Finally, the Panel developed its findings and recommendations after thorough discussions among its members.

This report explores the potential impact of advances in SBES on science and technology and identifies the challenges and barriers to further advances in SBES. For instance, we must overcome difficulties inherent in multiscale modeling, the development of next-generation algorithms, and the design and implementation of dynamic data-driven application systems. We must improve methods to quantify uncertainty and to model validation and verification. We must determine better ways to integrate data-intensive computing, visualization, and simulation. Importantly, we must overhaul our educational system to foster the interdisciplinary study that SBES requires. The payoffs for meeting these challenges are profound. We can expect dramatic advances on a broad front: medicine, materials science, homeland security, manufacturing, engineering design, and many others.

For more than a decade, researchers and educators in engineering and science have agreed: the computational and simulation engineering sciences are fundamental to the security and welfare of the United States. The findings and recommendations of this report strongly reinforce that contention.

Major Findings

1. SBES is a discipline indispensable to the nation's continued leadership in science and engineering. It is central to advances in biomedicine, nanomanufacturing, homeland security, microelectronics, energy and environmental sciences, advanced materials, and product development. There is ample evidence that developments in these new disciplines could significantly impact virtually every aspect of human experience.

2. Formidable challenges stand in the way of progress in SBES research. These challenges involve resolving open problems associated with multiscale and multi-physics modeling, real-time integration of simulation methods with measurement systems, model validation and verification, handling large data, and visualization. Significantly, one of those challenges is education of the next generation of engineers and scientists in the theory and practices of SBES.

3. There is strong evidence that our nation's leadership in computational engineering and science, particularly in areas key to Simulation-Based Engineering Science, is rapidly eroding. Because competing nations worldwide have increased their investments in research, the U.S. has seen a steady reduction in its proportion of scientific advances relative to that of Europe and Asia. Any reversal of those trends will require changes in our educational system as well as changes in how basic research is funded in the U.S.

Principal Recommendations

1. The Panel recommends that the National Science Foundation and other Federal research agencies make changes in their organizational structures to facilitate long-range core funding of SBES. The new Cyberinfrastructure at NSF is envisioned as a "portion of cyberspace" where scientists can "pursue research in new ways and with new efficiency" by utilizing: 1) high-performance, global-scale networking, 2) middleware, 3) high-performance computing services, 4) observation and measurement devices, and 5) improved interfaces and visualization services. Serious consideration should be given to the feasibility of developing a parallel program in SBES that interfaces to multiple divisions of NSF in concert with Cyberinfrastructure. Supporting SBES research should certainly be a goal of every division within the Directorate of Engineering at NSF, but the realization of the full potential of advances in SBES will require support across all directorates and from other federal agencies as well.
2. To maintain our leadership in science and engineering, the Panel recommends a minimum increase in NSF funding of $300 million per year over 2005 levels of SBES-related disciplines. We cannot maintain our leadership in engineering and the engineering sciences without substantial investments in SBES, because simulation is a key element in accelerating progress in engineering. Advances in computing speed alone or in measurement devices or in networking or interfaces cannot meet the great challenges before us without advances in the basic components of SBES. Similar observations have been made in the President's Information Technology Advisory Committee (PITAC) report, as well as in the results of several other related studies.
3. The Panel recommends a long-term program of high-risk research to exploit the considerable promise of SBES. The Panel strongly supports the observation made in the PITAC report and elsewhere that short-term investments and limited strategic planning will lead to excessive focus on incremental research rather than on long-range sustained research with a lasting impact. Progress in SBES will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. The work of these teams should be sustained for a decade or more to yield the full fruits of the investment.
4. The Panel recommends that NSF underwrite the work of an NRC committee to explore the issue of interdisciplinary education in detail and to make recommendations for a sweeping overhaul of our educational system. The problem of education in SBES-component disciplines, and in multidisciplinary programs in general, is large, pervasive, and critically important. The initiative for change will not likely come from academia alone; it must be encouraged by the engineering and scientific leadership and throughout the organizational structure of our universities.

Other important findings and recommendations of the Panel are given in the body of the report.

1.0 SBES: A National Priority for Tomorrow's Engineering and Science

Today the field of computer simulation is on the threshold of a new era. Advances in mathematical modeling, computational algorithms, the speed of computers, and the science and technology of data-intensive computing have prepared the way for unprecedented improvements in the health, security, productivity, and competitiveness of our nation. To realize these advances, however, we must overcome major scientific, engineering, sociological, and educational obstacles. Progress will require significant breakthroughs in research, changes in the research and educational cultures of our academic institutions, and changes in the organizational structure of our educational system. For the engineering fields, advances in computer simulation offer rich possibilities. Full exploitation of the new capabilities, however, must await basic research into the scientific components of modeling, simulation, and computing, among other areas. We refer to the combination of these basic research activities as *Simulation-Based Engineering Science*, or *SBES*.

In this report we describe this new discipline. We first identify some of the remarkable benefits SBES brings to technologies that make our lives healthier, safer, and better. Next, we survey the core issues of SBES, that is, the major obstacles to and opportunities for its development. We then explore the impact of SBES on our national research and educational resources, goals, and organizations. Throughout the report, we highlight our findings and recommendations. In making those recommendations, we attempt to reflect the views prevailing within the nation's scientific and engineering communities.

This much is certain: there is overwhelming concurrence that simulation is key to achieving progress in engineering and science in the foreseeable future. Indeed, seldom have so many independent studies by experts from diverse perspectives been in such agreement: computer simulation has and will continue to have an enormous impact on all areas of engineering, scientific discovery, and endeavors to solve major societal problems. This message is woven into the principal findings of many key investigations. For example, the PITAC report [4] emphasizes the need to develop computational science for national competitiveness, and the SciDAC [26] and SCaLeS [18, 19] reports identify opportunities for scientific discovery at the high end of today's simulation capabilities and call for a new scientific culture of interdisciplinary teamwork to realize those capabilities. In addition, the *Roadmap for the Revitalization of High-End Computing* [24] and the *Federal Plan for High-End Computing* [13] both call for innovations in computer architecture to accommodate advanced simulation. The *Future of Supercomputing* report [12] examines the role of the Federal Government in sustaining the leading edge of supercomputing, and the Cyberinfrastructure report [1] outlines a diverse program of interrelated research imperatives stretching well beyond simulation into communication and data technologies. Beginning with the Lax report of 1982 [20] and continuing with a number of reports already appearing in this young century [3, 8, 9, 23], the studies share a similar vision regarding the importance of simulation.

> *Seldom have so many independent studies been in such agreement: simulation is a key element for achieving progress in engineering and science.*

Consequently, the present report enters an arena already filled with voices calling for more vigorous research and training in computation-based simulation. The ideas in this report are in harmony with those voices, and in fact the report is as brief as it is because others have already eloquently articulated the case for simulation. Even so, this report addresses important elements of simulation that have been overlooked. Moreover, it adds the voice of engineering to the discussion, one that has not yet been fully heard.

Realizing the full potential of SBES will require a revolution in simulation technology. Simulation-Based Engineering Science is not "simulation as usual"; rather, it is research focused on the modeling and simulation of complex, interrelated engineered systems and on the acquisition of results meeting specified standards of precision and reliability. Indeed, the scope of SBES includes much more than the modeling of physical phenomena. It develops new methods, devices, procedures, processes, and planning strategies. Not only does it draw on and stimulate advances in our scientific understanding, it capitalizes on those advances by applying them to challenges in the engineering domain. For example, discoveries in SBES have direct applications to optimization, control, uncertainty quantification, verification and validation, decision-making, and real-time response. In short, SBES will lift simulation to a powerful new level, a level where we hope to solve the most stubborn problems of modeling, engineering design, manufacturing, and scientific inquiry. In fact, so profound are the implications of advanced simulation techniques that we can expect SBES to trigger the development of a host of aggressive new technologies and to foster significant new scientific discoveries.

SBES constitutes a new paradigm that will be indispensable in meeting the scientific and engineering challenges of the twenty-first century.

Consider, for example, a few of the breakthroughs that SBES offers: (1) the means to understand and control multiscale, multi-physics phenomena; (2) fundamental developments in nanotechnology, biomedicine, materials, energy and environment, and the earth and life sciences; and (3) dramatic enhancements to the fidelity and utility of computational predictions. Clearly, SBES ushers in a technology that not only expands the reach and capability of every field of engineering but also promises significant improvements in the health, security, competitiveness, and wealth of our nation.

If we are to reap the benefits of SBES, however, we must first overcome the obstacles. First, we must revolutionize the way we conceive and perform simulation. This revolution requires that we learn to incorporate new discoveries that simplify and enhance multiscale, multidisciplinary simulations. Second, we must make significant advances in the supporting technologies, including large-scale computing, data management, and algorithms. Third, we must overhaul our educational institutions to accommodate the needs of SBES research and training. Fourth, we must change the manner in which research is funded and conducted in the U.S.

So far, developments in simulation have ridden the wave of advances in hardware and software information technology. Because of these advances, simulation has become an increasingly effective tool in traditional science and engineering practices. Unlike most theory, which posits restricted, idealized systems, simulation deals with real systems. For that reason, simulation provides unprecedented access to real-world conditions. In addition, simulation has none of the limitations of experimental designs and tests, which are often hampered by cost constraints, unrealistic parameter ranges, and even restrictions imposed by treaties or health and environmental concerns. For these reasons, computer simulation is credited with numerous triumphs in the twentieth century. It has become indispensable, for example, in assessments of vehicle crashworthiness. It is fundamental to the generation of predictive models of the weather, climate change, and the behavior of the atmosphere. Its

> *Simulation has become indispensable in predictive methods for weather, climate change, and behavior of the atmosphere; and in broad areas of engineering analysis and design.*

importance in broad areas of engineering analysis and design are well known. It has become essential to product manufacturing. Its achievements in biomedical applications are widely discussed. Systems design in defense, communication, and transportation also rely on computer simulation.

At the heart of these successes, however, are simulation methodologies that are decades old, too old to meet the challenges of new technology. In many ways, the past successes of computer simulation may be its worst enemies, because the knowledge base, methods, and practices that enabled its achievements now threaten to stifle its prospects for the future.

Our nation prides itself in being the leader in computational science and simulation theory and technology. Unfortunately, many indicators suggest that the United States is quickly losing ground. Particularly in SBES, the country is no longer positioned to lead the world over the next few decades. Even today, the consequences of falling behind are penetrating deep into our technology and economy, as well as jeopardizing our position in the global community.

> *The importance and great potential of simulation have not gone unnoticed by our competitors around the world.*

Our global competitors are well aware of the great potential of computer simulation. Throughout Europe and Asia, governments are making major investments in computing, mathematical and computational modeling, algorithms, networking, and generally in computational engineering and science. Indeed, these nations are building on the technologies that the U.S. pioneered in the twentieth century. We are in danger, once again, of producing world-leading science but leaving it to our competitors to harvest the technological and economic advantages.

Yet, even our traditional lead in basic research is under threat. According to [4, p. 9]: “Since 1988, Western Europe has produced more science and engineering journal articles than the United States and the total growth in research papers is highest in East Asia (492 percent), followed by Japan (67 percent), and Europe (59 percent), compared with 13 percent for the United States. Worldwide, the share of U.S. citations in scientific papers is shrinking, from 38 percent in 1988 to 31 percent in 2001." In Germany, 36 percent of undergraduates receive degrees in science and engineering; in China, 59 percent, and in Japan, 66 percent. In contrast; only 32 percent of undergraduates receive such degrees in the United States [6, 25, 21].

The imbalance is beginning to reveal itself in international trade. "From 1980 to 2001, the U.S. share of global high-technology exports dropped from 31 percent to 18 percent, while the share for Asian countries rose from 7 to 25 percent" [4, p. 8]. Since 2001, the U.S. trade balance in high-tech products has been negative.

The chief global economic competitor of the United States is China. In 2004 China graduated approximately 498,000 bachelor's level engineers. By comparison, India graduated 350,000 engineers, and the U.S. graduated 70,000 [6, 25]. The employment of an engineer in China costs roughly one-tenth to one-sixth of what it costs in the United States. Some argue, however, that the U.S. production of engineers, computer scientists, and information technology specialists remains competitive in global markets when like-to-like data from the representative countries are compared [11]. Nevertheless, even our competitors in SBES believe that SBES research expenditures in Europe and Asia are rapidly expanding while they are stagnant or declining in the U.S.

The key to offsetting those disadvantages is leadership in simulation. The U.S. must be in the forefront of efforts to make simulation easier and more reliable. We must extend the capabilities of simulation to the analysis of more complex systems and the real-time acquisition of real-time data. Simulation must no longer be relegated to the peripheries of an engineering student's skill set; instead, it should be a core part of the engineering curriculum, where it plays a role in effective pedagogy.

Computer simulation has become indispensable to the development of all other technologies, including microelectronics, advanced materials, biotechnology, nanotechnology, pharmaceuticals, medicine, and defense and security. Many breakthroughs in these technologies derive from computer simulation and simulation-based scientific discovery. Clearly, we must integrate computer simulation into engineering education and practice. To do so, however, requires great intellectual resources and a national commitment to SBES.

In Chapter 2, we describe some of the remarkable applications of SBES, all of which represent enormous benefits to our society. If we are to realize such great potential, however, we must overcome many technical, mathematical, scientific, and computational challenges. So great are these challenges that they will require a sea change in our approach to engineering and science education. Chapter 3 surveys the greatest of those obstacles. In addition, the chapter identifies opportunities for broadening the impact of SBES through developments in visualization, sensors and image processing, and uncertainty quantification.

Finally, in Chapter 4 we describe the impact of SBES on our educational system. Our educational system must change if it is to equip future generations of engineering scientists with knowledge of SBES and its value in science and technology.

2.0 THE PAYOFF: Driving Applications and Societal Benefits of SBES

The applications and benefits of SBES are many. This chapter reviews some of the important applications of SBES and explores the challenges and benefits of each.

2.1 SBES in Medicine

Most diseases (such as heart disease, cancer, stroke, and respiratory diseases) and their treatments (whether surgical, transcatheter, or pharmacologic) involve complex physical responses and interactions between biological systems, from the molecular to organism scales. Simulation methods can therefore dramatically increase our understanding of these diseases and treatments, and furthermore, improve treatment. Computational science has already made significant inroads in many biomedical domains, most notably genomics and proteomics. A current challenge is the application of SBES to clinical medicine and to the study of biological systems at the cellular, tissue, and organ scales.

Both medical practice and engineering are problem-solving disciplines.

Medical practice and engineering have many similarities. Both are problem-solving disciplines, and both require an understanding of complex systems. Engineering design processes, however, are based upon predicted outcomes. Often, engineering solutions require the satisfaction of numerous criteria simultaneously. Those solutions often require sophisticated computer and analysis technologies. By contrast, medical practice uses a “build them and bust them” approach. Historically, the paradigm of medicine combines diagnosis and empiricism; that is, physicians use various tests to diagnose a medical condition and then plan a treatment or intervention based on empirical data and professional experience. Generally, medical practice precludes any formal process to predict the outcome of a treatment for an individual patient, although there may be some statistical data to indicate the success rate of the treatment.

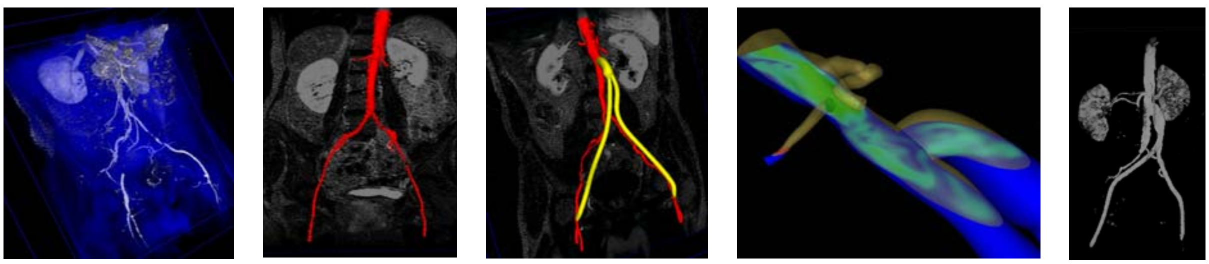

Figure 1: Example of a simulation-based medical approach applied to the design of a bypass surgery procedure for a patient with occlusive cardiovascular disease in the aorta and iliac arteries. Shown from left to right are magnetic resonance image data, a preoperative geometric solid model, an operative plan, computed blood flow velocity in the aorta and proximal end of bypass, and post-operative image data used to validate predictions. Advances contemplated in SBES disciplines could greatly improve these approaches by allowing real-time adaptive control of surgical procedures through the combination of simulation tools and imaging technologies.

A program in SBES could also lead to new approaches to medical practice, collectively called Simulation-Based Medicine.

A program in SBES could lead to new approaches to medical practice, approaches that could be collectively called *Simulation-Based Medicine*. New SBES methodologies, already leveraging tremendous advances in medical imaging and high-performance computing, would give the practice of medicine the tools of modern engineering. For example, doctors would be able to use simulations—initialized with patient-specific anatomic and physiologic data—to *predict* the outcomes of procedures and thereby *design* optimal treatments for individual patients. This ability to predict treatment outcomes and design procedures accordingly represents an exciting new possibility for medicine.

Not only could physicians devise better treatments for individual patients, but also manufacturers could use SBES methods to predict the performance of their medical devices in virtual patients. The physical and animal testing procedures currently used prior to human trials have significant limitations in their ability to represent variations in human anatomy and physiology. With SBES methods, manufacturers could conduct virtual prototyping of medical devices by simulating the performances of alternate device designs for a range of virtual

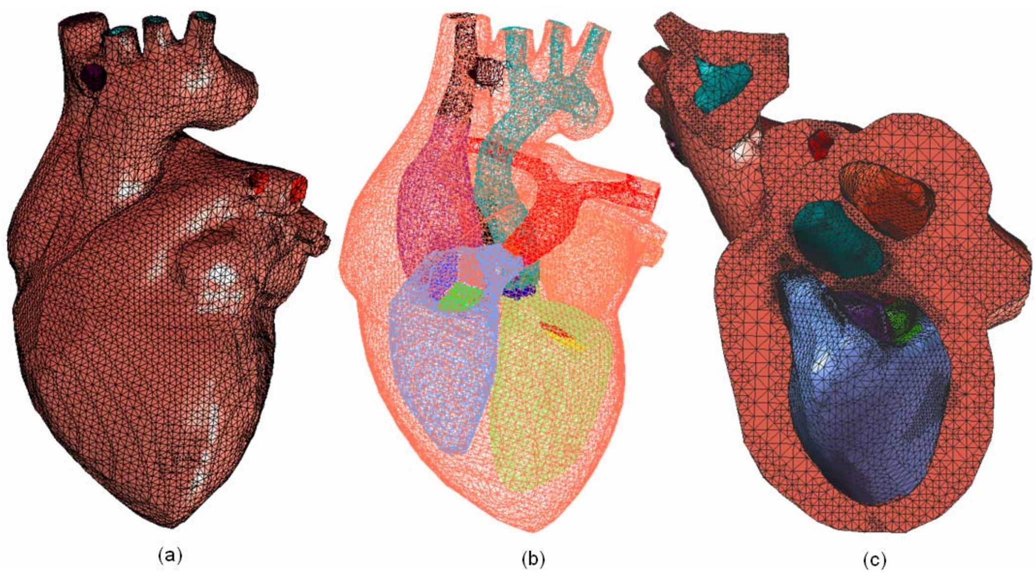

Figure 2: The modeling of biomedical systems is becoming increasingly sophisticated. Here is an example of a three-dimensional, tetrahedral-mesh, heart model [27] developed from surface data obtained from the New York University School of Medicine [22]. (a) Exterior view. (b) Boundary detection represented in wire frame. (c) Cross-sectional view of the mesh. Patient-specific modeling technologies need to be advanced significantly to make the vision of Simulation-Based Medicine a reality. The benefits, however, are impressive: dynamic models of deformation, blood flow, and fine-scale capillary effects may greatly advance cardiovascular medicine.

patients. In this way, manufacturers would be able to refine their designs for different patient conditions. As a result, these *virtual clinical trials* prior to animal and human trials could lead to safer, more effective devices, reduce development costs, and shorten time-to-market.

Manufacturers in pharmaceuticals and biotechnology could also benefit from SBES methods. For example, targeted drug-delivery techniques are being used increasingly to treat a range of diseases, including heart disease (for example, drug-eluting stents), cancer (for example, local chemotherapies), and chronic respiratory diseases (for example, therapeutic inhalants). In all those areas of innovation, simulation-based methods could be used to model the transport of drugs through the circulatory or respiratory systems and to determine the local concentrations to use in pharmacokinetic models of drug metabolism.

Currently, important topics in cancer research are the mechanisms of cell adhesion and invasion and signaling pathways. A better understanding of those mechanisms is critical to advances in cancer research and neurobiology. The developments of multiscale SBES technologies for investigations into cellular structures and cell mechanics, as well as the development of novel cellular force-measurement devices, will help explain dynamic cellular architectures and the mechanism of cell motility.

Of particular significance is cell motility. To understand cell motility we must first understand: (1) the mechanics of the cell interior, and (2) the mechanics of the cell-substrate or cell-ECM (extra-cellular matrix) interaction force. These complex mechanisms determine cell shape and migration, which in turn allow the cell to perform its critical functions, such as wound healing and embryonic morphogenesis. SBES technologies hold promise that we can improve our understanding of those cellular functions and increase our ability to differentiate normal cells from cancer cells. The stakes are high, because the invasion of transformed cells into other tissues—the process called metastasis—is believed to be the precursor of the development of cancer tissue.

2.2 SBES in Predictive Homeland Security

In the broadest sense, engineering design for security involves the development of systems to protect human populations and the artificial and natural infrastructures that support them. The systems protect us from a range of threats, whether hostile (for example terrorists), environmental (for example, air and water pollution), or natural (for example, earthquake or hurricane). The protective systems must guard our entire support infrastructure: buildings; transportation systems; food, water, and power distribution; communications; and waste disposal.

The methods of SBES can play an important role in the design and optimization of these protective systems. Most notably, SBES would allow our emergency planners to predict not only the consequences of threats (for example, the accidental or malicious release of a toxic chemical or biological agent), but also the effects of countermeasures. With the aid of predictive simulations, engineers would be able to design and optimize infrastructures that would be impervious to a wide range of threats. With the ability to conduct real-time simulations, moreover, an emergency team would be able to identify the most rational response to a crisis. The World Trade Center disaster of September 11, 2001 serves as a tragic example: if real-time simulation had been available, the emergency response team would have realized the importance of the immediate evacuation of the building complex.

> *SBES will allow the prediction of the consequences of threats and countermeasure responses.*

SBES can give engineers and planners a remarkably large operational view of the systems that make up our society. For example, SBES would give us the ability to simulate the operation of a whole city as a single system. It is able to do so because it integrates multiscale simulations of multiple subsystems and processes, such as structural responses, fluid transport of contaminants, power distribution, and transportation systems, as well as the response of the human population.

This vision of a “Digital City” would require the acquisition of data of unprecedented detail. Not only would the system have to acquire static data, that is, data regarding the installed infrastructure, but it would also have to continuously acquire dynamic data, that is, data undergoing constant change. Dynamic data, for example, would include continuous measurements of air- and water-contaminant concentrations; the flow rates of air, water, and effluents; the locations and velocities of transportation and other movable assets (for example, trains and heavy machinery); and the densities and movements of people and automobiles.

A logical extension of the Digital-City concept is that of the Digital Ecosystem, which may be artificial (such as a city) or natural (such as a forest, watershed, continent, or even the entire planet). Whatever the scale, the benefits are the same: we gain the ability to optimize human activity and infrastructures in respect to adverse events or trends, and, through real-time simulation, we are able to identify rational responses to crises.

The concepts and methods of SBES promise to revolutionize the practice of urban planning, transportation, structural and environmental engineering, and municipal and environmental management. To realize the visions of the Digital City and the Digital Ecosystem, however, we must acknowledge that a great amount of research must pioneer the way. The following are a few of the areas requiring development:

- Quantitative models of the processes to be simulated must be developed. For many of those processes, models of some level of fidelity already exist, or they are being developed for narrower engineering purposes. Obvious examples are structural models (of buildings and other structures), fluid-dynamics models (air and water flows), combustion models (for example, for predicting the spread of fires), and transportation models (for example, to analyze traffic flow). For other important processes, however, quantitative models are rudimentary or nonexistent. For example, we lack sociological models that can help us describe or predict the response of populations to crises. In addition, we need better models for the evolution of natural ecosystems such as forests or lakes.

- A comprehensive simulation system is required that integrates detailed models of a wide range of scales. The comprehensiveness of the simulation system is a requirement if SBES applications are to simulate multiscale complex systems. Some of the issues are generic, but others are problem specific.

- New models of exceptional fidelity are required. The development and validation of such models entail the acquisition of data of extraordinary detail. As a result, the development of the Digital City and Digital Ecosystem will inevitably put pressure on the experimental sciences and theoretical research to meet the demand for copious data. Furthermore, the real-time simulation of some applications will drive developments in sensors and the communication infrastructure, both of which must support streams of data. In addition, we need to develop the simulation techniques that can accommodate the data streams.

- A better understanding of the role of uncertainty is required. Some degree of uncertainty is inevitable in the ability of a model to reflect reality and in the data the model uses. We need to find ways to interpret uncertainty and to characterize its effects on assessments of the probable outcomes.

The rewards of meeting those challenges are great: enhanced security, safety, and convenience of life in the Digital City and the Digital Ecosystem; a social infrastructure of unparalleled efficiency; rational responses to natural events; and optimal interactions with natural environments. The following summarizes some of the major applications.

- **Protection Against Air Contaminants:** SBES technologies will detect and measure the presence of biological or chemical contaminants in the air and, given detailed weather data, identify the likely release location and magnitude of the release. The system will then design an optimal response plan.
- **Optimization of Infrastructures:** SBES technologies will optimize the designs of buildings and other infrastructural elements. Such designs would be site specific, interact well with natural and man-made surroundings, and blend with the urban system of which they are a part. In addition, the designs would take into account the effects of the structures both on normal operations and on operations during a wide range of large-scale emergencies.
- **Prediction of Long-Term Environmental Impacts:** SBES technologies will predict the effects of effluents from existing and proposed facilities on urban and natural environments. Such predictions would greatly increase the reliability and usefulness of environmental impact studies. In addition, they would allow planners to minimize the probability of unforeseen deleterious events.
- **Optimization of Emergency Responses:** SBES technologies would optimize emergency responses to fire and explosion (whether accidental or intentional). Planning for emergency responses would consider how the situation might evolve or escalate (for example, a fire might spread, building collapse, or the response intervention itself might adversely affect the situation).
- **Optimization of Security Infrastructures for Urban Environments:** SBES technologies would assist in the design and placement of air- and water-contaminant sensors and would help in the planning of countermeasures, such as contaminant dispersal and flood abatement.

2.3 SBES in Energy and the Environment

The energy-related industries rely on modern simulation methods to monitor the production of oil reservoirs, plan pollution remediation measures, and devise control strategies. Recent advances in simulation-related technologies may raise oil-reservoir management to a new level of sophistication. Those advances include distributed computing, multi-physics and chemistry modeling, parallel algorithms, and methods and devices for the dynamic use of well-bore and seismic data. In addition, the next generation of oilfield simulation tools could exploit developing technologies for data-driven, interactive, and dynamically adaptive strategies for subsurface characterization and reservoir management. Soon we could see multi-resolution reservoir models that can be executed on very large, distributed, heterogeneous, computational environments. Those models, moreover, could be fed data from sensors embedded in reservoir fields (for example, permanent downhole sensors and seismic sensors anchored on the seafloor). Such a model-and-sensors system could provide a symbiotic feedback loop between measurement data and computational models. This approach could lead to an instrumented oilfield, one that is more efficient, cost effective, and environmentally safe. The strategic and economic benefits are enormous:

> *An instrumented oilfield will result in more efficient, cost-effective, and environmentally safer reservoirs, with enormous strategic and economic benefits.*

- An increase in the volume of oil and natural gas produced from existing reservoirs. With our better understanding of existing oil and gas reservoirs, we can expect to deplete existing reserves more efficiently and to locate and produce bypassed reserves. The additional production could help us reduce our dependence on foreign oil.

- A better understanding of risks and uncertainties in exploration and lower finding costs. Better models of the subsurface would allow oil and gas companies to focus on prospects that offer the best return. As a result, they can allocate their capital much more efficiently.

The new SBES-related technologies have immediate application to other areas as well, including environmental remediation and storage of hazardous wastes. Again, these new application areas require an integrated and interactive simulation framework with multiscale capabilities. The development and use of such frameworks require the support of cross-disciplinary teams of researchers, including geoscientists, engineers, applied mathematicians, and computer scientists.

2.4 SBES in Materials

SBES-related technology may have its greatest societal impact where innovations in modeling and simulation methodologies intersect with innovations in materials. Multiscale modeling and simulation are transforming the science and technology of new-material development and the improvement of existing materials. This transformation is tantamount to a shift to a powerful new paradigm of engineering science. The new methods enable the unprecedented ability to manipulate metallic, ceramic, semiconductor, supramolecular, and polymeric materials. The results are material structures and devices that have remarkable physical, chemical, electronic, optical, and magnetic properties. We can now anticipate the molecular design of

> *With SBES, materials development becomes a unique opportunity for the integration of fundamental, interdisciplinary knowledge, with technological applications of obvious benefit to society.*

composite materials with undreamed-of functionalities. Moreover, to reap the advantages that SBES technology brings to materials development, researchers from many disciplines would have to integrate their knowledge in the materials sciences. Such collaboration maximizes the possibilities for developing materials of great technological value.

The principle of materials design is rooted in the correlation of molecular structure with physical properties. From those correlations, models can be formulated that predict microstructural evolutions. Such models allow the researcher to investigate the mechanisms underlying the critical behaviors of materials and to systematically arrive at improved designs.

The use of simulations to uncover structure-property correlations can be superior to relying only on experimental data. The reason is that simulation provides detailed information regarding the evolved microstructure, as well as complete control over the initial and boundary conditions. Another significant aspect of SBES, one that makes future materials development more robust, is that it links simulation methods across different length and time scales. A great deal of progress is being made in the first principles calculations of electronic structure and in atomistic simulations. Now progress is also being made in connecting these two powerful techniques of probing physical phenomena in materials.

The benefits from new materials development are amply evident in the current progress in nanoscience and technology, a world-wide enterprise that can be compared to drug design. Because of the multiscale nature of materials modeling and simulation, SBES is destined to play a key role in nanoscience. SBES provides the capability of linking electronic-structure methods, which are necessary for dealing with novel nanostructures and functional properties, with atomistic and mesoscale techniques. That linkage ensures that the different phases of materials innovation—from design to testing to performance and lifetime evaluation—can all be simulated, examined, and optimized.

The power of multiscale computation can be seen in a number of high-profile applications involving the behavior of known materials in extreme environments. For example, a problem that has occupied the attention of a sizable community of researchers for several years is the characterization of the mechanical behavior of plastic deformation in metals at high pressure and high strain rate. The challenge, which is relevant to national security, is to conduct multiscale simulation that links all of the following: calculation of the core of a dislocation using electronic-structure methods; the modeling of dislocation mobility using molecular dynamics simulation; and the determination of constitutive relations for continuum-level codes. Multiscale simulation can also help solve problems in the development of the structural components of nuclear power reactors. Such materials must not only be radiation resistant, but they must have lifetimes of over 40 years.

Even for materials that do not have to stand up to the extreme conditions of high pressure and intense radiation, the field of materials innovation is rich with challenges to our understanding of the underlying microstructures of the materials. By meeting those challenges, we can reap enormous benefits. For example, we could generate a molecular model of cement, the most widely used substance made by humans. Such a model would help us develop a new cement with greater creep resistance and environmental durability. Similarly, models would help us improve the performance of catalysts for fuel-cell electric vehicles. We could also improve techniques in oilfield exploration, where instrumentation and digital management of hydrocarbon reservoirs are issues. In all these examples, improvements in materials performance would have great impact.

Everywhere one looks there are problems important to society that require optimizing the functional properties of materials through control of their microstructure.

Everywhere one looks there are problems important to society that require optimizing the functional properties of materials through the control of their microstructures. Clearly, SBES will have a long-term impact on materials innovation. Three attributes of SBES in particular lead to this conclusion.

- **Exceptional Bandwidth:** The conceptual basis of materials modeling and simulation encompasses all of the physical sciences. It makes no distinction between what belongs to physics versus chemistry versus engineering and so on. This universality of SBES technology represents a scientific bandwidth that is at least as broad as the entire range of multiscale applications in science and engineering. In materials modeling and simulation, as in SBES more generally, traditional disciplinary barriers vanish; all that matters is "the need to know."
- **Elimination of Empiricism:** A virtue of multiscale modeling is that the results from both modeling and simulation are conceptually and operationally quantifiable. Consequently, empirical assumptions can be systematically replaced by physically-based descriptions. Quantifiability allows researchers to scrutinize and upgrade any portion of a model and simulation in a controlled manner. They can thus probe a complex phenomenon detail by detail.
- **Visualization of Phenomena:** The numerical outputs from a simulation are generally data on the degrees of freedom characterizing the model. The availability of this kind of data lends itself not only to direct animation, but also to the visualization of the properties under analysis, properties that would not be accessible to experimental observation. In microscopy, for example, researchers can obtain structural information but usually without the energetics. Through simulation, however, they can have both. The same may be said of data on deformation mechanisms and reaction pathways.

These three attributes of SBES, of course, are not restricted to materials development; they apply equally well to the other areas of SBES application. In this section, however, the focus has been on the application of SBES to materials development. The point that emerges is that, aided by SBES technology, materials modeling and simulation, or computational materials, is becoming the sister science of computational physics and computational chemistry.

2.5 SBES in Industrial and Defense Applications

Simulation is ubiquitous in industry. It plays an essential role in the design of materials, manufacturing processes, and products. Increasingly, simulation is replacing physical tests to ensure product reliability and quality. Fewer tests mean fewer prototypes, and the result is a shorter design cycle. Steady reductions in design cycles, in turn, are crucial to U.S. efforts to remain competitive in a world where the pace at which new consumer products are being developed is increasing every day. The need for shorter design cycles also applies to our national defense and security. World events are often unpredictable; our defense industry must be able to design, modify, and manufacture equipment in quick response to military and police exigencies. A case in point is the unanticipated need to reinforce armored vehicles in Iraq after several such vehicles were destroyed by improvised explosive devices.

To increase U.S. competitiveness, short design cycles are crucial if we are to keep up with the rapid pace of new-products throughout the world.

The use of simulation has proved effective in some industrial applications. For example, in crashworthiness studies the few instances that simulations replaced testing are frequently cited as success stories. Generally, however, simulation has yet to play a central role in important industrial and defense design applications. The reason is that large-scale simulation does not enter into the design cycle until its later stages. Model preparation, after all, requires a substantial amount of time and labor. Often it takes months to prepare a model, and even then the model needs to be calibrated with tests if the design is substantially different from previous designs.

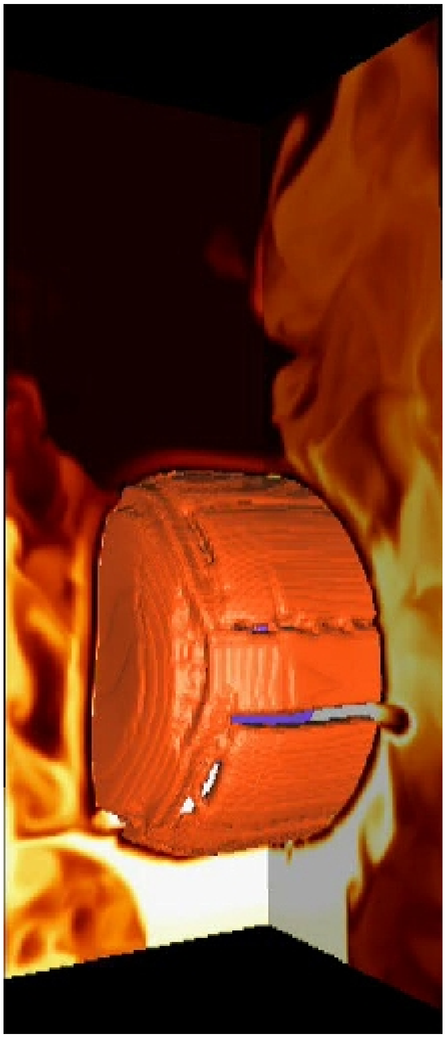

Figure 3: An example of contemporary visualization and simulation capabilities. Shown is a simulation of the explosion of a steel tank filled with explosive subjected to a jet of heated air. New methods are needed to capture multiscale effects and quantify uncertainties.

In addition, the preparation of a model usually requires considerable knowledge of and skill in finite-element analysis. For that reason, the challenge of generating models normally falls on engineers with advanced degrees, not designers. This separation between simulation and design activities results in delays and reduces the effectiveness of the simulation.

The difficulties of simulation are compounded when new materials, such as composites and metallics, are used in product designs. Before simulation can even begin, the new materials must be tested extensively to determine their properties. Such tests are time consuming, and they lengthen the time necessary to prepare and conduct useful simulations.

In addition, simulation capabilities are currently limited in their ability to model relevant phenomena. For example, in the simulation of a rear collision between two automobiles, it would be desirable to model the gasoline in the fuel tank and the effects of any fracture of the fuel tank. To date, such multi-physics simulations are not possible. Similarly, we are still unable to model the fracture of the interior panels and trim, which is important in determining occupant injury, or the fracture of sheet metal and structural members, which is common with aluminum.

If an industry is to replace testing with simulation, the simulation tools must undergo robust verification and validation procedures for effectiveness.

Thus, crashworthiness simulation technology is usually used to check designs near their final stages. Optimization of a design for crashworthiness in the early stages of the design process is simply not yet feasible. The complexity of model generation and the uncertainties are too great. Even if an industry were to replace testing almost completely with simulation, the changeover would still require robust verification and validation procedures to ensure the effectiveness of the simulation tools.

Similar limitations are found in many other industrial applications where, at least superficially, simulation has appeared to be a success. For example, in the simulation of sheet-metal forming, important phenomena, such as the tribology of the metal-die interface, are not modeled. Those phenomena are characterized by much smaller scales than the overall process, and they are subject to great variability because they depend on factors such as temperature and the age of the lubricant. In the tire industry, simulation is usually limited to determining the tire footprint; important performance characteristics such as pothole impact, hydroplaning, and cornering performance cannot be simulated because they involve multi-physics and many disparate length and time scales.

In the chemical processing industry, simulation would seem to have a significant role. In fact, most petrochemical plants use steady-state process simulation models to perform detailed real-time optimization. As a result, chemical plants are more energy and environmentally efficient. Even in the chemical industries, however, the use of simulation is limited. Current planning models capture only nominal plant capacities; they do not address the real performance of the plants and the processes at various scales, nor are they sensitive to uncertainties.

Over the past two decades the integrated circuit industry has been a major player in simulation-based engineering. Until now, the U.S. has been a leader in the development of highly integrated, easy-to-use software for circuit analysis, such as SPICE, and in the education of our engineering workforce in the application of that software. As a result, the U.S. was able to maintain its leadership in the high value-added segment of the market. As clock rates move into the gigahertz range, however, circuit theory is no longer applicable. Future - generation transistors, such as single electron transistors, low-threshold transistors, and quantum computing devices, will be based on new physics that links quantum mechanics and electromagnetics.

Overall, simulation in industry has yet to meet its full potential. The following list is a summary of its current limitations:

1. The development of models is very time consuming, particularly for geometries of complex engineering systems such as ships, automobiles, and aircraft. Moreover, the determination of material properties often requires extensive small-scale testing before simulation can be started, especially if statistical properties are needed. This testing also lengthens the time to obtain a simulation and hence the design cycle.

2. Methods are needed for linking models at various scales and simulating multi-physics phenomena.

3. Simulation is often separate from the design optimization process and cannot simultaneously deal with factors such as manufacturability, cost, and environmental impact.

Overcoming these barriers will require progress in our basic understanding and in the development of powerful new methods. Among these challenges are the following:

1. Multiscale methods that can deal with large ranges of time and spatial scales and link various types of physics.
2. Methods for computing macroscopic phenomena, such as material properties and manufacturing processes, in terms of subscale behavior.
3. Effective optimization methods that can deal with complex integrated systems, account for uncertainties, and provide robust designs.
4. Frameworks for validation, verification, and uncertainty qualification.
5. Methods for rapidly generating models of complex geometries and material properties.

Multiscale methods will provide extensive benefits. For instance, they will enable us to understand relationships and interactions of phenomena at different scales, which is crucial in the design of many products. In the design of products, it is often necessary to couple diverse physics, such as fluids with solids or electromagnetics with structures. Simulations of such couplings involve a large range of length and time scales. For example, to model live fire testing of defense products, it is necessary to incorporate phenomena of an immense range of scales associated with combustion and structures. Similarly, designs involving different components also have an enormous range of coupled time scales that determine overall system behavior.

Multiscale methods may also make possible the prediction of material properties in terms of basic building blocks, ranging from matrix and fiber properties of composite materials to the properties of atoms in metals. Demand is increasing for materials that reduce weight and cost; consequently, the availability of tools that, through simulation, can predict the behavior of a material from its basic building blocks would open tremendous possibilities for quickly developing better, less costly, and safer products. Such tools would eliminate the bottleneck of extensive materials testing, resulting in substantial reductions in design-cycle times. The methods we envision would be able to link models of different scales, such as models of micromechanics or even quantum mechanics linked to models of macroscale behavior.

Of course, as design processes increasingly rely on computer simulation, validation and verification procedures will become increasingly important. Although some efforts have been made at providing validation benchmark problems for linear analysis, nonlinear simulation software has not been subjected to extensive validation procedures. In fact, we find considerable controversy as to what appropriate validation procedures are, how broadly they apply, and whether they are even feasible. Clearly, a basic understanding of verification and validation procedures is urgently needed. After all, to be useful, the simulation tools used by industry and defense agencies must provide reliable results. Furthermore, since many real-world phenomena are not deterministic, statistical methods that can quantify uncertainty will be needed.

SBES has the potential to deliver, within a short design period, designs that are optimized for cost performance and total impact on the environment.

Design optimization is also in its infancy, and it too has many obstacles to overcome. The constraints on the optimization of a product design relate to manufacturability, robustness, and a variety of other factors. Optimality often needs to be defined in terms of complex criteria, and the frameworks currently in use are not readily amenable to that task. Moreover, to be effective for engineering design, optimization methods must be closely coupled with simulation techniques. Generally, however, we still lack a fundamental understanding of what constitutes an optimal design and how to find it in a complex multi-criteria design environment. Once optimization methods are developed that can deal with these complexities, we can expect to see chemical plants, automobiles, laptop computers, and a host of other industrial and consumer products that feature unprecedented efficiency at lower cost.

In summary, SBES has the potential to deliver designs that are optimized for cost performance and their total impact on the environment (from production to disposal or recycling), all within a short design cycle. This achievement is not possible, however, simply by extending current research methods and taking small, incremental steps in SBES development. The barriers to the realization of SBES relate to our entire way of conducting research and development and educating engineers. The next chapter discusses some of these core issues.

Finding

Because of the interdisciplinary character and complexity of SBES challenges, incremental, short-term research efforts are inadequate to achieving SBES goals. Instead, a long-term program of high-risk research will be needed to resolve the numerous obstacles standing in the way of SBES developments. The Panel agrees with the observation made in the PITAC report and elsewhere that short-term investments and limited strategic planning will lead to an excessive focus on incremental research rather than on the long-range, sustained research necessary to have a lasting impact. Moreover, progress in such research will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. The work of those teams should be sustained for a decade or more for the investment to yield its full fruits.

3.0 CORE ISSUES: Challenges, Barriers, and Opportunities in SBES Research

All of the driving applications discussed in the preceding chapter share common challenges, barriers, and requirements for research breakthroughs. We elaborate on the major issues in this chapter.

3.1 The Tyranny of Scales: The Challenge of Multiscale Modeling and Simulation

Researchers in the worldwide race toward miniaturization, nanoscience, molecular modeling of drugs and biological systems, advanced materials, and other applications, all of which involve events on atomistic and molecular levels, have run into a formidable roadblock: the *tyranny of scales*. Virtually all simulation methods known at the beginning of the twenty-first century were valid only for limited ranges of spatial and temporal scales. Those conventional methods, however, cannot cope with physical phenomena operating across large ranges of scale—12 orders of magnitude in time scales, such as in the modeling of protein folding [4, p. 4], or 10 orders of magnitude in spatial scales, such as in the design of advanced materials. At those ranges, the power of the tyranny of scales renders useless virtually all conventional methods. Confounding matters further, the principal physics governing events often changes with scale, so that the models themselves must change in structure as the ramifications of events pass from one scale to another.

The tyranny of scales dominates simulation efforts not just at the atomistic or molecular levels, but wherever large disparities in spatial and temporal scales are encountered. Such disparities appear in virtually all areas of modern science and engineering, for example, in astrophysics, atmospheric science, geological sciences, and in the design of complex engineering systems such as submarines, commercial aircraft, and turbine engines.

In many ways, all that we know about the physical universe and about the design and functioning of engineering systems has been partitioned according to categories of scale. The designer manipulating the electronic properties of materials sees the world as a myriad of infinitesimal atoms with clouds of orbiting electrons. The atmospheric scientist sees the world as the movement of great air masses that change climate conditions across thousands of miles of the earth's surface. Today, we are attempting technological advances that cannot tolerate any view of nature that partitions phenomena into neat categories of scale. The modeling and simulation tools we are seeking now must be commensurate in their applications with the great breadth of the phenomena they must simulate.

The development of effective multiscale modeling techniques will require major breakthroughs in computational mathematics and new thinking on how to model natural events occurring at multiple scales.

The tyranny of scales will not be defeated simply by building bigger and faster computers. Instead, we will have to revamp the fundamental ways we conceive of scientific and engineering methodologies, long the mainstays of human progress. Such a daunting challenge, historic in its significance, is beyond the capability of single individuals and disciplines. The necessary breakthroughs in computational mathematics and the development of new ways to model natural events at multiple scales will require the efforts of interdisciplinary teams of researchers and thinkers working in concert.

We can see instances already where preliminary and often ad hoc methodologies have retarded technological progress. The design of nanodevices is one example. Nanodevices are systems with tiny masses and relatively large surface areas. The design of such devices is in urgent need of new simulation tools, because they are at a scale too small to be captured by continuum mechanics. Another example is any biological application that requires methods that link diverse time scales. For instance, the sequence of events following a medical implant is initiated by the interactions between individual water molecules and the surface of the implant. This first set of interactions occurs on a timescale of nanoseconds. The resulting water "shell," in turn, has an influence on proteins and other types of molecules that arrive later. This second set of interactions has a timescale from microseconds to milliseconds. Thus, there is a significant time gap in the behavior that is difficult to model. Similarly, temporal gaps in the behavior of polymers cause problems for current simulation methods.

Numerous important applications of nanotechnology are being driven by homeland security. As a result, the need and urgency for developing multiscale tools has increased significantly. For example, we know that small concentrations of chemical and biological agents can have lethal effects on large segments of the human population. The recognition of that threat has prompted development of new mitigation methods, such as miniaturized intelligent sensors, protective clothing, and masks. The need for engineered nanostructured materials for homeland-security applications, as well as for optical and structural applications, has spurred much interest in the development of multiscale methods that can accommodate diversity in spatial scales.

Recent work in multiscale modeling has emphasized the synthesis of theories applicable to different scale ranges, such as quantum, molecular, and continuum descriptions [5, p. 1504]. Nevertheless, enormously important technological problems, such as turbulence modeling, remain unsolved. These problems involve a very broad range of scales amenable to a single description, such as continuum theory in the case of turbulence. In fact, turbulent-flow problems in practical engineering involve such an enormous range of scales that they cannot be currently solved on the world's largest and fastest computers. If we assume that progress continues at the rate of Moore's Law, the turbulence-flow problems will not succumb to solutions for many generations to come. The implications of solving these problems are great; for example, they have to do with our leadership in designing future generations of commercial and military aircraft. Before we can lead, however, we must find the path to fundamental developments in multiscale modeling.

The urgency of the development of multiscale simulation models has been felt worldwide. Over the past five years, virtually every conference, symposium, and international congress devoted to computational engineering and science has listed multiscale modeling as an important theme. Multiscale modeling has often been the subject of colloquia, study groups, or invited lectures. Three DOE workshops were recently held on multiscale mathematics [8, 23, 10], and programs at NSF and NIH are already in place for promoting the beginnings of new research in this area. In recent years, a large and growing body of literature in physics, chemistry, biology, and engineering has focused on various methods to fit together simulation models of two or more scales, and this has led to the development of various multi-level modeling approaches. To date, however, progress on multiscale modeling has been agonizingly slow. Only a series of major breakthroughs will help us establish a general mathematical and computational framework for handling multiscale events and reveal to us the commonalities and limitations of existing methods.

Finding

Formidable obstacles remain in linking highly disparate length and time scales and in bringing together the disciplines involved in researching simulation methods. These issues are common to many SBES applications. Fundamental discoveries will be needed to surmount these obstacles.

3.2 Verification, Validation, and Uncertainty Quantification

The ultimate goal of simulation is to predict physical events or the behaviors of engineered systems. Predictions are the basis of engineering decisions, they are the determining factor in product or system design, they are a basis for scientific discovery, and they are the principal reason that computational science can project itself beyond the realm of physical experiments and observations. It is therefore natural to ask whether specific decisions can rely on the predicted outcomes of an event. How accurate are the predictions of a computer simulation? What level of confidence can one assign a predicted outcome in light of what may be known about the physical system and the model used to describe it? The science, technology, and, in many ways, the philosophy of determining and quantifying the reliability of computer simulations and their predictions has come to be known as V&V, or verification and validation. The methods of V&V are fundamental to the success and advancement of SBES.

What level of confidence can one assign a predicted outcome in light of what may be known about the physical system and the model used to describe it?

To appreciate the subtleties and goals of V&V, one must first dissect the process of simulation. Beginning with the conceptual understanding of certain physical events of interest and with scientific theories that explain them (the target physical phenomena or engineering system identified for study), the analyst (the modeler, scientist or engineer) constructs a mathematical model of the event. The mathematical model is a collection of mathematical constructions, equations, inequalities, constraints, etc., that represent abstractions of the reality, and are dictated by the theory or theories characterizing the events. The analyst then develops a computational model of the event. The computational model is a discretized approximation of the mathematical model, and its purpose is to implement the analysis on a computer. Validation is the subjective process that determines the accuracy with which the mathematical model depicts the actual physical event. Verification is the process that determines the accuracy with which the computational model represents the mathematical model. In simple terms, validation asks, “Are the right equations solved?” while verification asks, “Are the equations solved correctly?”

The entire field of V&V is in the early stage of development. Basic definitions and principles have been the subject of much debate in recent years, and many aspects of the V&V remain in the gray area between the philosophy of science, subjective decision theory, and hard mathematics and physics. The twentieth century philosopher of science Karl Popper asserted that a scientific theory could not be validated; it could only be invalidated. Inasmuch as the mathematical model of a physical event is an expression of a theory, such models can never actually be validated in the strictest sense; they can only be invalidated. To some degree, therefore, all validation processes rely on prescribed acceptance criteria and metrics. Accordingly, the analyst judges whether the model is invalid in light of physical observations, experiments, and criteria

The most confounding aspect of V&V has to do with uncertainty in the data characterizing mathematical models of nature.

based on experience and judgment.

Verification processes, on the other hand, are mathematical and computational enterprises. They involve software engineering protocols, bug detection and control, scientific programming methods, and, importantly, *a posteriori* error estimation.

Ultimately, the most confounding aspect of V&V has to do with uncertainty in the data characterizing mathematical models of nature. In some cases, parameters defining models are determined through laboratory tests, field measurements, or observations, but the measured values of those parameters always vary from one sample to another or from one observation to the next. Moreover, the experimental devices used to obtain the data can introduce their own errors because of uncontrollable factors, so-called noise, or errors in calibration. For some phenomena, little quantitative information is known, or our knowledge of the governing physical processes is incomplete or inaccurate. In those cases; we simply do not have the necessary data needed to complete the definition of the model.

Uncertainty may thus be due to variability in data due to immeasurable or unknown factors, such as our incomplete knowledge of the underlying physics or due to the inherent nature of all models as incomplete characterizations of nature. These are called *subjective uncertainties*. Some argue that since the data itself can never be quantified with absolute certainty, all uncertainties are subjective. Whatever the source of uncertainty, techniques must be developed to quantify it and to incorporate it into the methods and interpretation of simulation predictions.

Although uncertainty-quantification methods have been studied to some degree for half a century, their use in large-scale simulations has barely begun. Because model parameters can often be

The use of stochastic models can represent gigantic increases in complexity in data volume, storage, manipulation, and retrieval requirements.

treated as random fields, probabilistic formulations provide one approach to quantifying uncertainty when ample statistical information is available. The use of stochastic models, on the other hand, can result in gigantic increases in the complexity of data volume, storage, manipulation, and retrieval requirements. Other approaches that have been proposed for uncertainty quantification include stochastic perturbation methods, fuzzy sets, Bayesian statistics, information-gap theory, and decision theory. The development of reliable methodologies—algorithms, data acquisition and management procedures, software, and theory—for quantifying uncertainty in computer predictions stands as one of the most important and daunting challenges in advancing SBES.

Finding

While verification and validation and uncertainty quantification have been subjects of concern for many years, their further development will have a profound impact on the reliability and utility of simulation methods in the future. New theory and methods are needed for handling stochastic models and for developing meaningful and efficient approaches to the quantification of uncertainties. As they stand now, verification, validation, and uncertainty quantification are challenging and necessary research areas that must be actively pursued.

3.3 Dynamic Simulation Systems, Sensors, Measurements, and Heterogeneous Simulations

One of the most challenging applications of SBES, but one that may yield the greatest dividends, is the linkage of simulation tools directly to measurement devices for real-time control of simulations and computer predictions. Some preliminary investments in the research into this new idea have been made under NSF's program in dynamic data-driven applications systems (DDDAS) [7, 9]. The full development of this revolutionary and fundamentally important discipline will take years of research and technological development.

The concept of DDDAS is envisioned as a new paradigm in computer simulation, one involving a "symbiotic feedback control system" [7, 9] in which simulations and experiments (or field data) interact in real time to dramatically improve the fidelity of the simulation tool, its accuracy, and its reliability.

The document that originally put forth the idea [7], now over five years old, described the goal of DDDAS as one of developing "application simulations that can dynamically accept and respond to 'online' field data and measurements and/or control such measurements. This synergistic and symbiotic feedback control loop among applications, simulations, and measurements is a novel technical direction that can open new domains in the capabilities of simulations with a high potential payoff, and create applications with new and enhanced capabilities. It has the potential to transform the way science and engineering are done, and induces a major beneficial impact in the way many functions in our society are conducted, such

This synergistic and symbiotic feedback control loop among applications, simulations, and measurements has the potential to transform the way science and engineering are done.

as manufacturing, commerce, transportation, hazard prediction/management, and medicine, to name a few."

A half-decade later, these words are still true, but we also better appreciate the size of the challenge. To develop DDDAS, we must resolve issues involving the complexity of the systems, the breadth of expertise and technologies required to implement the systems, the new software infrastructures, and the efficiency and capacity of the computational and data management systems required. Success on all those technological fronts will mandate a sustained and well-funded program of basic and applied research over possibly a decade or more. The payoffs, however, are immense—so important, in fact, that the highest priority should be given to developing and exploiting this fundamental SBES discipline. DDDAS is a concept conceived, defined, and promoted in the United States. To capitalize on our own initiatives, however, we must become aggressive in our development of DDDAS. Our current complacency in this technology is allowing our competitors to gain on us, once again.

The basic building blocks of DDDAS include the following: 1) a hierarchy of heterogeneous simulation models, 2) a system to gather data from archival and dynamic sources, 3) algorithms to analyze and predict system behavior by blending simulation models and data, 4) algorithms to steer and control the data gathering and model validation processes, and 5) the software infrastructure supporting model execution, data gathering, analysis prediction, and control algorithms.

Dynamic data-driven application systems will rewrite the book on the validation and verification of computer predictions.

In many ways, DDDAS will rewrite the book on the validation and verification of computer predictions. No longer will validation be a one-shot operation to judge the acceptability of a simulation problem on the basis of a static data set. In DDDAS, validation becomes a part of the dynamic control process that identifies and assesses deficiencies of the computational model and upgrades and improves the model on the fly. This incorporation of validation into the dynamics of the model dramatically enriches the predictability of the model and increases confidence in the predicted results.

DDDAS dynamically incorporates measurement data into a simulation as that simulation is executing. The simulation, in turn, dynamically steers the measurement process. To perform these operations, DDDAS integrates large-scale numerical computing with data-intensive computing, sensors, imaging, grid computing, and other measurement devices. The development of this technology requires new concepts in software infrastructure, algorithms, control protocols, and solvers. Once in place, however, the technology offers an endless list of applications. Surgical procedures, homeland security, control of hazardous materials, environmental remediation, drug delivery, manufacturing processes, oil reservoir management, and vehicle flight control are just a few.

Finding

Research is needed to effectively use and integrate data-intensive computing systems, ubiquitous sensors and high-resolution detectors, imaging devices, and other data-gathering storage and distribution devices, and to develop methodologies and theoretical frameworks for their integration into simulation systems. Concomitant investments are also required in sensory-data computing, the collection and use of experimental data, and the facilitation of interactions between computational models and methods, all of which are necessary to achieve dynamic adaptive control of the computational process.

3.4 New Vistas in Simulation Software

Many contemporary engineering communities regard simulation software as a commodity that vendors provide for well-defined, specific, and independent domains of application. Occasionally, these long-lived codes for engineering analysis receive incremental improvements, usually in the form of functional extensions. This leisurely approach to software development will not support the next generation of engineering problems—multiscaling with real-time data interaction and abundant uncertainties in the data. As the PITAC report states [14], “Today it is altogether too difficult to develop computational science software and applications. Environments and toolkits are inadequate to meet the needs of software developers in addressing increasingly complex interdisciplinary problems. Legacy software remains a persistent problem because the lifetime of a computational science application is significantly greater than the three- to five-year life cycle of a computing system. In addition, since there is no consistency in software engineering best practices, many of the new applications are not robust and cannot easily be ported to new hardware.”

Entirely new approaches are needed for the development of the software that will encapsulate the models and methods used in SBES.

For those reasons, entirely new approaches are needed for the development of the software that will encapsulate the models and methods used in SBES. Researchers must identify the methodologies that support the interoperability of individual components of simulation software. Then they must develop those methodologies and integrate them into the next generation of engineering software. This search for new methods and tools to support simulation software development is fraught with difficulties. Not only do the new simulation components require complex algorithms, they must also function efficiently on an evolving range of architectures designed for large-scale parallel computations.

Tomorrow's SBES software requires extraordinary degrees of robustness, efficiency, and flexibility. The new software must not only execute simulation algorithms, but must also dynamically manage data throughput and model adaptivity and control. It must steer observational and measurement systems to optimize data collection and use. It must navigate efficiently across models of multiple scales and accommodate multiple physical theories, and it must have scalable methods that interact seamlessly with data-gathering devices.

Much of our contemporary software development tools—libraries (for instance, linear equation solvers), language interoperability tools, component coupling and data transfer tools, and simulation development frameworks—do not meet the demands of SBES. To define the real requirements for the implementation of SBES technologies, we require a new paradigm of software development. Such a fundamental change calls for a great deal of "out-of-the-box" thinking about the way we approach software development and practice engineering. The change will even affect the way scientific computing is taught and perceived in our universities. Not only will tomorrow's software developers have to cope with more complex systems and heterogeneous hardware systems, but they will also have to understand the important details of the applications.

> Not only will tomorrow's software developers have to cope with more complex algorithms, but they will also have to understand the important details of the applications.

Whereas the future of SBES software is largely uncharted, some path-finding work is under way. A Federal government group, for instance, has taken a similarly aggressive software philosophy and developed software with which to bootstrap. This effort is called the Scientific Discovery Through Advanced Computing (SciDAC) initiative [26] (see also Chapter 2 of [18]). Organized in 2001, SciDAC is a highly interdisciplinary program tasked with finding methods by which state-of-the-art mathematics and domain-specific application sciences can be embodied in robust codes that run efficiently on current terascale supercomputers. The initiative is driven by research into science applications relevant to the goals of DOE's Office of Science. Those applications include fields such as global climate modeling, plasma fusion, quantum chromodynamics, accelerators, combustion, and supernovae, as well as the mathematics and computer science relevant to those disciplines. Most of this research portfolio involves the coordinated efforts of dedicated domain scientists in collaboration with mathematicians, computer scientists, and computational scientists throughout the nation. One of the principal products of SciDAC is sharable software, and development of such software takes the sustained effort of a permanent staff. For this reason, the center of gravity for most of the work in this field is at national labs. In addition, U.S. universities continue to play a key role in that research. At any rate, it is clear that the questions are too large and complex for any single institution to manage alone. Instead, we must encourage the formation of teams of researchers, working in a collaborative software environment, where they can profit from distributed resources and expertise.

The DOE's National Nuclear Security Agency is also heavily involved in computational science. In the mid-1990s, that agency embarked on an ambitious program of Stockpile Stewardship. Part of the program was the Accelerated Strategic Computing Initiative (ASCI, now ASC). With ten times the funding of SciDAC, the ASCI program, among other goals, seeks to use simulation to manage our nuclear stockpile. Simulation, in this case, would be a substitution for our actual testing of the devices, which is prohibited by international treaty. Five centers were established at U.S. universities to

> The new paradigm for SBES software research and development will allow for specialization with cross-accountability.

develop the computational science for ASCI.

As both DOE programs exemplify, if the engineering sciences are to realize the full benefits of the rapid advances in computing technologies, we must somehow integrate the knowledge and discoveries of mathematics, computer science, engineering, and the domain sciences. We also need to recognize that SBES is located at the intersection of those disciplines. In that sense, we can think of SBES as a super-discipline.

The new paradigm for SBES software research and development will allow for specialization with cross-accountability. As envisioned, mission-driven teams, primarily practicing engineers, will define and model the engineering systems that require breakthroughs in simulation methods (for example, artificial organs or distribution networks). In addition, the engineers will tentatively identify data interfaces and the computational tasks between those interfaces. From there, teams of "enabling technologists," primarily mathematicians and computer scientists, will tackle the abstract requirements identified by the mission-driven teams and develop software components that port across the target architectures (for example, massively parallel distributed memory computers). The component development will track the research frontier for each algorithmic area of expertise (for example, error estimation or eigenanalysis) while also conforming to mission requirements.

Finding

Much of our current software in computational engineering science is inadequate for dealing with the multifaceted applications and challenges of SBES. New software tools, paradigms, and protocols will need to be developed so that software is more transferable between fields and not wastefully duplicated. In the multidisciplinary teams we establish for SBES research, we must incorporate experienced software developers who will work closely with engineering scientists to develop tomorrow's SBES software.

3.5 The Emergence of Big Data in Simulation and the Role of Visualization in SBES

Since the advent of computing, the world has experienced an information "big bang," an explosion of data. Information is being created at an exponential rate. Since 2003, digital information makes up 90 percent of all information production, vastly exceeding the amount of paper and film. One of the greatest scientific and engineering challenges of the twenty-first century is to understand and make effective use of this growing body of information.

> *The era in which data-intensive computing and large-scale scientific computing were essentially disjoint camps is over.*

In the computational engineering and science environment that existed near the end of the previous century, data-intensive computing and large-scale scientific computing were essentially disjoint camps. One transported, stored, and manipulated large data sets, and the other implemented scalable parallel computing strategies for resolving very large computational models of scientific and engineering problems. That era of separation has passed. In all the applications of SBES discussed in this chapter, the use and generation of immense data sets are integral components. For example, uncertainty quantification, a key component of SBES, will require data sets many orders of magnitude larger than those of traditional deterministic computing. DDDAS, by definition, will demand new methods that rapidly generate, store, access, and transfer large data sets over computational grids or high-bandwidth networks. Then there is the issue of interpreting the results of the simulation itself, a problem that can involve gigantic data sets.

As we work to harness the accelerating information explosion, visualization will be among our most important tools. Indeed, visualization capabilities will have a dramatic impact on scientific, biomedical, and engineering research; defense and national security; and industrial innovations.

The reason visualization is such a powerful tool is that it is fundamental to our ability to interpret models of complex phenomena, such as multilevel models of human physiology from DNA to whole organs, multi-century climate shifts, or multidimensional simulations of airflow past a jet wing. Visualization reduces and refines data streams rapidly and economically, thus enabling us to winnow huge volumes of data – an ability important in applications such as the surveillance of public health at a regional or national level in order to track the spread of infectious diseases. Visualization for solving problems in applications like hurricane dynamics and homeland security are generating new knowledge that crosses traditional disciplinary boundaries. Finally, the use of visualization is rapidly transforming business and engineering practices for the better [15], thereby increasing the competitive edge of our industry.

Visualization is fundamental to our ability to interpret models of complex phenomena, such as multilevel models of human physiology from DNA to whole organs, multi-century climate shifts, or multidimensional simulations of airflow past a jet wing.

Visualization allows people to comprehend visual representations of data much more rapidly than they can digest the raw numbers or text. The designers of computer visualization tools exploit the high-bandwidth channel of human visual perception. Software systems may provide either static or interactive visual representations of data, depending on user needs and on whether the final goal is the explanation or the exploration of the data.

Visual representation of information has a rich historical tradition, primarily in manually created depictions such as anatomical drawings, spread sheets or basic graphics. Now, however, computer graphics has the scalability to handle datasets much larger than any that could be manually depicted. In addition, computer graphics offers new possibilities in animation and interactivity. Visualization is useful for detecting patterns, assessing situations, and prioritizing tasks. Computation alone does not lead to understanding. The end user also needs a comprehensible interface with the computational output. Visualization provides that interface, and in so doing becomes the key to the interpretation of the data.

Engineers need assistance in making complex decisions and analyses, especially with tasks involving large amounts of data. Often, engineers have to deal with over-specified situations, and visualization of the situation helps them filter out the irrelevant data. Engineers can use visual analysis systems to explore “what if” scenarios and to examine data under multiple perspectives and assumptions. They can identify connections between any number of attributes, and they can assess the reliability of any conclusions [15].

We need to create an SBES visualization framework for uncertainty and to investigate and explore new visual representations for characterizing error

Visualization research must continually respond to and address the needs of the scientific community. For example, the ability to visualize measures of error and uncertainty will be fundamental to a better understanding of three-dimensional simulation data. This understanding will allow the validation of new theoretical models, improve the interpretation of data, and facilitate decision-making. With few exceptions, however, visualization research has ignored the need for visual representation of errors and uncertainty for three-dimensional visualizations [16]. We need to create an SBES visualization framework for uncertainty and to investigate new visual representations for characterizing error and uncertainty.

Within DDDAS and SBES applications, visualization of time-dependent data will be crucial. Currently, however, most interactive visualization techniques make use of static data only. The prevailing method for visualizing time-dependent data is first to select a viewing angle and then to render time steps off-line and play the visualization back as a video. Whereas this approach is often adequate for presentational purposes, the inability to engage in interactive exploration undermines the effectiveness and relevancy of visualization for investigative purposes. Thus, new methods for interactively visualizing large-scale, time-dependent data are needed. In addition, we need methods for visualizing vector and tensor fields, field data collected experimentally from multiple sources, and the ability to visualize data from both a global and local perspective.

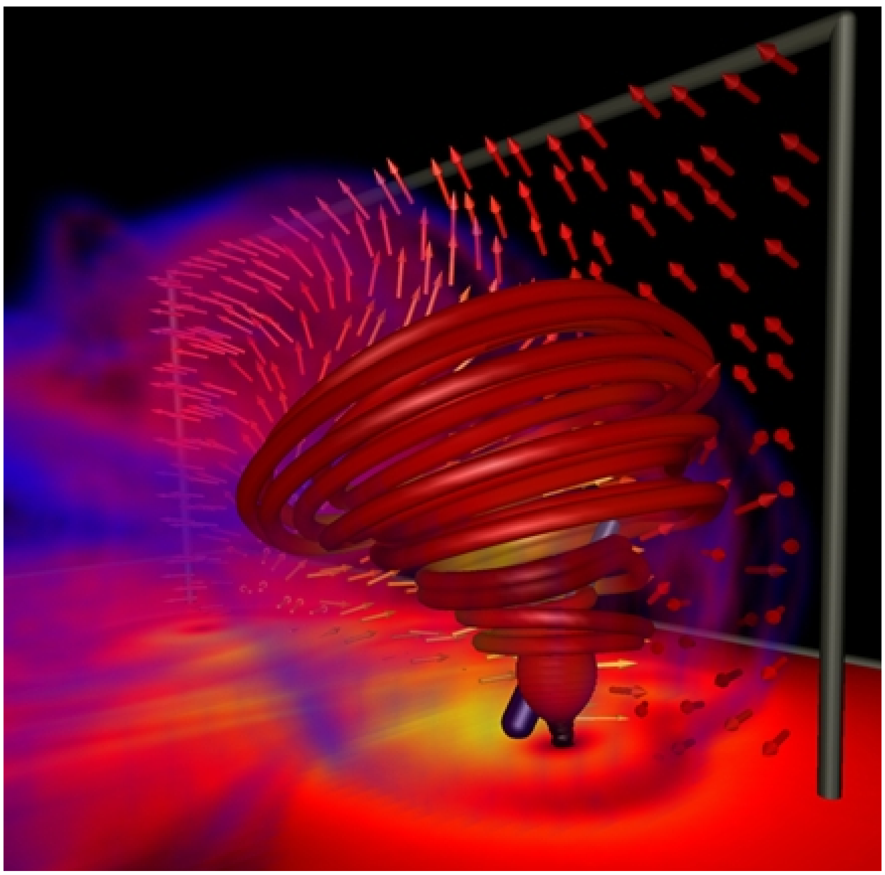

Figure 4: State-of-the-art visualization of turbulence in combustible flow. Tomorrow's capabilities may include parallel, interrogative visualization tools, integration of visualization with large-scale dynamics simulations of complex multi-physics events, and zooming techniques to visualize events at multiple scales.

New approaches to algorithmic visualization will be needed that focus on the needs of SBES. One approach is interrogative visualization, which is another way of saying that quantitative querying through analysis must be supported hand-in-hand with fast rendering of domains and computed function fields. A second approach is interpretive visualization. Interpretive visualization focuses on informatics and techniques to interpret imaging data, as well as various quantitative-analysis data. For example, going from imaging data to the construction of a domain model is an arduous task. In particular, to capture spatial domain realism at each of the desired scales of simulation is daunting, and may in fact be impossible.

A third approach is repetitive visualization. Humans have several biorhythms. We have the daily circadian rhythm of mental efficiency, and we alternate between periods of work and rest. We should accommodate biorhythms in our methodologies for quantitative or interpretive visualization. In other words, we should develop a mathematical framework for visualizations that allows our perceptions of information to change with repeated visualizations of that information. Additionally, if we are simulating the same function using models at varying scales, we would have a natural opportunity to revisit our earlier visualizations and make comparisons at multiple scales [2].

Because of the complexity and the massive amounts of data from simulations, researchers will turn to semi-automated techniques from the multidisciplinary field of scientific data mining to extract useful information from the data. To meet this purpose, data-mining techniques exploit ideas from image and video processing, statistics, pattern recognition, mathematical optimization, and other fields. Scientific data-mining techniques can be used to quantitatively compare simulations to each other and to experiments, to extract summary statistics from high-fidelity simulations for use in building models, and to analyze experimental data.

Whereas data-mining techniques can be effective in the extraction of information from simulation data, several open challenges remain. Those challenges include the extraction of features of interest from adaptive mesh refinements and unstructured grids, the processing and interpretation of experimental images that are often of low quality, the definition of metrics used in comparisons of simulations and experiments, and the analysis of distributed data sets resulting from simulations on parallel systems [17].

Finding

Visualization and data management are key technologies for enabling future contributions in SBES. In addition, they hold great promise for scientific discovery, security, economic competitiveness, and other areas of national concern. Computer visualization will be integral to our ability to interpret and utilize the large data sets generated in SBES applications.

3.6 Next-Generation Algorithms and Computational Performance

Algorithms, the recipes for turning mathematical into computational processes, provides the bridge between the models describing physical and engineered systems, on the one hand, and the computational devices that generate the digital representations of simulations, on the other. Too often, only the speed of a computational device is cited as the figure of merit for simulation performance, and the impact of algorithms on reducing the time complexity (number of operations) and space complexity (size of memory) is unappreciated. For more than three decades, progress in microprocessor capabilities has been described by Moore’s Law, the observation that the number of transistors per unit area on a processor doubles every 18 months, with corresponding increases in practical performance for a fixed algorithm. Faster and more cost-effective hardware is a strong driver for simulation-based engineering. However, algorithmic improvements have been far more important.

In tomorrow's SBES environment, the computing performance of individual microprocessors will be just one of many important factors. New metrics will be needed to judge the effectiveness of systems based on SBES principles. More fundamental metrics include: time to solution in a multiprocessor environment, the wall-clock time that elapses from the initiation of the simulation process to the predicted outcome, and a measure of the confidence level for the predicted result. If the time to solution is short, but the quality of and confidence in the solution are low, the prediction may be of little value.

Improved algorithms have resulted in significant performance gains as measured by time to solution. Recent studies have noted remarkable progress in this area [3, 13, 18]. Figure 5 shows an example of that progress. The figure depicts improvements in performance for large-scale simulations of turbulent gas-phase combustion [19, p. 79]. As the example shows, advances in simulation algorithms have tripled the effective performance over that due to advances in processor speed alone over a period of a couple of decades. Similar results have been documented in many other domains, such as magnetohydrodynamics and radiation transport, and should inspire efforts to obtain and document super-Moore's Law gains in all areas of SBES

Among the most challenging problems for new algorithms are optimization and inverse problems. Simulation-based decision-making gives rise to complex optimization problems, which are governed by large-scale simulations. These optimization problems appear in engineering design (in which the decision variables represent the configuration and constitution of the system) and in manufacturing and operations (in which the decision variables represent control parameters). Moreover, decision-making informed by predictive simulation requires estimations of uncertain parameters that characterize the simulation. The response to the resulting inverse problems is to seek estimates for those parameters that minimize discrepancies with observations.

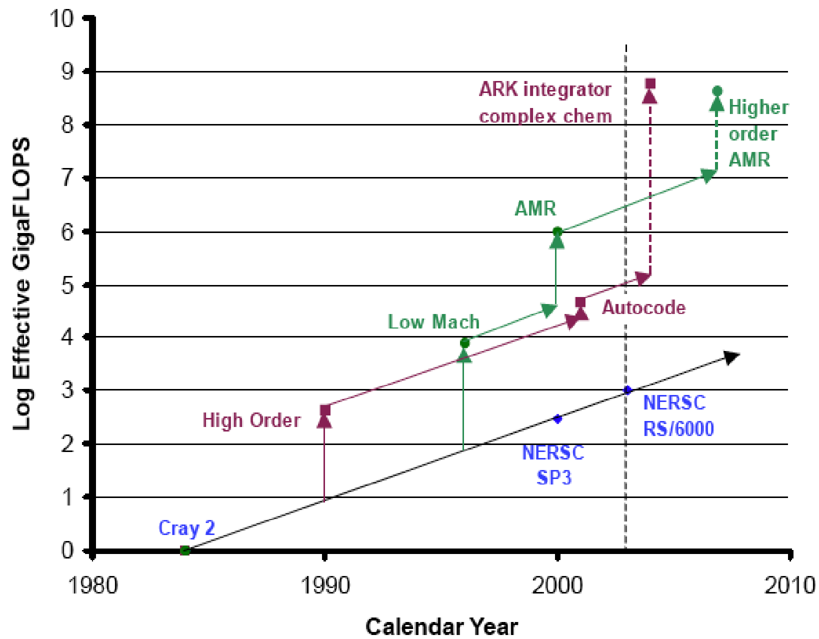

Figure 5. Increases in time to solution due to new algorithms, given in effective gigaflops over a period of years during which Moore's Law, the bottom line on this log-linear plot, remains valid (from [19, p. 79]).

Unfortunately, simulation-based optimization—whether in the form of optimal design, optimal control, or inverse problems—is notoriously more challenging than the corresponding simulation. First, the optimization problem is typically ill-posed, even though the simulation problems themselves are usually well-defined. Second, optimization usually results in a four-dimensional space-time boundary-value problem, despite the evolutionary nature of the forward problem. Third, the optimization problem is often formulated in probabilistic terms. Fourth, the simulation is merely a subproblem associated with optimization, which can be orders of magnitude more computationally challenging. Indeed, when the simulation problem requires terascale resources, the optimization problem will be in the petascale realm.

Contemporary optimization methods are inadequate for those tasks. We need entirely new classes of scalable, efficient, and robust optimization algorithms that are tailored to the complex multiscale, multi-physics simulations engendered by SBES. The resulting challenges are of the highest order; yet, they must be overcome to fulfill the promise of SBES: to elevate decision-making from a practice relying on simple interpolative models to a more rigorous science based on high-fidelity predictive simulation.

Finding

Investment in research in the core disciplines of science and engineering at the heart of SBES applications should be balanced with investment in the development of algorithms and computational procedures for dynamic multiscale, multiphysical applications.

4.0 THE CRISIS OF THE KNOWLEDGE EXPLOSION: SBES Education for Tomorrow's Engineers and Scientists

In Volume Two of the SCaLeS Report [19], one finds mention of the "crisis of the knowledge explosion." This expression refers to the dramatic expansion of the knowledge base required to advance modern simulation. The expansion ignores the traditional boundaries between academic disciplines, which have long been compartmentalized in the rigid organizational structures of today's universities. The old silo structure of educational institutions has become an antiquated liability. It discourages innovation, limits the critically important exchange of knowledge between core disciplines, and discourages the interdisciplinary research, study, and interaction critical to advances in SBES.

The PITAC report [4] lists the following as one its principal recommendations [4, p. 9]: "Universities must significantly change their organizational structures to promote and reward collaborative research that invigorates and advances multidisciplinary science. Universities must implement new multidisciplinary programs and organizations that provide rigorous, multifaceted education for the growing ranks of computational scientists the nation will need to remain at the forefront of scientific discovery." The report goes on to ask: Will research and educational study in the twenty-first century be "medieval or modern?"

The Panel strongly supports the viewpoint of the PITAC Report. If simulation is to become a discipline, an engineering tool, and a life-long learning opportunity, then the university-level engineering educational system in this country must be restructured. The current system does not provide the broad range of interdisciplinary knowledge that tomorrow's engineers and scientists in SBES require. To succeed, they must acquire substantial depth in computational and applied mathematics, as well as in their specific engineering or scientific disciplines. Graduate students, moreover, must be able to build foundations that allow them to access quantum and molecular science; statistical and continuum mechanics; biological science and chemistry; applied and computational mathematics; computer science and scientific computing; and imaging, geometry, and visualization. Participation in multidisciplinary research teams and industrial internships will give students the broad scientific and technical perspective, as well as the communication skills that are necessary for the effective development and deployment of SBES.

The integration of SBES into the educational system will broaden the curriculum for undergraduate students. Undergraduates, moreover, will have access to educational materials that demonstrate theories and practices that complement the traditional experimental and theoretical approaches to knowledge acquisition. In addition, SBES will provide a rich new environment for undergraduate research, in which students from engineering and science can work together on interdisciplinary teams.

NSF will need to collaborate with other federal agencies to open the door for a new generation of multidisciplinary research.

As in any entrenched culture, change is hard to come by. To change the culture of separate disciplines in U.S. universities will require well-directed, persistent, and innovative federal initiatives. The NSF has already done much to encourage multidisciplinary research and education through initiatives like the ITR and IGERT and DOE has the highly successful SciDAC program. Serious consideration should be given to turning successful cross-cutting programs into permanent (but still cross-cutting) administrative structures, just as the disciplinary divisions are permanent.

It is unlikely that the necessary changes in educational structure will come without strong directives from leaders from academia, industry, and government laboratories. Exactly what changes are needed and how they can best be implemented are issues well beyond the scope of this Panel. A detailed study of these issues, perhaps undertaken by an NSF-funded committee of the National Research Council, could trace out the new educational framework needed for effective interdisciplinary study and research.

The NSF needs to take the lead in "legitimizing" multidisciplinary research. One possibility might be the introduction of CAREER awards in multidisciplinary research areas. In some areas, NSF will need to collaborate with other federal agencies to open the door for a new generation of multidisciplinary researchers. A core base of funding should be provided that will allow multidisciplinary research and education to flourish. Best practices in multidisciplinary education should be identified and then encouraged. NSF programs like IGERT or DOE's Computational Science Graduate Fellowship Program provide much-needed funding and guidance for multidisciplinary graduate education, but they only have the resources to fund a very few such efforts in a given area. More funding is urgently needed for multidisciplinary graduate education programs that offer students an integrated approach of team research and career development.

Finding

Meaningful advances in SBES will require dramatic changes in science and engineering education. Interdisciplinary education in computational science and computing technology must be greatly improved. Interdisciplinary programs in computational science must be encouraged, and the traditional boundaries between disciplines in higher education must be made pervious to the exchange of information between discipline scientists working within multidisciplinary research teams.

5.0 CONCLUSIONS

This report has documented the findings and recommendations of the Blue Ribbon Panel on Simulation-Based Engineering Science, or SBES. As defined in this report, SBES is a discipline that focuses on the computer modeling and simulation of complex, interrelated engineered systems and on the acquisition of data meeting specified standards of precision and reliability. SBES draws on advances in scientific understanding and incorporates that understanding into new approaches to problems in the engineering domain through computer simulation.

The need for SBES as a distinct field of research comes at a crossroads in our nation's technological development. For almost half a century, developments in mathematical modeling, computational algorithms, and the technology of data-intensive computing have led to remarkable improvements in the health, security, productivity, quality of life, and competitiveness of the United States. We have now arrived at an historic moment. As described in this report, we are on the verge of an enormous expansion in our ability to model and simulate an almost limitless variety of natural phenomena. That expansion has profound implications:

First, computer modeling and simulation will allow us to explore natural events and engineered systems that have long defied analysis, measurement, and experimental methodologies. In effect, empirical assumptions will be replaced by science-based computational models.

Second, modeling and simulation will have applications across technologies—from microprocessors to the infrastructure of cities. Not the least of these new technologies will be effective systems for national security.

Moreover, new simulation methods will lay the groundwork for entire technologies that are only now emerging as possibilities.

Third, modeling and simulation will enable us to design and manufacture materials and products on a more scientific basis with less trial and error and shorter design cycles.

Fourth, modeling and simulation will greatly improve our ability to predict outcomes and optimize solutions before committing resources to specific designs and decisions.

Fifth, modeling and simulation will expand our ability to cope with problems that have been too complex for traditional methods. Such problems, for example, are those involving multiple scales of length and time, multiple physical processes, and unknown levels of uncertainties.

Sixth, modeling and simulation will introduce tools and methods that apply across all engineering disciplines—electrical, computer, mechanical, civil, chemical, aerospace, nuclear, biomedical, and materials science. For instance, all engineering disciplines stand to benefit from advances in optimization, control, uncertainty quantification, verification and validation, design decision-making, and real-time response.

There is little wonder that independent studies into the future of the nation's technology are unanimous in their conclusions that computer modeling and simulation are *the key elements* for achieving progress in engineering and science. The challenges of making progress, however, are as substantial as the benefits. We must, for example, find methods for linking phenomena in systems that span large ranges of time and spatial scales. We must be able to describe macroscopic events in terms of subscale behaviors. We need better optimization procedures for simulating complex systems, procedures that can account for uncertainties. We need to build frameworks for validation, verification, and uncertainty quantification. Finally, we need methods for rapidly generating high-fidelity models of complex geometries and material properties.

We are not alone in recognizing the urgency of our need to find solutions to these problems. Many of our international competitors are well ahead of us in committing the necessary funding and intellectual resources to overcome the technical problems described in this report. Indeed, the technological superiority Americans have so long taken for granted seems to be slipping away.

To arrest that trend and to help restore the U.S. to its leadership role in this strategically critical technology, the Panel has made four recommendations (see page xiv of this report for details):

(1) The Panel recommends that the NSF change its organizational structures to facilitate long-range core funding of SBES.

(2) The Panel recommends a minimum sixfold increase in funding over 2005 levels of SBES-related disciplines.

(3) The Panel recommends a long-term program of high-risk research to exploit the considerable promise of SBES.

(4) The Panel recommends that NSF underwrite an effort to explore the possibility of initiating a sweeping overhaul of our engineering educational system to reflect the multidisciplinary nature of modern engineering and to help students acquire the necessary modeling and simulation skills.

These recommendations call for NSF to take decisive and aggressive action to support SBES. Unfortunately, over the past decade, NSF and other agencies have persistently funded far fewer simulation-related research projects than recommended. The difference was sometimes a factor of three and occasionally a factor of ten. Moreover, even projects receiving support were frequently under-funded and the grant periods were so short that researchers could only hope to achieve incremental advances in the development of key disciplines. By contrast, over the same period, funding for SBES research in Europe and Asia increased many fold. To overcome these combined shortcomings in funding and duration, the Panel recommends at NSF, an annual fund of $300 million be made available to advance the SBES components critical to the nation's security, leadership, and competitiveness.

The Panel recognizes that improvements in the speed and efficiency of computers remain important components of advances in SBES. Nevertheless, efforts in these improvements should not supersede efforts in other disciplines underlying simulation. Instead, NSF should focus on initiatives in SBES that promote interaction between multiple disciplines that fit naturally and strategically in parallel with or within the Cyberinfrastructure framework. Within NSF, SBES should represent a new and fundamental thread of the Cyberinfrastructure theme, one that could well call for a parallel program that interfaces every division within the Directorate of Engineering, if not across the entire Foundation.

Appendix A: SBES Workshop Attendees

April 2004 Workshop

Workshop Organizers

Ted Belytschko *(Northwestern*)
Jacob Fish *(Rensselaer)*
Thomas J. R. Hughes *(U Texas-Austin)*
J. Tinsley Oden *(U Texas-Austin)*

Universities

Narayan Aluru, *(U Illinois-UC)*
William Curtin *(Brown U)*
Leszek Demkowicz *(U Texas-Austin)*
Charbel Farhat *(U Colorado-Boulder)*
Omar Ghattas *(Carnegie Mellon)*
Anthony Ingraffea *(Cornell)*
Chris Johnson *(U Utah)*
David Keyes *(Columbia*)
Donald Millard *(Rensselaer)*
Robert Moser *(U Illinois-UC)*
Alan Needleman *(Brown U)*
N. Radhakrishnam *(N Carolina A&T U)*
Mark Shephard *(Rensselaer)*
Charles Taylor *(Stanford)*
Mary Wheeler *(U Texas-Austin)*

Government Laboratories

Thomas Bickel *(SNL)*
John Red-Horse *(SNL)*
Roshdy Barsoum *(ONR*)
Luise Couchman *(ONR)*
Craig Hartley *(AFOSR)*
Walter Jones *(AFOSR)*
Raju Namburu *(ARL)*
Noam Bernstein *(NRL)*
Jonathan B. Ransom *(NASA)*

NSF

Kamal Abdali *(NSF)*
John Brighton *(ENG)*
Ken Chong *(ENG/CMS)*
Sangtae Kim *(NSF)*
George Lea *(NSF)*
Priscilla Nelson *(NSF)*
Michael Plesniak *(ENG/CTS)*
Galip Ulsoy *(ENG)*

September 2005 Workshop

Universities

Richard Alkire *(U Illinois-UC)*
Narayana Aluru *(U Illinois-UC)*
Kyle Anderson *(UTC SimCenter)*
Chandrajit Bajaj *(U Texas-Austin)*
Jon Bass *(U Texas-Austin)*
Ted Belytschko *(Northwestern)*
Larry Biegler *(Carnegie Mellon)*
Wei Cai *(Stanford)*
Alok Chaturvedi *(Purdue)*
Leszek Demkowicz *(U Texas-Austin)*
Abhi Deshmukh *(U Mass)*
Craig Douglas *(U Kentucky)*
Charbel Farhat *(Stanford)*
Jacob Fish *(Rensselaer)*
Roger Ghanem *(USC)*
Omar Ghattas *(U Texas-Austin)*
Michael Heath *(U Illinois-UC)*
K. Jimmy Hsiah *(U Illinois-UC)*
Thomas J. R. Hughes *(U Texas-Austin)*
Tony Ingraffea *(Cornell)*
Chris Johnson *(U Utah)*
Ramdev Kanapady *(U Minnesota)*
Carl Timothy Kelley *(NC State)*
Yannis Kevrekidis *(Princeton)*
David Keyes *(Columbia)*
Alan Laub *(UCLA)*
David Levermore *(U Maryland-CP)*
Michael Levine *(Pittsburgh)*
David Littlefield *(U Alabama)*
Wing Kam Liu *(Northwestern)*
Raghu Marchiraju *(Ohio State)*
J. Tinsley Oden *(U Texas-Austin)*
Steven Parker *(U Utah)*
Linda Petzold *(UC-Santa Barbara)*
Robert Pennington *(U Illinois-UC)*
N. Radhakrishnan *(NC A&T U)*
Mark Rashid *(UC-Davis)*
Tom Russell *(U Mass)*
Mark Shephard *(Rensselaer)*
David Srolovitz *(Princeton)*
Fanis Strouboulis *(Texas A&M)*
Andrew Szeri *(UC-Berkeley)*
Brian Wirth *(UC-Berkeley)*
Jacob White *(MIT)*
Sidney Yip *(MIT)*

DOE, Government Laboratories, and NIH

Roshdy Barsoum *(ONR)*
Peter Castle *(INL)*
Luise Couchman *(ONR)*
Stephen Davis *(ARO)*
Evi Dube *(LLNL)*
Francois Gygi *(LLNL)*
Chandrika Kamath *(LLNL)*
Dimitri Kusnezov *(DOE)*
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