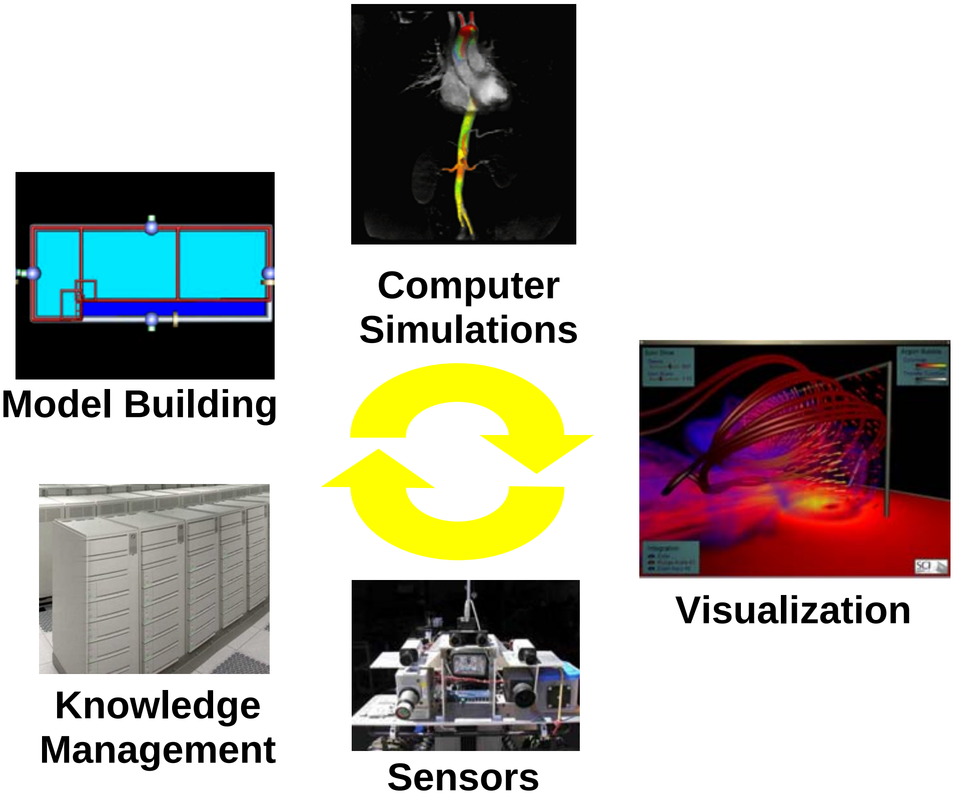
Simulation Based Engineering Science

A Report on a Workshop
Held Under the Auspices of the

National Science Foundation

April 15-16, 2004



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Preface

The unprecedented successes of modern computer simulation approaches and the enormous potential of enhancing the utility, fidelity, and reliability of simulation due to advances in data-related systems foretells the emergence of a new discipline, referred to as Simulation Based Engineering Science (SBES). Enhancement and acceleration of research in SBES could have a dramatic, beneficial impact on society in many areas, such as improved products at reduced cost, improved health and environment, and improved security and safety. Efficient mechanisms for managing and funding the research needed to advance SBES, however, may not exist in NSF or other agencies due to its interdisciplinary character. Collectively, these issues motivated the National Science Foundation to organize a two-day workshop on SBES to discuss the subject, to provide a more detailed definition of the field and its place in contemporary engineering, and to explore ways in which research in this field can be accelerated and brought to bear on pressing problems of broad national interest.

The workshop was held on April 15 and 16, 2004, in Arlington, Virginia under the auspices of the Directorate of Engineering and was attended by key NSF managers and a cross section of specialists in SBES from universities and government laboratories. The following groups and individuals were in attendance:

Workshop Organizers

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

Invited Workshop Participants

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

Government participants

Thomas Bickel (Sandia National Labs)
John Red-Horse (Sandia National Labs)
Roshdy Barsoum (ONR)
Luise Couchman (ONR)
Craig Hartley (AFOSR)
Walter Jones (AFOSR)
Raju Namburu (ARL)
Noam Bernstein (NRL)
Jonathan B. Ransom (NASA)
Kamal Abdali (NSF)
John Brighton (NSF)
Ken Chong (NSF)
Sangtae Kim (NSF)
George Lea (NSF)
Priscilla Nelson (NSF)
Michael Plesniak (NSF)
Galip Ulsoy (NSF)

This document surveys and summarizes the principal findings of the SBES Workshop and lists major recommendations for future development of SBES under NSF.

SBES Workshop Participants.

EXECUTIVE SUMMARY

A new discipline of engineering and applied science is emerging, referred to here as Simulation-Based Engineering Science (SBES), in which modern computational methods and devices and collateral technologies can be combined to resolve fundamental issues far outside the scope of traditional scientific and engineering methods. Advances in SBES offer hope of resolving a variety of fundamental problems that affect every branch of engineering and science, and the health, security, and quality of life of all Americans. SBES in an interdisciplinary field, arising from the intersection of more mature disciplines where many of the important developments of the next century will be made: computational and applied mathematics, engineering science, computer science, distributed and grid computing, all enriched by the host of developing technologies in such areas as imaging, sensors, and visualization.

This document surveys and summarizes the principal findings of an NSF sponsored two-day Workshop on SBES and lists recommendations for future development of SBES under NSF.

A remarkable feature of this discipline is that it simultaneously provides powerful tools for addressing many important problems facing the nation while also providing natural interfaces between the diverse disciplines concerned with these problems. The problem areas may be mapped into the organizational units of NSF while the interfaces provide a unique opportunity to develop cross-cutting activities within the organization. Among the areas reported at the workshop are the following:

Biomedicine and Health: Many of the major diseases that affect or will affect most Americans are yielding slowly to traditional medical paradigms. SBES provides opportunities for a paradigm shift in medical practice in which modern simulation tools and an engineering approach give promise for dramatic improvements in many areas of biomedicine.

Manufacturing: With a move toward micro-scale devices and nano-technology, extreme demands are being put on tomorrow’s manufacturing enterprises that cannot be met by today's technology. New science and technology is needed to lift the fidelity and sophistication of today’s processes to a new level.

Education and Research: With the development of new scientific approaches, computer hardware, measuring and imaging devices, and the emerging cyberinfrastructure technologies, a redirection in the way science and engineering is taught at the graduate and undergraduate levels is needed so that the next generation of engineers is equipped with the latest knowledge and tools in the various disciplines. Many of these very important tools will be based on knowledge developed through interdisciplinary research and will be firmly embedded in tomorrow’s computational environment.

National Security: The increased frequency of threats to the security of the nation’s cities and infrastructure due to both natural hazards and hostile actions by our nation’s enemies must be met with technological advances that will provide new tools for coping with natural events and with adversaries. These tools will range the gamut from mathematical models for predicting and anticipating natural disasters to developing methods that foretell the effects of hostile events and provide data for determining how the effects of these events can be controlled, avoided or even how the threat of such events can be detected in advance.

Energy and Environment: A host of energy and environmental issues present immediate concerns for the future well-being of the nation. These range from issues of determining and controlling the production of oil and other natural resources to the development of modern technologies for understanding and controlling environmental factors that impact health and quality of life. These include new technologies to determine the dispersion of toxic substances and the development of procedures to mollify and control their effect on the environment.

Successful developments in these areas must overcome the absence of effective methods for: bridging a wide range of length and time scales; integrating simulation capabilities and extensive data acquisition methods to speed model development; increasing the efficiency of decision making by incorporating validation and random aspects of data; managing complex, multidisciplinary models; and handling and quantifying uncertainty, management of large statistical data sets, and coping with chaotic behavior and random events.

The consensus of those participating in the Workshop on SBES is that NSF should give strong consideration to developing a cross-cutting activity or priority area in SBES that, in its beginning stages, could combine goals and resources from the Engineering Directorate, CISE, and the developing initiative in Cyberinfrastructures. Exactly what position SBES may ultimately take in the NSF organizational framework is an issue that leaders at NSF will determine. The strong consensus of those participating in this workshop is that SBES is a critical discipline, indispensable for continued leadership of the U.S. in science and technology and fundamental as a tool to resolve many major national problems affecting all Americans.

1. SIMULATION-BASED ENGINEERING SCIENCE: THE NEW ERA IN ENGINEERING AND SCIENCE

Computation has had a remarkable impact on contemporary engineering and science. The use of computational methods and devices to simulate physical phenomena and the behavior of engineered systems has made possible dramatic advances in technology that have affected virtually every aspect of human existence. Today, a new era is emerging in which revolutionary new developments may be made that could advance the discipline far beyond the boundaries thought possible only a few years ago. The birth of this new era is imminent because of the rising opportunity to integrate and extend developing capabilities in modeling and large scale computer simulations with the developing technologies in data-intensive computing, distributed and grid computing, and the development of the cyberinfrastructure. Concomitant with these developments are dramatic advances in new methodologies for multi-scale and multi-physics simulations that span enormous spatial and temporal scales. This emerging discipline is referred to here as Simulation Based Engineering Science (SBES). It is highly interdisciplinary; it involves the development of methods to model multi-scale, multi-physics events; it will employ dynamic data driven methods, sensors, imaging modalities, distributed and grid computing, and other features that constitute tomorrow's computing infrastructure. The exploitation of the full potential of these emerging technologies so as to push forward the capabilities, scope, and reliability of simulation-based engineering should be an important goal of agencies that support research and development in engineering and science.

The importance of SBES and proof of its interdisciplinary nature can be appreciated in a review of major problem areas of national concern. A partial list follows:

Biomedicine and Health: Cardiovascular disease, cancer, diabetes, kidney, and chronic liver disease and cirrhosis are among the top health problems, and causes of death, faced by Americans today. To combat these growing health risks interdisciplinary research and enhancements of surgical procedures are critical to ensure a higher rate of recovery and long range beneficial effects. This is an issue effecting tens of millions of Americans and could affect a significant percentage of the population during their lifetime.

Manufacturing and Engineering Design: This past decade has seen a gradual shift from the traditional prototype construction and testing approach to simulation-based engineering design. However, the process is in its infancy, because today's computational engineering tools lack the robustness, the high bandwidth linkage to data acquisition needed for model construction, validation, and the multi-scale, multi-physics capabilities that are essential. Nevertheless, the thrust from testing to simulation is unabated because of the following:

- experimental limitations in various engineering disciplines, ranging from the impossibility of conducting tests (in nuclear safety problems for example) to the hazards and huge expense of experiments and tests in areas such as environmental engineering and seismic engineering;

- the need for reliable rapid-cycle design of engineering products and medical systems;
- the need for a fundamental paradigm shift in many fields of engineering to provide a reliable tool for decision making, analysis, and design;
- the need for dynamic access to huge datasets to enhance the fidelity of computational models and to quantify and control uncertainty in predictions;
- the need for tools to generate data, store and retrieve it, for computational models of systems of great complexity evolving in time.

With a move toward micro-scale devices and nano-technology, extreme demands will be put on tomorrow’s manufacturing enterprises that cannot be met by today's technology. New simulation based science and technology is needed to lift the fidelity and sophistication of today’s processes to a new level.

Education and Research: With the development of new scientific approaches, computer hardware, measuring and imaging devices, and the emerging cyberinfrastructure technologies, a redirection in the way science and engineering is taught at the graduate and undergraduate levels is needed so that the next generation of engineers is equipped with the latest knowledge and tools in the various disciplines. Many of these very important tools will be based on knowledge developed through interdisciplinary research and will be firmly embedded in tomorrow’s computational environment.

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To these examples one can add the fields of communications, transportation, basic science, pharmaceuticals, earth sciences, biology-based systems, materials science, and many others. **Responses to these major national problem areas and many more can be greatly enhanced by new developments in SBES. Simulation based engineering science provides a common theme and resource for addressing all of these issues and the glue that connects a diverse collection of disciplines represented within NSF and other agencies.** Among the common needs are software systems for new computer architectures to rapidly receive, process, store, and transmit data; new algorithms to treat a multitude of multi-physics, multi-scale phenomena; new algorithms and modeling techniques to greatly increase the speed and reliability of computational simulations; interfaces with devices as well as the technologies that will provide interfaces with computer and computational systems that can give information in real time of physical systems including the human body, cities and communities, electronic materials, reservoirs, and many other physical and environmental systems too numerous to name.

Successful developments in these areas must overcome the absence of effective methods for:

1) bridging a wide range of length and time scales,
2) integrating simulation capabilities and extensive data acquisition methods to speed model development,
3) increasing the efficiency of decision making by incorporating validation and random aspects of data,
4) managing complex, multidisciplinary models, and
5) handling and quantifying uncertainty, management of large statistical data sets, and coping with chaotic behavior and random events.

Traditional areas of science and technology that do not employ simulation face limitations of growing proportions that could affect the way our nation responds to many critical needs in security, health care, manufacturing, energy, communications, material science and other areas. SBES could be an indispensable tool for resolving these needs. It could further enhance experimental science and technology by providing fundamental tools for determining how physical events are perceived and understood and how engineered systems are observed to perform; it could make possible the attainment of new levels of sophistication in decision making vital to all areas of technology; it could impact design and even the codes used in engineering design; it could impact education, permeating to the undergraduate and graduate curricula in major universities nationwide.

Beyond the obvious scientific importance of the discipline, preliminary indications are that rapid basic improvements in engineering applications made possible by SBES have the potential to save and improve lives and to annually save billions of dollars in direct engineering and product cycle costs throughout the spectrum of manufacturing, transportation, energy, communications, and medical industries in the U.S.

1.1 “Moore’s Law” for Simulation: Computation versus Computing

Moore’s Law, the assertion of Gordon Moore in 1965 that the number of transistors per square inch on integrated circuits would double every couple of years has become commonly used as a measure of progress in computing capability over time.

Unfortunately, advances in computer performance do not necessarily translate into simulation or design capability or advances in computational engineering and science. One can conceptualize new versions of Moore’s Law applied to engineering simulations that would include advances in problem solving, complexity, and overall fidelity of simulations due to advances in hardware, but also in improved algorithms and mathematical models. One such characterization is given in Figure 1 for a particular application in magnetohydrodynamics simulations. An "effective speed" of increased capability is given in which increases due to the development of major new algorithms are provided. In this case, the payoff in developing new models and more efficient parallel algorithms can outstrip increases in computer performance by as much as four orders of magnitude over the same time period. Similar trends and developments can be cited in many other application areas.

Despite the fact that simulation is becoming critical and ubiquitous in engineering and science, it has not evolved as an independent discipline. For example, in the current NSF organization, computational science and engineering is spread out in many different programs. Many of these programs, for example CISE, focus on the development of specific computer hardware infrastructure and accompanying enabling technologies, but do not provide focus on the general software and algorithmic technologies needed to advance SBES across all disciplines. As a consequence, the development of simulation based engineering has also lagged as an academic discipline and the training of engineers and scientists in this discipline has also lagged.

NSF has a history of ground-breaking initiatives that have become mainstream programs for other national endeavors, particularly programs in DoE, NASA,DoD, and internationally (Escience, EU). Many of its previous initiatives, such as the Grand Challenges, KDR and ITR, have fostered underlying technology that provides a basis for the next step. Previous NSF initiatives were "HPCC", "methods/algorithms", and "technology" driven. SBES can build upon and leverage these initiatives to develop the new capabilities that will significantly advance engineering and science. Simulation-based research and educational programs at universities can profoundly improve the way engineering is done. But a concerted effort is needed to bring this potential to fruition.

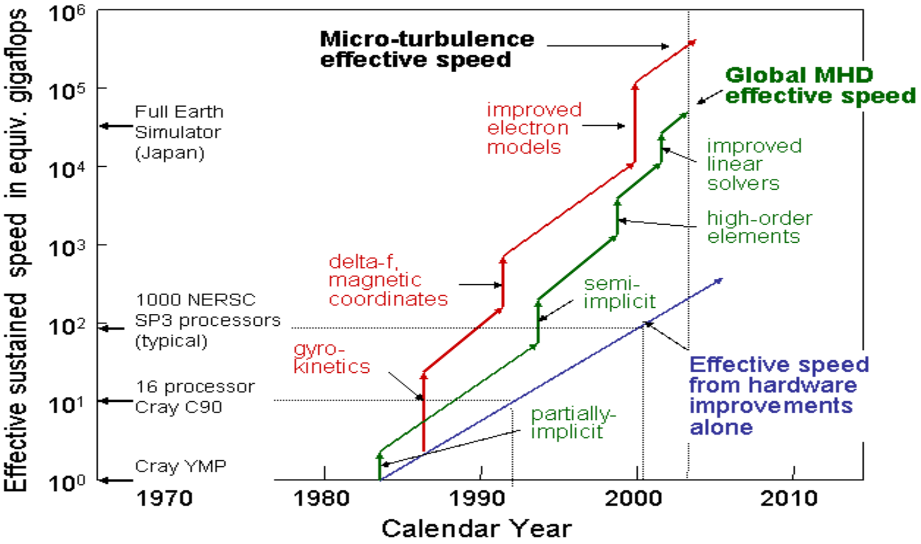

Figure 1: An example of improvements in performance of computational simulations over time due to improvements in algorithms, methods, and software as well as advances in hardware.

1.2 Barriers, Challenges, and Opportunities

While the promise of simulation is immense, the limitations of today's capabilities are often not appreciated. Many of today's simulation capabilities are built on large-scale phenomenological models that have required many years of development and entail extensive testing prior to simulation. Moreover, traditional models presume that the data is deterministic, static, and do not include it as a major part of the simulation modeling process. Modeling with large-scale simulators can no longer be distinct from data-acquisition technologies; the entire arsenal of tools, mathematical methods and algorithms, and networked systems must be integrated into a new view of computational engineering science.

One of the main barriers is to link large-scale models with the behavior at much smaller scales, where the behavior can be obtained by computation without full scale testing. Another barrier is the important area of *model verification and validation:* the development of mathematical, computational, and data acquisition and management tools that will ensure that models are correctly solved and produce results with quantifiable reliability.

The challenge for NSF lies in the intrinsically interdisciplinary nature of the research and deliverable knowledge and technology in SBES generated by the convergence between engineering, scientific computation, and a diverse collection of application disciplines ranging from medicine to material science to earth and environmental science. From a research perspective, the position of an NSF initiative in SBES should be carefully considered relative to the focus on the development of specific computer hardware infrastructure and accompanying enabling technologies currently supported by CISE. An SBES program will ultimately be distinguished by the features noted above – (i) simulation-focus, (ii) multi-scale/multi-physics models, (iii) an engineering systems-approach, (iv) leveraging the decades of simulation expertise in the engineering and applied mathematics communities, and (v) a design/problem-solving emphasis, will help to distinguish the SBES program. From an educational perspective, it will become essential that a growing percentage of tomorrow's scientists, engineers and clinicians become fluent in the language and concepts of SBES. Emphasis should be placed on this "bilingual education" and the knowledge-exchange between the engineering and scientific computing communities.

The opportunity derives from the NSF's leadership in supporting a number of the component sciences and technologies that benefit most the development of simulation-based engineering. First, NSF leads the world in supporting computer engineering and computer science and in the development of modern theories and algorithms. Second, NSF has historically had a leading position in attempts to organize information into data resources that can bring the latest and best information and technology, in a comprehensive and comprehensible way, to the scientific and engineering communities. Third, NSF has played a leading role in the development and support of high performance computing. Computer technologies, such as parallel processing, distributed and grid computing, and, ultimately, the cyberinfrastructure, could provide the data communication and data processing platform for SBES. Finally, by committing itself to an explicit effort in SBES, NSF can assure itself continued leadership well into a future in which simulation will be essential to all aspects of engineering, biomedicine, and science.

2. EXAMPLES OF POTENTIAL SBES APPLICATIONS

In this section examples are given of how SBES could change the way engineering, medicine, and basic science is done.

2.1 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 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.

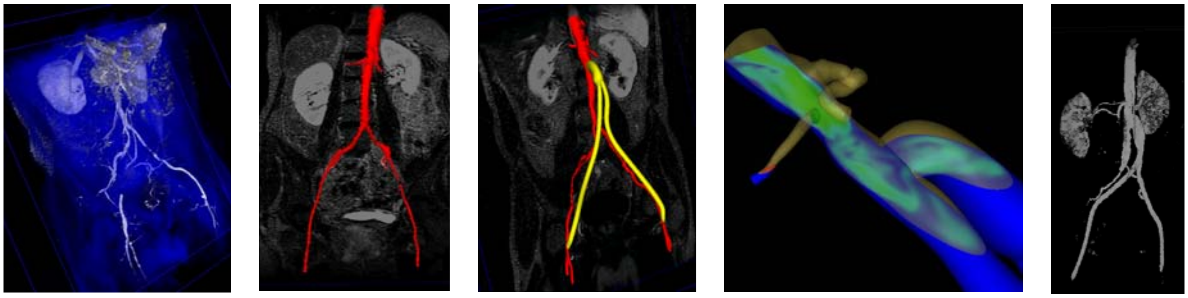

Figure 2: Example of simulation-based medicine approach as applied to designing bypass surgery for patient with occlusive cardiovascular disease in aorta and iliac arteries. Shown from left are magnetic resonance image data, preoperative geometric solid model, operative plan, computed blood flow velocity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

A program in SBES could also lead to a new approach to medical practice, that of Simulation-Based Medicine. New simulation-based engineering methods, 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 and determine local concentrations to use in pharmacokinetic models of drug metabolism.

A possible avenue for the development of a comprehensive computer simulation-based theoretical framework of human anatomy and physiologic function is through the creation of a *Digital Human*. The construction of a Digital Human has the potential to unify centuries of scientific inquiry in biology, medicine and bioengineering by synthesizing theoretical models of living systems. Much of the current research in biology, medicine and bioengineering is focused on acquiring data to test individual theoretical hypotheses using observational and experimental methods. Often, the experiments that are performed focus either on the molecular biology of individual cells in culture, or on system-level observations in animals and humans. The results of these experiments are peer-reviewed and then are “stored” in scientific journals. While it is generally possible to access this information, it is generally difficult to directly utilize the biologic data in new theoretical models. In contrast to hypothesis-driven research, much of the work in biomedical modeling is technology-driven. The focus of this research is the development of mathematical tools to simulate human function. In general, these tools focus on individual organ systems, e.g. musculoskeletal or cardiovascular or on individual proteins. The current tools for biomedical simulation are not integrated across organ systems or temporal and physical scales.

A theoretical framework is needed to serve as a repository of anatomic, biologic and physiologic data as well as providing computer simulation methods to use this input data to model human function. The construction of such a theoretical framework of human function would be of great value by allowing the testing of hypotheses related to the onset and progression of disease, the evaluation of new pharmaceuticals and medical devices, the implementation of new medical treatments, and the deployment of new tools for medical and surgical education through simulation. These models would ultimately include the interaction between molecular, cellular and system-level events. The Digital Human could be a generic human for pharmaceutical and device design and medical education, or could be patient-specific and incorporate methods for pharmacogenomics, diagnostic radiology, medical simulation and treatment planning, image-guided therapies and surgical robotics. As it applies to clinical medicine, the goal of such an initiative would be to develop a unified model of a patient to enable the seamless transfer of data and computational models all the way from a patient’s past medical history to diagnostic data to the final treatment. The development of high performance computers and sophisticated numerical methods has made it possible, for the first time in history, to realize this theoretical framework, and individual research programs are starting to assemble individual components of a Digital Human.

While similar efforts have been considered (e.g. the Physiome and the DOE Virtual Human projects) the creation of a digital human would have five distinguishing features. First of all, such a program would be centered not just on developing a computer-based repository of experimental data, but rather working simulation models. Second, since the program would be centered in the National Science Foundation, and pursued as part of the initiative on SBES, it would leverage the decades of research in modeling complex systems, many of which share the multi-scale and multi-physics character of biological systems. Rather than reinventing theoretical models and computational algorithms, the Digital Human paradigm would engage the expertise of the computational engineering science and applied mathematics communities that have proven experience in modeling complex systems. Third, rather than follow a biologic reductionist approach whereby living systems are studied at the molecular scales working up, this initiative should adopt the engineering methodology of starting at the organism and organ-system scales and working down to cellular and molecular scales only as required to increase the fidelity of the models and design tools under development. Fourth, a Digital Human approach would promote the development of multi-physics simulation methods to couple organ systems (e.g. the cardiovascular and respiratory systems or even the blood stream and blood vessels). Finally, the focus of a Digital Human paradigm would, while enabling scientific discovery, emphasize the design and optimization of medical therapies, devices and delivery systems for improving the health of individual patients.

The construction of a Digital Human would be a monumental task requiring decades to complete – a 21st century “moon-shot”. However, a sustained commitment to such a vision and a concerted focus on creating the enabling technologies could reap great societal benefits over the short-term and lay the groundwork for Simulation-Based Medicine over the longer term.

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 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 for this purpose includes the entire support infrastructure, such as buildings, transportation infrastructure, food, water and power distribution infrastructure, communications infrastructure, 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, 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," 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, water-shed 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, 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:

- The development of the quantitative models of the processes to be simulated. 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 there are many others. Quantitative modeling of other processes is not currently as well developed. For example, sociological models of the response of populations, models of the evolution of natural ecosystems such as forests or lakes.
- The integration of numerous detailed models at a wide range of scales 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.
- Design and optimize a building, or other infrastructure element for the site it is to occupy, accounting for all of its interaction with its natural and man-made surroundings, and its affect on the entire urban "system" of which it is a part, including effects in both normal operation and in wide ranging emergency/disaster situations.
- Predict 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, greatly increasing the reliability and usefulness of environmental impact studies, and allowing optimization to minimize probability of deleterious impacts.
- During and after a fire or explosion (whether accidental or purposeful), optimize emergency responses based on analysis of the probable evolution of the situation (spread of fire, integrity of buildings, effects of response interventions etc.).
- Design and optimize security infrastructure for the urban environment. This could include sensor design and placement, countermeasure design (e.g. contaminant dispersal, flood abatement).

2.3 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 requires 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.

2.4 SBES in Biomimetic Sensors and Devices:

Nature has inspired many technological breakthroughs and advances in the past. For example, very early designs for an airplane were based on the observation of birds. Biomimetics refers to the concept of taking ideas from nature and mimicking them to create revolutionary advances in engineering and sciences. There is now an even greater opportunity in biomimetics because of advances in micro and nanofabrication technology – by replicating biological processes in the cell (and life in general) it is now possible to create nanometer scale sensors that promise unprecedented sensitivity and selectivity in detecting single molecules. There are many other examples in biology and life – the mimicking of which will lead to tremendous advances. Examples include artificial muscles, automatic assembly and self-repairing of engineering components by understanding the self-assembly processes in organisms, designing new materials (e.g. soft materials) to create cell-like constructs, creation of smart fabrics by analyzing the insulation layers of animals, creation of micro and nanostructures by understanding the sensory systems of parasites and insects and many others. The use of experimental techniques alone to make rapid advances in biomimetic technology can be very expensive, time consuming and sometimes practically impossible. The application of SBES, with a judicious combination of experiments, can lead to rapid prototyping of biomimetic devices. Predictive simulation tools for biomimetic technology can shed fundamental insights into the physical and biological principles that govern the system behavior, as well as identification of the significant parameters that need to be controlled and optimized during the design process.

As an example, the mimicking of biological ion channels is described in some detail here. Ionic channels are a class of proteins found in the membranes of all biological cells. Ionic channels provide a compelling biological template for the conception of biomimetic structures because of the wide range of biological functions they exhibit. Ionic channels are the molecular basis for the movement of electrical currents across membranes, resulting in signal transduction. From a physiological point of view, ionic channels regulate the transport of ions in and out of the cell, and in and out of compartments inside cells like mitochondria and nuclei, thereby maintaining the correct internal ion composition that is crucial to cell survival and function. Many channels have the ability to selectively transmit or block a particular ion species and most exhibit switching properties. Malfunctioning channels cause or are associated with many diseases, and a large number of drugs act directly or indirectly on channels.

The key features of ion channels that give rise to their extraordinary range of biological functions include variations in: 1) their *selectivity* (what ions can pass through), 2) their *conductance* (how rapidly can ions get through), and 3) their *sensitivity* (how the conductance is modulated by such factors as the chemical composition of their environment, the transmembrane voltage, the membrane surface tension, and the chemical binding of the ion, etc.). Some of the various biological functions of channels that potentially have enormous significance for device design and engineering include – signaling and computation, triggers for cellular events, electrical power generation, energy transduction, fluid pumping and filtration, chemical sensing and mechanotransduction.

The wide range of functions exhibited by ionic channels has already generated a great deal of interest in the engineering community. A clear understanding of channel operation may provide a template for the design of synthetic channels with specific conductance and selectivity properties. One approach to create artificial ion channels is to use single-walled carbon nanotubes. Shown in Figure 3 is a functionalized carbon nanotube that has been considered to mimic certain aspects of biological ion channels. Since carbon nanotubes are hydrophobic, water and electrolytes don’t enter small diameter carbon nanotubes spontaneously. To overcome this problem, carbon nanotubes have been functionalized with chemical groups and an electrical field is used in molecular dynamics simulations to demonstrate that such an idea indeed works and can be used to mimic ion channels. Such SBES studies make it easier for further experimentation on the use of carbon nanotubes as biomimetic channels.

The interest in biomimetic devices is growing steadily, motivating diverse communities of scientists that range from mechanical, electrical, chemical and bioengineering to biophysics, chemistry and biology. While the benefits from biomimetic devices are clear, the challenges are many. A partial list of challenges that can be addressed by SBES in the area of biomimetics is discussed below:

- By creating computer models of living systems, SBES can be used to understand the physical and biological processes that give rise to the specific function of the living systems. In addition, the significance of the structural complexity as well as the techniques nature uses to build the living systems can be addressed in detail by using SBES.

- The design and optimization of materials that mimic biological tissues is an important issue. SBES can be used to understand materials behavior at various length and time scales.
- The interaction between wet (biology) and dry (e.g. solid-state) systems needs to be understood in detail to create biomimetic systems. SBES can be used to understand fluid-solid interfaces, surface chemistry, charged double layers and other intermolecular forces that are encountered in wet and dry systems.
- Multi-scale approaches, combining models ranging from density functional theory to tight-binding to molecular dynamics/Monte Carlo to continuum, are critical to describe the function of biomimetic sensors and devices. SBES provides a platform and framework to integrate the models at various length and time-scales.
- SBES can be used for rapid computational prototyping of a variety of biomimetic sensors and devices, which find applications in single molecule detection, medicine, health care (e.g. detection of cancer), and defense and consumer products.

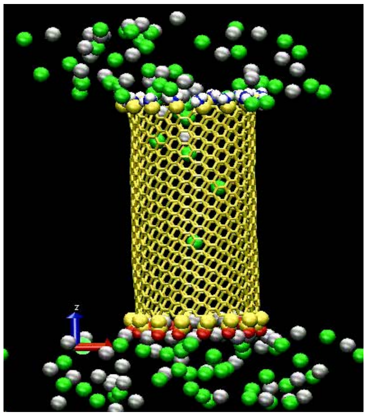

Figure 3: A functionalized carbon nanotube to mimic biological ion channels.

In summary, biomimetics requires an interdisciplinary effort involving scientists from various disciplines and SBES provides the unique platform to enable revolutionary advances through such interdisciplinary collaborations.

3. SBES IN ENGINEERING DESIGN

To enhance and maintain the United States' lead in technology-based industries, new technologies must be developed that enable the design and manufacture of increasingly complex products at lower cost and in less time than international competitors. Although current simulation technologies, in the form of computer-aided engineering systems, are having a major impact, simulation in engineering design tends to be limited to two classes of situations. The first consist of the application of well qualified methods to determine specific design performance parameters. An example of this type is geometric interference checking such as that applied by Boeing in the design of the 777. The second consists of situations where the cost associated with the application of the classic methods of prototype construction and tests is prohibitively time consuming and expensive, thus warranting the development of advanced simulation technologies. An example in this class is automotive crashworthiness analysis, which all the major automotive manufacturers have invested in and now rely on heavily. These current methods fall far short of providing engineering practitioners with simulation technologies that account for the full set of performance criteria to produce optimum designs considering variables from material microstructures through overall system configuration.

An examination of the current capabilities, recent advances in simulation technologies, continued increases in low cost computing power, and various industry roadmaps indicate that future simulation-based engineering science technologies can provide practitioners the engine needed to support the design of engineered products accounting for all steps from fundamental materials design through the life-cycle of the product. The products produced with these SBES technologies will include everything from the most technologically advanced systems, through a full range of medical systems, to the most basic of every day consumer products. Furthermore, the designs of these products will be validated through the application of virtual prototyping combined with selected physical experiments at the materials and component level.

The Opportunity and Challenge:

Fundamental advances in physical and biological sciences and the development of new measurement and characterization tools have made it possible to understand spatial and temporal phenomena on the atomic, molecular, microscopic, and macroscopic scales. Microelectronics has led this revolution through the development of integrated circuits. Recent progress in nanotechnology and biotechnology has extended the envelope of scales, making it possible to design starting from nanoscale building blocks. The ability to translate these advances into the engineering of new products and processes will require a transformation in the methodologies of engineering modeling, simulation, and design. Interactions at all scales affect the ultimate behavior of the complete system, and engineers must learn to model and design across this range of scales (see Figure 4).

The SBES developments needed to realize the potential of multi-scale design include:

- The ability to model and analyze the appropriate physical phenomena across the full range of spatial and temporal scales.
- Technologies to ensure the analyses performed by practitioners, that range from design engineers to medical doctors, produce reliable results.
- The ability to carry out risk-informed design decisions and optimize designs accounting for the variables at all scales.

Methods to model and analyze behavior at the relevant physical scales from quantum level interactions to the life prediction of full scale products has a long history and provides the back-bone of the needed coupled multi-scale analysis procedures. The most obvious area needing fundamental developments is the ability to couple information across 15 orders of temporal and 12 orders of spatial scales. The differences in the model representations used at the different scales, and the necessity to change models as scales are bridged to maintain computational tractability, make this a complex process. Future research developments must strive to develop mathematically sound frameworks capable of bridging the scales that are powerful enough to capture the physical behaviors required. As research progresses on the development of the needed mathematical frameworks and increased understanding at the interacting scales is obtained, it will also be possible to eliminate levels of empiricism that exists in many engineering models and replace them with more physically-based models, thus greatly increasing the robustness of the modeling technologies available.

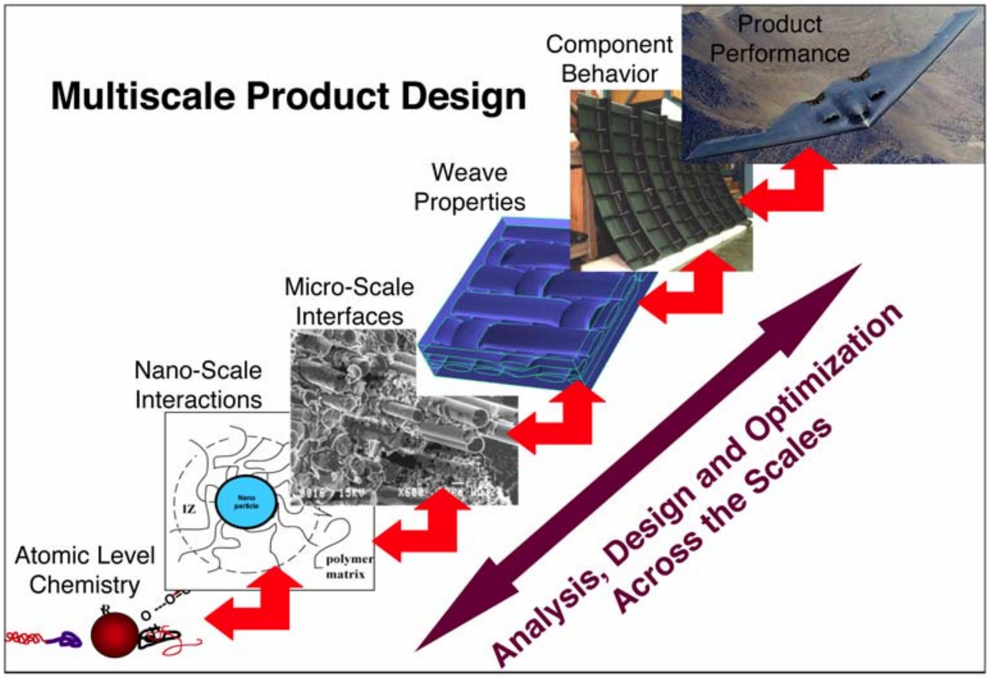

Figure 4: Multi-scale design of a composite component of an aircraft.

Even for the situations where current engineering analysis technologies are capable of accurately predicting the parameters of interest, today such predictions can only be obtained by highly trained experts. Therefore, current analysis technologies do not properly support the application of simulation-based design processes where all needed engineering analyses can be automatically executed to reliably predict the required parameters to the level of fidelity needed at that point in the design process. Meeting the objectives of simulation-based design requires the development of an entirely new level of verified analysis technologies in which adaptive control of all steps in the engineering analysis process is applied. These adaptive control methods will be responsible for determining the scales that must be considered, controlling the selection of models at each scale and the interactions between the scales, and controlling the applications of the numerical discretizations applied in each analysis. Furthermore, these analyses must be properly validated using an effective combination of material and component level tests including codification of the ranges of parameter variation that have been validated within the design system.

The proper application of a new generation of SBES technologies will support the effective application of risk informed design decision processes in which the analyses account for variabilities and uncertainties allowing consideration of the impact of a full range of outcomes. This information will be used by a new generation of optimization methods capable of optimizing a set of probabilistic variables across multiple scales.

4. EDUCATION IN SBES

A number of features of SBES distinguish it from traditional engineering academic disciplines. Among the most important are its different educational objectives. Studies in SBES:

- Should present engineering in a broad context and its relationship to data and prediction; it should include the multi-scale, multi-physical aspects, and explain the potential and limitations of computer simulation;
- Should be done with greater depth and breadth, e.g. with connections to scientific computing, applied mathematics, and physical sciences;
- Should require the ability to synthesize knowledge from these areas and apply it to complex realistic systems: SBES must be applications driven.

With these objectives in mind, several key issues concerning educational programs in SBES at several levels are discussed below.

SBES Issues at the Graduate Level

There is a shortage of American students prepared to pursue graduate studies in SBES. The absence of identifiable programs in SBES is an impediment to attracting more. Only a few undergraduate programs produce students qualified for graduate studies in SBES: a pipeline is possible and needs to be primed.

SBES graduate students should take a different course sequence, and the courses should have different content than those taken by traditional students. For example, the applied mathematics and computer science foundations for SBES are focused and deep: they need a firm foundation in traditional applied mathematics and computer sciences, and topics not covered or not well covered in traditional courses in these areas. There are opportunities for NSF Integrative Graduate Education and Research Traineeship (IGERT) projects in these areas for SBES.

Currently, most SBES-oriented engineering faculty synthesize interdisciplinary courses in an *ad hoc* manner to teach the focused, relevant content for SBES within the time constraints of a graduate program. They interact with faculty in applied mathematics and computer sciences in new ways to get this job done. The emergence of SBES is reflected in the development of new communities of faculty and students, and a new language of communication among them. Further streamlining of these interactions and course development process is expected.

The target for doctoral research in SBES is in the creation of new simulation capabilities for situations where existing methods or models or codes break down, but with validation via application to specific application area(s). Attracting good students to this area requires SBES presence, in some forms, in the undergraduate curriculum.

SBES at the Undergraduate Level

At present, new undergraduate degree programs in SBES do not seem viable. However, the increased pervasiveness of modeling and simulation is a precursor to the infusion of SBES throughout the undergraduate curriculum. It is important that examples of SBES be added to existing courses where feasible, especially in upper-level design courses. These examples can take the form of case studies from industry, interactive modules emphasizing multi-scale and multi-physics simulations, deployment of commercial simulation software for student projects.

Opportunities for undergraduate research projects in SBES proper should also be encouraged. Such projects present particular challenges due to the level of expertise required. However, because they are by their nature interdisciplinary, there is the opportunity for teamwork by students in computer science and applied mathematics in engineering research at the undergraduate level. This jumpstarts the process of cross-disciplinary learning and may be a significant pipeline towards graduate study in SBES.

Creation of cross-departmental courses in SBES at the senior technical elective level would form the basis of a concentration in SBES within disciplinary majors. Such infusions of SBES into the undergraduate experience are opportunities for NSF funding through its many engineering education programs (See, for example, the opportunities within the Advanced Technological Education Program (ATE) at http://www.ehr.nsf.gov/due/programs/ate/).

SBES Educational Outreach Opportunities: K-12 to Lifelong Learning

The real-life applications that drive SBES, and its inherent computer simulation basis, can be natural attractors to K-12 students, especially those from underrepresented groups. The notion of using computers to simulate complex realistic situations is not foreign to today's youth. SBES can be an exciting means to recruit students to careers in science, mathematics, engineering and technology.

A list of potential K-12 connections is:

- Web-based science/engineering modules emphasizing computer simulation, e.g. www.simscience.org;
- Science/engineering museum shows and other public arenas, e.g. Engineering Day at The Mall, with simulation-based exhibits;
- Summer programs for teachers and students at universities with SBES educational programs;

Again, opportunities abound through the many NSF programs directed towards K-12 technological education, especially the Division of Elementary, Secondary, and Informal Education (ESIE).

5. CONCLUSIONS AND RECOMMENDATIONS

Simulation Based Engineering Science is an important evolving discipline that could have a dramatic impact on the way engineering is done in the future. By integrating a multitude of developing technologies, traditional physical sciences, biomedicine and medical practice, computational and computer sciences, it could lift computer simulation to an unprecedented level that would benefit many areas important to the nation. Much research and development needs to be done to realize this great potential in SBES.

The core of SBES is modern engineering, but it draws from many other disciplines. Chief among these are computer science and computer engineering, computational mathematics, biomedicine, physical sciences, materials, earth sciences, and geosciences. This broad structure is difficult to accommodate in either traditional university organizational structures or that which exists at NSF.

The consensus of those participating in the NSF Workshop on SBES is that NSF should give strong consideration to developing a cross-cutting activity or priority area in SBES that, in its beginning stages, could combine goals and resources from the Engineering Directorate, CISE, and the developing initiative in Cyberinfrastructures across the Foundation. Exactly what position SBES may ultimately take in the NSF organizational framework is an issue that leaders at NSF will determine. The strong consensus of those participating in this workshop is that SBES is a critical discipline indispensable for continued leadership of the U.S. in science and technology.