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**Simulation-Based  
Engineering Science:**

***Revolutionizing Engineering and Science  
through Intelligent Simulation***

***August 28, 2005***

**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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## EXECUTIVE SUMMARY

[DRAFT OPENING PARAGRAPHS AND OUTLINE]

*Simulation*: the act or process of simulating, creating a likeness, the imitation or representation of the functioning of one system or process by means of the functioning of another. In this document, simulation refers to computer-generated imitations obtained from discretization of mathematical and conceptual models of physical events or of features of the behavior of engineered systems. Computer simulation represents an extension of theoretical science; it can and generally is based on mathematical models characterizing scientific theory, but it can be much more, because simulation can be used to explore the consequences of situations in which well-established theory breaks down. Simulation also provides a unique alternative to experimental science and observation, for it can be used to study events not observable or for which measurements are impractical or too expensive. Thus, the vast technological base on which modern computer simulation rests, the enormous pool of scientific, mathematical, computational, and engineering knowledge and methodologies it draws upon, make simulation an extremely important, intellectually deep, and powerful discipline that transcends the traditional pillars of science. It brings to engineering science a rich collection of ideas and a remarkable collection of tools that could revolutionize the way engineering and science are done in the 21<sup>st</sup> century.

While the use of computer simulation in engineering science began over a half century ago, the remarkable developments in computational and computer sciences, in computing equipment and infrastructure over the past decade have brought simulation theory and technology to the brink of a new era, one that can have a dramatic impact on all areas of engineering science. But Simulation-Based Engineering Science has emerged as a key discipline for other reasons as well: a host of critical technologies are on the horizon that cannot be understood, developed, or utilized without simulation methods. Simulation-

Based Engineering Science, SBES, is a discipline indispensable in the nation's continued leadership in science and engineering.

This report is from a Blue Ribbon Panel convened by the Assistant Director of the Engineering Directorate of the National Science Foundation (NSF) to explore opportunities and potential advances in SBES and to make strategic recommendations as to how NSF should structure its programs to respond to them.

The Panel's findings and recommendations have developed from interactions with major factors in the computational engineering and science communities, by building upon the results of numerous studies by other panels and bodies accumulated over the last decade on major issues in computational and computer science, on input from key leaders in the computer simulation community during two national NSF-supported workshops on SBES, and on the results of 8 meetings of the panel over a six-month period.

This document explores the potential impacts of advances in SBES on science and technology and the challenges and barriers to advancement. These include formidable challenges in multi-scale modeling, in the development of next-generation algorithms, in the design and implementation of dynamic data-driven application systems, in methods for uncertainty quantification and model validation and verification, in coping with the integration of data-intensive computing and visualization with simulation, and with overhauling our educational system. But the payoffs are incredible, encompassing dramatic advances in medicine and medical practice, in materials science, in homeland security systems, in manufacturing, engineering design, and many others.

There is little doubt that simulation and computational engineering science are of fundamental importance to the United States. This fact has been emphasized in numerous studies that have appeared over the last decade, and is strongly documented in the present report. What is of paramount concern is that the urgency and importance of this fact may be underappreciated by those

involved in setting the research-funding agenda for the country or those in academia who manage our educational institutions.

[Summary of Principal Recommendations]

[Emphasis on the fact that we are losing our standing to competitors at an increasing rate.]

## **1.0 SBES – A NATIONAL PRIORITY FOR TOMORROW’S ENGINEERING AND SCIENCE**

Advances in mathematical modeling, computational algorithms, in the speed of computers, and in the science and technology of data intensive computing have brought the field of computer simulation to the threshold of a new era, an era in which unprecedented improvements in the health , security, productivity, and competitiveness of our nation may be possible. However, to achieve these advancements, major obstacles must be overcome, including major scientific, engineering, sociological, and educational obstacles that may require significant breakthroughs in research, changes in the research and educational culture in our academic institutions, and changes in the organizational structure of our educational systems. The great benefits of these advances are in the realm of engineering, but they will require basic research in the scientific components of modeling, simulation, computing, and other areas. For this reason, we refer to the discipline as simulation-based engineering science: SBES. In this report we will describe this new discipline, the major obstacles standing in the way of its advancement, some of the remarkable benefits it can make possible, and we will record findings and recommendations of our panel that reflect our understanding of the consensus of a large segment of the nation's scientific and engineering community involved in computational engineering and sciences.

There is overwhelming consensus that simulation is a key element for achieving progress in engineering and science in the near future. Indeed, seldom have so many independent studies by experts from diverse perspectives reached conclusions that are in such agreement: computer simulation is a discipline of fundamental importance that is having and will continue to have an enormous impact on all areas of science, on scientific discovery, and on major problems

affecting humankind. This message is woven into the principal findings of many key investigations. We acknowledge in particular: the PITAC report [4], which emphasizes the development of computational science for national competitiveness; the SciDAC [17] and SCaLeS [12,13] reports, which emphasize opportunities for scientific discovery at the high-end of today's simulation capabilities and the need for a new scientific culture of interdisciplinary teamwork to realize them; the Roadmap for the Revitalization of High-End Computing [16] and the Federal Plan for High-end Computing [10], which emphasize the need for innovation in computer architecture in order to advance simulation; the Future of Supercomputing report [9], which examines the role of the federal government in sustaining the leading edge of supercomputing; and the Cyberinfrastructure report [1], which outlines a diverse program of inter-related research imperatives stretching well beyond simulation into communication and data technologies. Other related reports appeared in this new century alone [3,6,7,8,15], and many others shared the same vision going back to the Lax report of 1982 [14a].

The present report enters a domain already reverberating with recent calls to increase the vigor of research and training in computation-based simulation in the United States. It is in harmony with its predecessors and owes its brevity to their effective presentations, but it also sounds new notes, emphasizing additional and extremely important elements of simulation that have been overlooked, and adds a voice that has not been fully heard.

Attaining the potential of SBES will require a revolution in simulation technology. Simulation-Based Engineering Science constitutes a new paradigm in computer simulation and related technologies that will be indispensable in meeting the scientific and engineering challenges of the twenty-first century. It is not "simulation as usual." SBES is focused on modeling and simulation of complex, interrelated engineered systems and obtaining results of a specified precision and reliability. It involves modeling physical phenomena, but goes beyond to address methods, devices, procedures, processes, and planning. It

draws on and stimulates advances in scientific understanding, extending it to the engineering domain through optimization, control, uncertainty quantification, verification and validation, planning, decision-making, and real-time response. It involves the aggressive development of a host of new technologies that lift simulation to a new level, a level essential for addressing the most difficult aspects of modeling, engineering design, manufacturing, and scientific discovery. SBES will: (1) provide the means to understand and control multi-scale, multi-physics phenomena; (2) be a vital tool in fundamental developments in nanotechnology, biomedicine, materials, and earth and life sciences; (3) dramatically enhance the fidelity and utility of computer predictions; and (4) provide a technology that will tremendously benefit almost every field of engineering and the health, security, competitiveness, and wealth of our nation. Meeting these challenges will require: (1) a revolution in the way simulations are conceived and performed; including new discoveries in simplifying and enhancing multiscale, multidisciplinary simulations and a knowledge base for the field; (2) great advances in supporting technologies, including large-scale computing, data management, and algorithms; (3) an overhaul of our educational institutions; and (4) changes in the manner research is funded and conducted.

Simulation has ridden the crest of a hardware and software information technology wave that has made it increasingly effective relative to current standard science and engineering practice. Simulation treats real systems rather than the restricted, idealized systems of most theory. Simulation provides unprecedented access to real-world conditions, rather than being restricted to affordable experiments and tests within unrealistic parameter ranges or limited by treaty or health and environmental concerns. The triumphs of computer simulation in the twentieth century are well known: simulation has become indispensable in assessing vehicle crash worthiness; in predictive models of the weather, climate change, and behavior of the atmosphere; in broad areas of engineering analysis and design; in product manufacturing; in an expanding list of biomedical applications; and in designing systems for defense,

communications, and transportation. However, many of the simulation methodologies at the heart of these successes are decades old and are completely inadequate for the myriad of challenges on the horizon. In many ways, the past successes of simulation may be the worst enemy of the discipline for it has led to a knowledge base, methods, and practices that are not adequate for the impending challenges. At a time in which our nation claims to be the leader in computational science and simulation theory and technology, many indicators suggest that the United States is quickly losing ground and is, in fact, no longer positioned to lead the world over the next few decades in SBES. The consequences of falling behind in this race will have a profound impact on US technology, the US economy, and the US position in the global community.

The importance and great potential of simulation have not gone unnoticed by our competitors around the world. Our competitors in Europe, Asia, and South America are already building on U.S.-pioneered developments of the twentieth century in computing, mathematical and computational modeling, algorithms, networking, and generally in computational engineering and science. They are making major investments in simulation research. We are in danger, yet again, of producing world-leading science that is being converted into technology and economic growth overseas rather than at home.

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.”

“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 trade balance in high-tech products has been negative.

China is emerging as the chief global economic competitor of the United States. In 2003 China graduated approximately 700,000 engineers at the bachelor's level, compared with 60,000 in the United States. To employ an engineer in China costs roughly one-tenth to one-sixth of what it costs in the United States. This large productivity disadvantage must be overcome through better training and tools. Simulation is the key to overcome this disadvantage. Simulation must become easier to use reliably and its capabilities must be extended to more complex systems and real-time results. It must be made a core part of the engineering curriculum, not only as a desirable engineering skill outcome, but also as a means for more effective pedagogy.

New frontiers in engineering and science hold the promise of changing the way the industrialized world functions. Simulations will underpin advances in all future technologies, including microelectronics, advanced materials, biotechnology, nanotechnology, pharmaceuticals, medicine, defense and security, and many other areas. Breakthroughs in each of these areas will be made through simulation-based scientific discovery and simulation-based expansion of this understanding to engineering practice for technological developments. This will require the most advanced know-how, significant resources, and a national commitment to SBES.

The road toward advances in key SBES components is a rough and winding one, and many challenges must be met and overcome. They include technical, mathematical, scientific, and computational issues, and a sea change in our approach to engineering and science education. The greatest obstacles are discussed in the following sections. We address next the incredibly difficult but fundamentally important area of multi-scale modeling, which stands as a barrier to many advances in SBES. Then the equally important area of reliability of computer simulations is discussed, and the exciting possibilities of dynamically-controlled simulation systems are described. Advances in SBES will bring about dramatic changes in how scientific and engineering software is designed, maintained, utilized, and how the performance of computational systems is

measured. These issues are discussed in Chapters 5 and 6. We provide only a small sample of the multitude of driving SBES applications that are on the horizon. All will have enormous benefits to society. We discuss in Chapter 8 the revolution in our educational systems that will be required to equip future generations of engineering scientists with knowledge of SBES and its value in science and technology. Finally, a list of major recommendations for accelerating the advancement of SBES is given. The Panel regards these recommended actions as vital to the nation's leadership in computational engineering and science.

## 2.0 THE TYRANNY OF SCALES: THE CHALLENGE OF MULTI-SCALE MODELING AND SIMULATION

Those involved in the world-wide race toward miniaturization, nanoscience and technology, molecular modeling of drugs and biological systems, new advanced materials, and other applications involving events occurring on the atomistic and molecular scale have run into a huge and formidable roadblock that is due to the *tyranny of scales*. Virtually all simulation methods known at the beginning of the twenty-first century were valid for a limited range of spatial and temporal scales. When confronted with the requirements of modeling physical phenomena that range over 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, one appreciates the enormity of the tyranny and the unlikelihood of defeating it with conventional simulation tools.

The tyranny of scales does not occur just at the atomistic level. The need for simulation models involving a disparity of spatial and temporal scales is confronted in virtually all areas of modern science and engineering: in astrophysics, atmospheric science, geological sciences, and in the design of complex engineering systems, such as submarines, commercial aircraft, and modern turbine engines.

In many ways, the entire body of existing knowledge of the physical universe and all accumulated knowledge on the design and functioning of all engineering systems is partitioned according to scale. The designer of electronic properties of materials sees the world as galaxies of atoms with clouds of electrons in orbit about them, while the atmospheric scientist observes changes in climate conditions that occur over thousands of miles. Tomorrow's technological advances cannot tolerate this partitioned view of nature. New thinking, very likely by interdisciplinary teams of researchers, will be needed to

develop models and simulation tools that transcend many scales. The tyranny of scales will not be overcome easily, and will not be resolved by simply building bigger and faster computers. 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 urgency of the development of multi-scale simulation models has been felt worldwide. Over the past five years, virtually every conference, symposium, or international congress devoted to computational engineering and science has listed multi-scale modeling as an important theme, often as the subject of colloquia, study groups, or invited lectures. Three DOE workshops were recently held on multiscale mathematics [7, 15], and programs at NSF and NIH are already in place for promoting research in this subject. Over the last three years, a large and growing body of literature has been produced 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, many akin to new versions of the multigrid methods popular at the end of the 90s. Progress on multi-scale models, has been agonizingly slow. Breakthroughs in this fundamental area are needed along with significant increases in the support of research.

### 3.0 VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION

The ultimate goal of simulation is to make predictions of physical events or of attributes of the behavior of engineered systems. Such predictions are the basis of engineering decisions, they are the determining factor in product or system design, they may be a basis for possible scientific discovery, and they are a principal aspect of computational science that projects it beyond the realm of physical experiments and observations. It is therefore natural to ask if the predicted outcomes of an event are reliable. 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 and 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 and V: verification and validation. It is a subject fundamental to the success and advancement of SBES.

To appreciate the subtleties and goals of V and 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 phenomenon 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 computational model of the event is a discretized corruption of the mathematical model developed so that its analysis can be implemented on a computer – a digital computing device. Validation is the process, or collection of processes, designed to determine the accuracy with which the mathematical model depicts

the actual physical event. Verification is the process of determining 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 right?”.

Remarkably, the entire field of V and V is in an early stage of development. Basic definitions and principles have been the subject of much debate in recent years, and many aspects of the subject remain in the grey realm between the philosophy of science and 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, and as much as the mathematical model of a physical event is a manifestation of a theory, such models can actually never be validated in a strict sense – they can only be invalidated. Thus, all validation processes involve the prescription of acceptance criteria and metrics that would allow the analyst to judge if the model is invalid in the light of physical observations and experiments and measured against criteria 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 and 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 are always variable in measured data from one sample to another or from one observation to the next. Moreover, the experimental devices used to obtain the data can have error due to uncontrollable factors, so-called noise, or errors in calibration. Then there are phenomena for which little quantitative information is known about the data needed to complete the definitions of the model, or for which knowledge of the governing physical processes is incomplete or inaccurate. Uncertainty may thus be due to variability in data, referred to as aleatoric uncertainty, or due to immeasurable or unknown

factors, which is so-called subjective uncertainty. In either case, techniques must be developed to quantify uncertainty and to incorporate such measures into the interpretation and use of simulation predictions.

Uncertainty quantification methods for large-scale simulations are in an early stage of development and much research remains to be done. Since model parameters can often be treated as random fields, probabilistic formulations provide one approach to uncertainty when ample statistical information is available. The use of stochastic models, on the other hand, can represent gigantic increases in complexity in data volume, storage, manipulation, and retrieval requirements. Other approaches to uncertainty qualification include stochastic perturbation methods, fuzzy sets, Bayesian statistics, information-gap theory, decision theory, and other methodologies. 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.

## **4.0 DYNAMIC SIMULATION SYSTEMS, SENSORS, MEASUREMENTS, AND HETEROGENOUS SIMULATION**

One of the most challenging thrusts of SBES, but one which may yield the richest dividends, is concerned with the new and revolutionary idea of tying simulation tools directly to measurement devices for real time control of simulations and computer predictions. Some preliminary investments in research in this direction have been made under NSF's program in Dynamic Data Driven Applications Systems (DDDAS) [6] but the full development of this new and fundamentally important discipline will take years of research and new technological developments in many areas.

DDDAS is envisioned as a new paradigm in computer simulation involving a "symbiotic feedback control system" [6] in which simulations and experiments (or field data) interact in real-time to dramatically improve the fidelity of the simulation tool, its accuracy and reliability.

The original document putting forth the idea, now over five years old, described the goal 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 between applications/simulations and measurements is a novel technical direction that can open new domains in the capabilities of simulations with 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 as manufacturing, commerce, transportation, hazard prediction/management, and medicine, to name a few."

A half-decade later, these words still ring true, but the enormity of the

task of developing such DDDAS systems, the complexity of the issues involved, the breadth of expertise and technologies required to implement such systems, the new software infrastructures, and the efficiency and capacity of computational and data management systems required, will mandate a sustained and well-funded program of basic and applied research over possibly a decade or more. The payoffs, however, are so immense and important 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. We must aggressively begin to develop it before our competitors once again gain ground because of our complacency.

The basic building blocks of DDDAS include: 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.

In many ways, DDDAS will rewrite the book on validation and verification of computer predictions. No longer will the validation process be a one-shot proposition to judge the acceptability of a simulation problem on the basis of a static data set; it will be a dynamic control process in which the deficiencies of one computational model can be assessed, upgraded, and improved on the fly to dramatically enrich the predictability of the model and increase confidence in the predicted results.

It is a technology that will integrate large-scale numerical computing with data-intensive computing, sensors, imaging, grid computing, and other measurement devices. It will require new concepts in software infrastructure, algorithms, control protocols, and solvers. It will strive to dynamically incorporate data into an executing simulation, and, in turn, to dynamically steer

the measurement process. The possible applications are endless: surgical procedures, homeland security, control of hazardous materials, environmental remediation, drug delivery, manufacturing processes, oil reservoir management, vehicle flight control, and many others.

## 5.0 NEW VISTAS IN SIMULATION SOFTWARE

Many contemporary engineering communities regard simulation software as a commodity provided by vendors for well-defined applications. Long-lived codes for engineering analysis in specific, independent domains of application are incrementally improved by providing functional extensions. The demands of the next generation of engineering problems – multiscale, with real-time data interaction and abundant uncertainties in the data – cannot be supported by such an approach. The PITAC report [11] says: “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 on 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 to the development of the software that will encapsulate the models and methods needed for full-orbed SBES. Methodologies that support the interoperability of individual simulation software components must be identified, developed, and integrated into the next generation of engineering software. In addition, the algorithmic complexity of new simulation components, coupled with the requirement that these components function efficiently on an evolving range of architectures designed for large-scale parallel computations, will require entirely new methods and tools to support simulation software development.

Many contemporary software libraries (for instance, linear equation solvers), language interoperability tools, component coupling and data transfer

tools, and simulation development frameworks, will not survive the requirements of robustness, efficiency, and flexibility of tomorrow's SBES software. The SBES software paradigms needed will require "out-of-the-box" thinking, to define the real requirements for the implementation of SBES technologies. Tomorrow's software will not only execute simulation algorithms, but also dynamically manage data throughput and model adaptivity and control. It must also be designed to steer observational and measurement systems to optimize data collection and use. It must be designed to navigate across implementations of models of multiple scales based on multiple physical theories efficiently, with scalable methods that interact seamlessly with data-gathering devices. To meet this demand, new approaches to software development and engineering must be developed, and this will require changes in the way scientific computing is taught and perceived in our universities. Tomorrow's software developers must not only cope with the challenges of more complex algorithms and heterogeneous hardware systems, but also understand important aspects of the applications for which the software is to be developed.

While the software vista for SBES is uncharted as to details, there is a path-finding program in the federal government with a similarly aggressive software philosophy and some software with which to bootstrap. This is the Scientific Discovery through Advanced Computing (SciDAC) initiative [17] (see also chapter 2 of [12]), which targets a handful of science applications relevant to the Department of Energy: principally accelerators, combustion, global climate, plasma fusion, quantum chromodynamics, and supernovae. Each application requires the concerted attention of applied mathematicians, computer scientists, and domain-specific scientists. In a similar way, close integration of three disciplines—engineering, computer science, and applied mathematics—and a new super-discipline in their intersection (SBES) are needed to realize the full benefits of the fast-moving advances in computing technologies in engineering science.

Software research and development under SBES should set a new paradigm for specialization with cross-accountability. Mission-driven teams, primarily practicing engineers, must define and model the engineering systems requiring breakthroughs through simulation (e.g., artificial organs, distribution networks), tentatively identifying data interfaces and the computational tasks between them. Teams of “enabling technologists,” primarily mathematicians and computer scientists, must tackle the abstract requirements identified by the mission-driven teams and develop software components that port across the target architectures, (e.g., massively parallel distributed memory computers). Component development should track the research frontier for each algorithmic area of expertise (e.g., error estimation, eigenanalysis) while being driven by mission requirements.

## **6.0 THE EMERGENCE OF BIG DATA IN SIMULATION AND THE ROLE OF VISUALIZATION**

Since the advent of computing, the world has experienced an information “big bang”, and explosion of data. Information is being created at an exponential rate and, since 2003, digital information makes up 90% of all information production, vastly exceeding paper and film. One of the greatest scientific and engineering challenges of the 21<sup>st</sup> century is to effectively understand and make use of this growing body of information.

In the computational science environment that existed near the end of the 20<sup>th</sup> century, data intensive computing and large-scale scientific computing were essentially disjoint camps, one involved in transporting, storing, and manipulating large data sets and the other with implementing scalable parallel computing strategies for resolving very large computational models of scientific and engineering problems. However, that era is very much over. In all of the SBES challenges mentioned earlier in this report and in the driving applications to be discussed later, the use and generation of immense data sets is clearly an integral component of SBES applications. Uncertainty quantification, for example, will require data sets many orders-of-magnitude larger than those of traditional deterministic computing. DDDAS, by definition, will demand that new methods be developed to 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. Computer visualization may provide the only answer to interpreting and utilizing the large data sets generated in SBES applications.

Visualization provides the means to explore and explain data through software systems that provide a static or interactive visual representation. The designers of computer visualization tools exploit the high-bandwidth channel of

human visual perception to allow people to comprehend information orders of magnitude more quickly than they could digest the raw numbers or text. Visual representations of information have a rich historical tradition, but the advent of computer graphics brought scalability to handle much larger datasets than could be manually depicted, and introduced the possibility of animations and interactivity. Visualization is useful for detecting patterns, assessing situations, and prioritizing tasks. Understanding, and ultimately knowledge, cannot be delivered directly from computation. Visualization is the tool for providing a face for computation to an end user, and in this role is the key to deriving knowledge from data. Visualization is a key technology for enabling future contributions in SBES, as well as scientific discovery, security, economic competitiveness, and other areas of national concern.

## 7.0 NEXT-GENERATION ALGORITHMS AND COMPUTATIONAL PERFORMANCE

Algorithms, the recipes for implementing mathematical and computational processes, provide the bridge between the models describing physical and engineered systems, and the computational device, the computing system, that generates a digital representation of a simulation. Too often, only the speed of the device is identified as a measure of efficiency and performance, and not the finesse with which clever algorithms can be used to accelerate the solution process. For more than three decades, it has been commonplace in the world of computation to measure progress in computing capabilities over time using Moore's Law, the assertion that the number of transistors per unit area in a computer chip would double every couple of years and, correspondingly, so would the speed and performance of the computers that utilized them. Such measures of computing performance are virtually irrelevant in tomorrow's SBES environment. New metrics will be needed to judge the effectiveness of new systems based on SBES principles. In the final analysis, the metrics for performance in tomorrow's computer simulation environment will be two-fold: time-to-solution, 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 and confidence in results is low, the prediction may be of little value. In any case, the simplistic measure of gigaflops is of fading importance in tomorrow's simulation arenas.

The gains in performance as measured by time-to-solution made possible by improved algorithms should not be underestimated. Remarkable possibilities in this area have been noted in recent studies and as reported in [12] and [3]. Figure 1 contains a representative depiction of improvements in performance for a large-scale simulation in turbulent gas-phase combustion [13, p. 79]. In this

example, possible advances in simulation algorithms could almost triple the effective gigaflop performance over that due to processor speed alone, thus repealing Moore's law in a definite and convincing way.

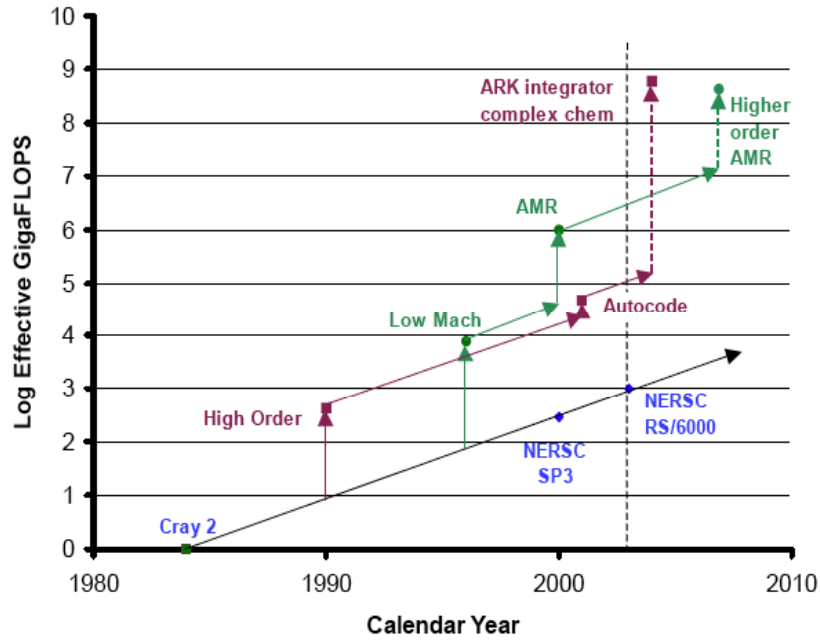


Figure 1. Increases in time-to-solution due to new algorithms given in effective gigaflops over a period of years during which Moore's law, the linear variation, remains valid. (From [13 , p. 79]).

## **8.0 THE PAYOFF: SOME DRIVING APPLICATIONS AND SOCIETAL BENEFITS OF SBES**

The applications and benefits of SBES are many. In the sections to follow, some of the important areas are described in the context of the core challenges listed earlier.

### **8.1 *SBES IN INDUSTRIAL AND DEFENSE APPLICATIONS***

Simulation has become ubiquitous in industry. It plays an essential role in the design of materials and manufacturing processes, and in the design of products. For example, prototype test simulation is increasingly used to replace prototype tests in many industries; it has enabled design cycle times to be reduced by decreasing the number of tests that need to be performed and the number of prototypes that need to be built.

However, in many important industrial processes, simulation methods still do not play a central role in design and its potential usefulness has not been exploited for several reasons:

1. the development of models is very time consuming; this is particularly true for defining parameters such as material properties, which often require extensive small-scale testing before simulation can be started, especially if statistical properties are also required;
2. the interpretation of data is difficult;
3. methods do not exist to link simulation models seamlessly with tests so that the overall decision process is facilitated;
4. simulation is separate from the design optimization process and can

not simultaneously deal with factors such as manufacturability, cost, and environmental impact.

Overcoming these barriers will require progress in basic understanding and new methods in various areas. Among these are:

1. multi-scale methods that can predict material behavior in terms of subscale properties, which are often known as multi-scale methods;
  2. effective optimization methods that can deal with complex constraints;
  3. frameworks for validation, verification, and uncertainty qualifications;
- and
4. methods for rationally interpreting nonlinear behavior.

The first is particularly important in view of the increasing use of new materials; the engineer must have at his disposal tools that can predict the behavior of a material in terms of its basic building blocks, which requires linking predictions at subscales, such as micromechanics or even quantum mechanics, to the macroscale behavior. While such linkages are well established for linear response, the crucial element that is not available today is the link between the scales for nonlinear behavior, particularly failure.

Design optimization is also in its infancy and there are many challenges to be overcome. There are many constraints in the optimization of a product design which are related to manufacturability, robustness, and a variety of other constraints. Furthermore, optimality often needs to be defined in terms of complex criteria that are not readily amenable to the frameworks currently in use. In addition, optimization methods must be closely coupled with the simulation tools to be effective for engineering applications in design. The entire question of what constitutes an optimal design and how to find it in a complex multifaceted environment is not understood today.

SBES has the potential to provide designs that are optimized for cost performance and its total impact on the environment (from production to disposal

or recycling) within a short design time. However, this cannot be achieved by incremental progress in extending current methods. There are many fundamental barriers that need to be resolved before nonlinear simulation can fulfill its promise in industry.

## **8.2** *SBES IN MEDICINE*

While computational science has made significant inroads in some biomedical domains, most notably in genomics and proteomics, it has had little impact thus far on the study of biological systems at the cellular, tissue, and organ scales, and only a limited impact on clinical medicine. Most diseases (including heart disease, cancer, stroke, respiratory diseases, etc.) and treatments (including surgical, transcatheter, and pharmacologic methods) involve complex interactions between biological systems from the molecular to organism scales. It is clear that computational science could have a much greater impact on biomedicine if simulation-based methods to analyze biological systems were developed.

It is interesting to compare medical practice with engineering. Both are problem-solving disciplines. Both require an understanding of complex systems. However, in engineering one endeavors to accurately predict the performance of a product or procedure. The entire design process is based upon predicted outcomes. Very often numerous criteria may need to be simultaneously satisfied. Sophisticated computer and analysis technologies are employed. By comparison, medical practice is a “build them and bust them” approach. The historical and current paradigm in medicine is based on a diagnostic/empirical approach. Physicians use various tests to diagnose a medical condition and then plan a treatment or intervention based upon experience and empirical data. There is generally no formal process employed to predict an outcome of a treatment for an

individual patient although there may be some statistical data to indicate the success rate of a procedure.

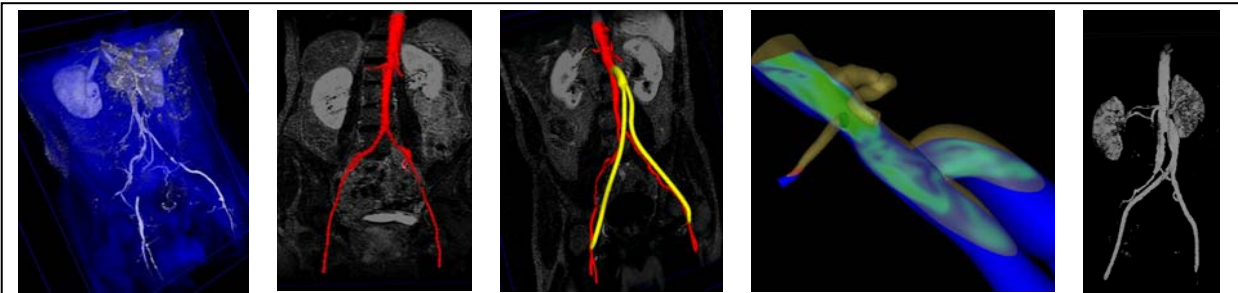


Figure 2: Example of simulation-based medicine approach as applied to designing bypass surgery for patient with occlusive cardiovascular disease in aorta and iliac arteries. Shown from left are magnetic resonance image data, preoperative geometric solid model, operative plan, computed blood flow velocity in aorta and proximal end of bypass, and postoperative image data used to validate predictions.

A program in SBES could also lead to new approaches to medical practice, that of Simulation-Based Medicine. New SBES methodologies, leveraging the tremendous advances in medical imaging and high-performance computing, could ensure that the practice of medicine in the future will resemble the practice of modern engineering more closely. In particular, an entirely new era in medicine could be created whereby doctors utilize simulation-based methods, initialized with patient-specific anatomic and physiologic data, to *design* optimal treatments for individuals based on *predicted* outcomes.

In addition to enabling physicians to devise better treatments for individual patients, simulation-based engineering methods could enable medical device manufacturers to predict the performance of their devices in virtual patients prior to deployment in human trials. Current physical and animal testing procedures (now used prior to human trials) have significant limitations in representing variations in human anatomy and physiology. Virtual prototyping of medical devices could be conducted by simulating the deployment of alternate device-designs in a group of virtual patients representing the range of conditions

likely to be encountered. These *virtual clinical trials* prior to animal and human studies, could result in safer designs, reduced development costs, and shorter time-to-market. Finally, the pharmaceutical and biotechnology manufacturers could benefit from SBES methods. For example, targeted drug deliveries are being increasingly used in treating a range of diseases including heart disease (e.g., drug-eluting stents), cancer (e.g., local chemotherapies), and chronic respiratory diseases (e.g., therapeutic inhalants). Simulation-based methods could be used to model the transport of drugs through the circulatory or respiratory systems and determine local concentrations to use in pharmacokinetic models of drug metabolism.

## **SIMULATION-BASED ARTIFICIAL ORGAN DESIGN**

According to the United Network for Organ Sharing, the number of Americans awaiting organ transplantation has grown to 90,000, while fewer than 15,000 organs are donated per year. Over 6,500 people die annually while on organ waiting lists. For many of these patients, the development of artificial organs—heart, lung, kidney, liver, and pancreas—offer the best hope for restoring health and prolonging their lives. Despite decades of research and a critical unmet demand, the development of artificial organs has progressed at an unacceptably slow pace. To bring an artificial organ to market requires up to 10 years of *in vitro*, animal, and clinical evaluation at a cost between \$30 and \$65 million [*these are 1993 figures; need to update*]. Such long lead times and prohibitive up-front costs have discouraged all but a few large corporations from continuing to pursue the development of these products—despite their critical need by the American public.

To fulfill the promise of artificial organs, computation-based simulation of natural and artificial organ function must be developed. This will allow extensive virtual testing and optimization of proposed designs prior to expensive animal and clinical trials. The result will be a reduction in the incidence of

suboptimal devices entering the clinical trials phase, where failure is catastrophic and redesign is not economically feasible. Computation-based modeling will not only reduce the design cycle time, but will also provide greater insight into the behavior of these devices, leading to superior designs and higher rates of success.

Unfortunately, simulation-based design of blood-wetted artificial organs—such as heart, lung, kidney, liver, and pancreas—has remained a formidable challenge. This is, in part, associated with the complexities of modeling blood flow and damage in complex devices, and the difficulty in performing design optimization under complex flow models and constraints. The major challenge in modeling blood flow is to accommodate its microstructure-induced behavior, which stems from the presence of deformable cellular bodies that are suspended in blood plasma. The design goal is to maximize performance while minimizing blood damage and blood element deposition, within constraints placed by anatomy, physiology, manufacturability, and cost. While blood damage is a cell-scale phenomenon, performance is usually quantified at device scales. Clearly, design optimization must address a wide range of spatio-temporal scales.

Figure 3 illustrates the cascade of length scales describing a proposed toddler ventricular assist device (TVAD), ranging from the centimeter device scale on the left, to the sub-millimeter non-Newtonian flow scale, to the sub-micron red blood cell flow dynamics scale, to the nanometer molecular scale of the cell membrane on the right. The challenges of simulation-based design of such a device are manifold and include the development of multiscale blood flow and damage models, stable discretization methods, scalable numerical solvers, verification and validation procedures, and optimization methods that employ coarse-scale representations for tractability while reverting to fine scales where necessary to avoid compromising feasibility and optimality. By accelerating research in these areas, SBES has the potential to revolutionize artificial organ design, resulting in vastly improved devices that are brought to market much more rapidly and economically.

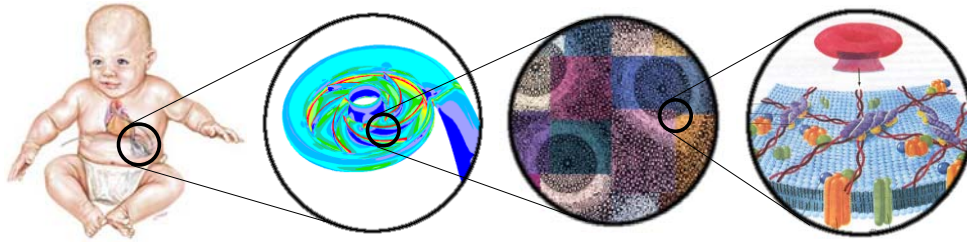


Figure 3: Multiscale model hierarchy of a toddler ventricular assist device

### 8.3 *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 infrastructure that support them from a range of threats, both hostile (e.g., terrorist), environmental (e.g., air and water pollution), and natural (e.g., earthquake or hurricane). Overall, the system for which security systems are to be designed and optimized includes the entire support infrastructure, such as buildings, transportation infrastructure, food, water and power distribution infrastructure, communications infrastructure, and waste disposal infrastructure. The application of SBES in this area will allow the prediction of the consequences of threats (e.g., accidental or malicious release of a chemical or biological agent), and possible countermeasure responses. Predictive simulations will allow the design and optimization of infrastructure for a wide range of objectives, and real-time simulations will enable the rational selection of responses during a crisis. For example, such real-time simulation capability for the World Trade Center could have indicated the importance of immediate evacuation of the building on September 11, 2001.

The comprehensive simulation of a city as a system requires integrated multi-scale simulation of many sub-systems and processes such as structural

response, fluid transport of contaminants, power distribution, and transportation systems, as well as the response of the human population. As with the previous Digital Human example, this vision of a *Digital City*, will require the acquisition of data of unprecedented detail. These data include detailed “static” descriptions of the installed infrastructure, and dynamically acquired data regarding the current state of the system, including such data as continuous measurements of air and water contaminant concentrations, flows of air, water, effluents etc., locations and velocities of transportation and other movable assets (e.g., trains, heavy machinery), densities and flows of the human population and their automobiles, etc.

A natural generalization of the Digital City concept is that of a Digital Ecosystem, whether artificial (such as a city) or natural (such as a forest, watershed, or even a continent or the world). The benefit is essentially the same: the ability to optimize human activity and infrastructure (in this case with regard to impact on the environment), and, through real-time simulation, allow rational selection of responses in a crisis, in this case an environmental crisis.

The application of SBES in this general area promises to revolutionize the practice of urban planning, transportation, structural and environmental engineering, and municipal and environmental management, as well as many other fields. The research required to realize this vision of a Digital City or Digital Ecosystem is in several general areas:

- Quantitative models of the processes to be simulated must be developed. For many of these processes, models of some level of veracity exist or are being developed for narrower engineering purposes. Obvious examples of this are structural models (of buildings and other structures), fluid dynamics models (air and water flows), combustion models (e.g., for fire spread), transportation models (e.g., traffic flow), and many others. Quantitative modeling of other processes is not currently as well developed. For example, sociological models of the response of populations or models of the evolution

of natural ecosystems such as forests or lakes.

- Detailed models at a wide range of scales must be integrated into a comprehensive simulation tool. This is a requirement for the application of SBES to almost any multi-scale complex system. Many of the issues are generic, but many are also problem specific.
- A general feature of SBES research and development is that new models or models of unprecedented veracity are required, and data of unprecedented detail are required to support model development and validation. Thus development of the Digital City or Digital Ecosystem will inevitably push experimental and theoretical research in the numerous fields relevant to this application. Further, the continuous real-time data needed for some applications will drive the development of the sensors and communication infrastructure required to support its acquisition, and the simulation techniques to assimilate the data into the simulations.
- There will of course continue to be uncertainties in the models and the data that drives them. To support rational decision making these uncertainties will need to be characterized and included in the modeling, so that design and decisions can be made based on assessments of the probable outcomes.

The application of SBES to the broadly defined security issues described here, and the development of Digital Cities and Digital Ecosystems present unparalleled opportunities to improve the function of the infrastructure supporting human populations and its interaction with the natural environment. A few of the likely applications of such simulations are listed below. There are obviously many more possible applications than can be listed here, and perhaps the most exciting possibilities are yet to be conceived.

- After detection of a dangerous contaminant in the air (biological or chemical), and based on detailed data regarding winds, identify likely release locations, magnitude of release, and design response plans for affected areas,

optimized for the particular situation.

- SBES technologies could enable the design optimization of buildings or other infrastructure elements for the site it is to occupy, allowing for all of its interaction with its natural and man-made surroundings, and its effect on the entire urban system of which it is a part, including effects in both normal operation and in wide-ranging emergency/disaster situations.
- The long-term effects of the effluent of existing or proposed facilities, or of proposed changes to facility operations on urban and/or natural environments must be predicted. This will greatly increase the reliability and usefulness of environmental impact studies, and allow optimization to minimize probability of deleterious impacts.
- SBES will make possible the optimization of emergency responses to fire or explosion (whether accidental or purposeful) based on analysis of the probable evolution of the situation (spread of fire, integrity of buildings, effects of response interventions, etc.).
- SBES technologies will make possible the design and optimization of security infrastructures for the urban environment. This could include sensor design and placement, countermeasure design (e.g., contaminant dispersal, flood abatement).

## ***8.4 SBES IN ENERGY AND ENVIRONMENT***

The use of modern simulation tools has become an indispensable component to energy-related industries for monitoring production of oil reservoirs and as an aid in developing pollution remediation and control strategies. With new advances in distributed computing, multi-physics and chemistry modeling, parallel algorithms, and methods and devices for dynamic

use of well-bore and seismic data, a new level of sophistication in oil reservoir management could be achieved. The next generation of oilfield simulation strategies may exploit developing technologies for data-driven, interactive, and dynamically adaptive strategies for subsurface characterization and reservoir management. The possibility of combining multi-resolution reservoir models that can be executed on very large distributed heterogeneous computational environments, with sensors embedded in reservoir-fields (e.g., permanent downhole sensors and seismic sensors anchored at the seafloor) monitoring, could provide a symbiotic feedback loop between measured data and the computational models. This could lead to an “instrumented oilfield”: more efficient, cost-effective, and environmentally safer with enormous strategic and economic benefits including:

- An increase in the volume of oil and natural gas produced from existing reservoirs. With better understanding of the existing oil and gas reservoirs, the potential exists to more efficiently drain existing reserves and to locate and produce bypassed reserves. The new technologies developed could help in reducing dependence on foreign oil.
- Better understanding of risk and uncertainty and lowered finding costs. Better models of the subsurface will allow oil and gas companies to more efficiently allocate their capital by focusing on those prospects that offer the best return.

These new technologies have immediate application to other areas, including environmental remediation and storage of hazardous wastes. Again, these new application areas require an integrated and interactive simulation framework with multi-scale capabilities supported by a cross-disciplinary team of researchers, which could include geoscientists, engineers, applied mathematicians, and computer scientists.

## 8.5 *SBES IN MATERIALS: COMPUTATIONAL MATERIALS*

The overlap of modeling and simulation with materials research and development highlights an area of great strategic significance for SBES. The field of materials is rich with long-standing problems of obvious importance for which the underlying science is not well understood. Developing a microstructural understanding of cement to enhance creep resistance and environmental durability is one challenge that requires no motivation, given that it is the most widely used man-made substance in the world. No less important are metals like iron and semiconductors like silicon which all face similar challenges regarding optimizing their functional properties through the control of microstructure. The spirit of SBES is to develop models and simulation methods that will allow macroscopic properties to be manipulated by microscopic insights. The challenges of materials innovation and utilization, critical to practically all science and technology of societal importance, present formidable problems at the conceptual (modeling) level as well as demands on large-scale simulations. If one were to examine the reasons why SBES will have profound impact on materials science and engineering, it will be seen that the same logic would apply to physics, chemistry, engineering, etc. The success of SBES will be significantly aided by the emergence of materials modeling and simulation, or computational materials, as an equal partner to the familiar fields of computational physics and computational chemistry.

We see three overarching themes portraying the challenges and opportunities for SBES in materials: 1) *Exceptional Bandwidth* – The conceptual basis of computational materials covers all of physical science without regard to what belongs to physics versus chemistry versus engineering. This means the scientific bandwidth of SBES is as broad as all the multiscale aspects of science and engineering. In materials modeling and simulation, as in SBES more generally, traditional disciplinary boundaries have vanishing barriers. What

governs is “the need to know”. 2) *Removing Empiricism* – A virtue of multiscale modeling is that results pertaining to both model and simulation are conceptually and operationally quantifiable. This means that empirical assumptions can be systematically replaced by physically-based descriptions. Quantifiability implies any part of the modeling and simulation can be scrutinized and upgraded in a controlled manner, thus allowing a complex phenomenon to be probed part by part. 3) *Visual Insights* – The numerical outputs from a simulation are generally data on the degrees of freedom characterizing the model. Their availability allows not only direct animation, but also visualization of analyzed properties which are not accessible to experimental observation. In microscopy, for example, one has structural information but usually without the energetics, whereas by simulation one can have both. The same may be said of deformation mechanisms and reaction pathways.

Structure-property correlation is the materials science approach to probing complex systems and controlling their behavior. A bottleneck in practice is that the information needed for the correlation, necessarily obtained from more than one set of measurements, is not specific enough or not available. The advent of robust modeling and simulation will allow any materials property to be determined for a fully characterized structure, thus enabling the implementation of the correlation in a fully self-consistent manner. Once established, this paradigm can be extended to hypothetical systems which are of interest for innovation and design.

Linking the different length and time scales of models and simulation methods is a grand challenge for SBES (see Sec. 2.0). In the arena of computational materials, serious efforts are being made to connect the electronic structure and atomistic scales in one direction to obtain more reliable interatomic potentials for molecular dynamics and Monte Carlo simulations, and in the other direction to provide pre-conditioning structures for first principles calculations. How to transfer information from the molecular level to the mesoscale is widely acknowledged in the community of multiscale modeling to be the critical

bottleneck for realizing the potential of computational materials for industrial applications. This is an issue that will not be quickly resolved in the foreseeable future. Besides linking adjacent scales, one can jump scales such as using electronic-structure information directly in mesoscale simulations. Given that the difficulty of matching system descriptions involving completely different sets of degrees of freedom is not confined to materials, bridging scales is truly a cornerstone issue in SBES.

In computational materials there are a number of high-profile applications which push the limits of capabilities in modeling and simulation. These generally have to do with understanding and designing materials for extreme environments. In mechanical properties the plastic deformation of metals at high pressure and high strain rate, is one such problem which has occupied the attention of a sizable community for several years. The challenge is multiscale, from calculating the core of a dislocation using electronic-structure methods to modeling dislocation mobility using molecular dynamics simulation, to developing constitutive relations for continuum-level codes using dislocation dynamics simulation. The requirements of high pressure, greater than 10 Mbar, and high strain rate, greater than  $10^8$ , put the problem essentially out of reach for conventional experiments. Ensuring greater fidelity in modeling and new levels of simulation power will be the legacy of SBES.

## **9.0 THE CRISIS OF THE EXPLOSION OF KNOWLEDGE: SBES EDUCATION FOR TOMORROW'S ENGINEERS AND SCIENTISTS**

In Volume Two of the SCaLeS Report [13], one finds reference to the “crisis of knowledge explosion”, referring to the fact that the knowledge base required to advance modern simulation spills across many of the academic disciplines now compartmentalized in rigid organizational structure of today’s universities. This silo structure of educational institutions 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 as one of the 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 sciences the nation will need to remain at the forefront of scientific discovery. ” It asks, will research and educational study in the twenty-first century be “medieval or modern?”.

Restructuring of university-level engineering educational systems will be necessary to integrate simulation as a discipline and an engineering tool into the educational experience and the lifelong learning opportunities for practitioners. Educating tomorrow’s engineers and scientists in SBES will require that the student acquire substantial depth in computational and applied mathematics and underlying scientific disciplines. This must be made possible through multidisciplinary interactions. New educational materials that demonstrate the theory and practice associated with SBES are therefore needed. Initially,

graduate-level curricula in SBES will be developed, and, as the graduate-level curriculum matures, SBES must become part of the undergraduate curriculum as well.

## 10.0 FINDINGS AND RECOMMENDATIONS

- Because of the complexity and many facets of applications driven by SBES research, its goals cannot be achieved by incremental, short-term research efforts. A long-term program of high-risk research will be needed to resolve the numerous obstacles standing in the way of SBES developments. We believe that short-term investments, and limited strategic planning will lead to excessive focus on incremental research rather than on long-range sustained research with lasting impact.
- Formidable fundamental obstacles remain in linking highly disparate length and time scales and disciplines in simulation methods. These issues have a commonality across many SBES applications and fundamental discoveries are needed to surmount these obstacles. In addition, bringing SBES to fruition requires better understanding of highly nonlinear and rough systems, error control, adaptivity, and orders of magnitude improvements in algorithms.
- Progress in SBES will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. The work of these teams must be sustained for a decade or more to yield the full fruits of the investment.
- 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 in simulation systems.
- Concomitant investments on sensory data computing, the collection and use of experimental data, and the facilitation of interactions with computational models and methods are needed that can provide dynamic adaptive control of

the computational process.

- 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. It will be necessary to incorporate in the multi-disciplinary teams involved in SBES research, experienced software developers who will work hand-in-hand with engineers and engineering scientists to develop tomorrow's SBES software.
- Investment in research in the core disciplines of science and engineering at the heart of SBES applications should not outweigh the investment in the development of algorithms and computational procedures for dynamic multi-scale, multi-physics applications, and these algorithms must be designed to adaptively adjust to dynamic data input.
- SBES will bring with it dramatic changes in science and engineering education. Interdisciplinary education in computational science and computing technology must be greatly improved. New interdisciplinary programs in computational science must be encouraged and traditional discipline boundaries in higher education must be made pervious to the exchange of information between discipline scientists within multi-disciplinary research teams. Curriculum development in SBES should be funded and a path toward the development of a pool of younger researchers in SBES who will be tomorrow's leaders in this discipline must be constructed.

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