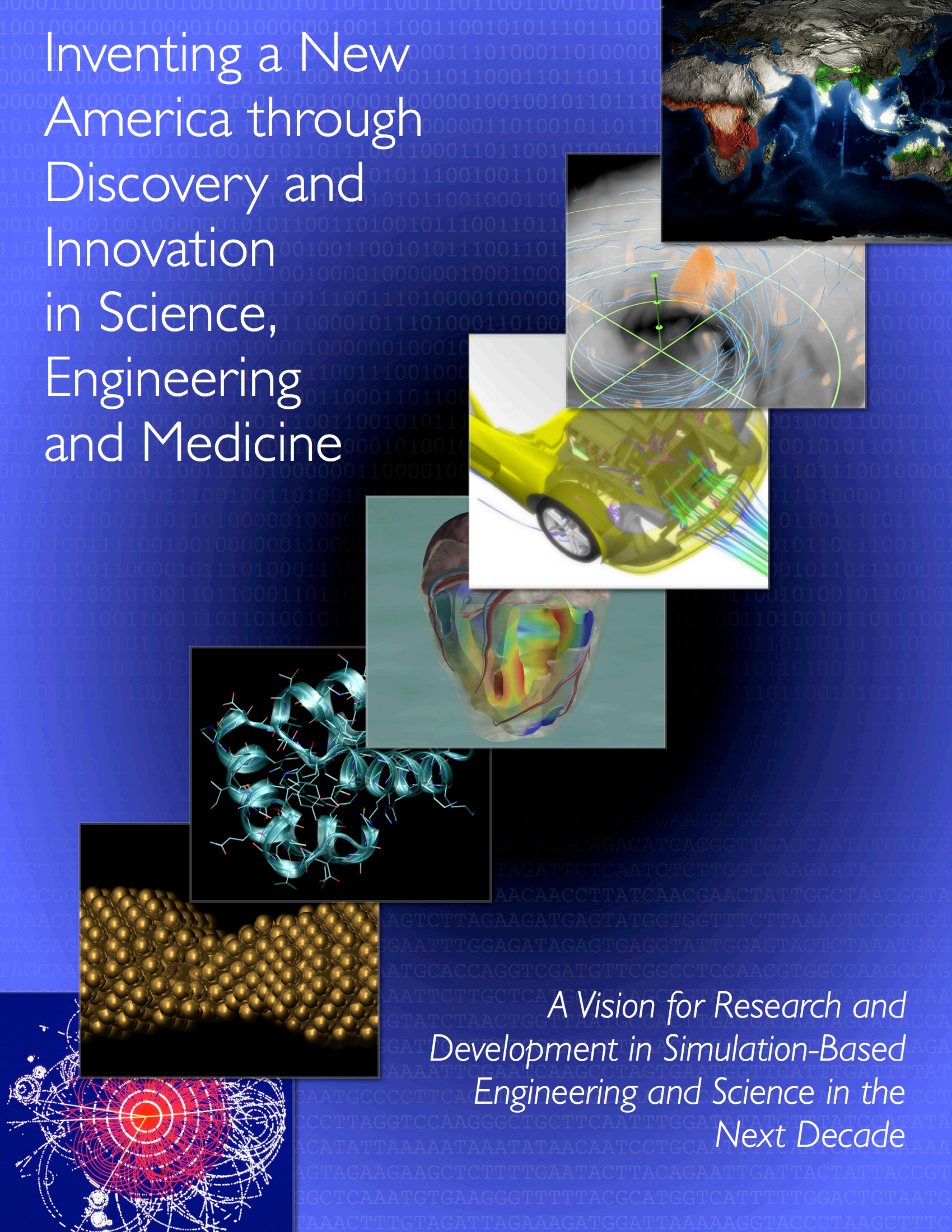
Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine



A Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade

Research Directions Workshop

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WTEC also organizes workshops, like this one, and provides other research services to Federal clients. Dr. R. D. Shelton, President, is the WTEC point of contact: telephone 410-467-9832 or email Shelton@ScienceUS.org.

Inventing a New America through Discovery and Innovation in Science, Engineering, and Medicine

A Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade

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Acknowledgments

This document reports the findings and recommendations from the workshop "Research Directions: Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade," held over the two-day period April 22-23, 2009 at the National Academies and George Washington University in Washington D.C. Further details are provided in the Preface, Executive Summary and Introduction.

This report was prepared by the workshop chair, Peter Cummings and co-chair Sharon Glotzer, with contributions from Jim Davis (UCLA) and John Allison (Ford Motor Co.) [Chapter III], Brian Athey (University of Michigan) and Sangtae Kim (Morgridge Institute for Research) [Chapter V], Padma Raghavan (Pennsylvania State University) [Chapter VI], and Max Bronstein (University of Michigan) who provided commentary on earlier drafts of the entire report. We gratefully acknowledge their invaluable contributions.

We also wish to express our thanks to all of the workshop attendees, speakers and break-out participants (listed in the Appendix), to the World Technology Evaluation Center (WTEC) for its facilitation of the workshop for making it a success, to Pat Johnson and Ben Benokraitis of WTEC for final production of the report, and to the National Science Foundation (NSF) for financial support. We particularly acknowledge Phil Westmoreland, Clark Cooper and Julia Lane of NSF for their support and encouragement.

— Peter T. Cummings and Sharon C. Glotzer

Preface

Peter T. Cummings and Sharon C. Glotzer

Simulation-Based Engineering and Science (SBE&S) involves the use of computer modeling and simulation to solve mathematical formulations of physical models of engineered and natural systems. The impacts of SBE&S can be observed in critical industries, such as pharmaceuticals, medical imaging, and telecommunications. In addition, the infrastructure of the nation relies on SBE&S as it enables the efficient construction and design of our highways, automobiles and aircraft, buildings and power grids. While these examples are far from exhaustive, it is clear that SBE&S is an integral component of research and development (R&D), with far-reaching impacts on our lives and national competitiveness.

Historically, the United States has been the world leader in SBE&S due to sustained investment in high-performance computing (HPC), its adoption by leading U.S. industries, and continued government support of the SBE&S researchers that mold the cutting edge.[1] However, there is concern that this leadership is eroding, especially as the cost of entry into HPC is dropping to the point where anyone can play, and no one can afford not to. Recognition of this trend led a number of Federal agencies – the National Science Foundation (NSF), Department of Energy (DoE), Department of Defense (DoD), National Institutes of Health (NIH), National Aeronautics and Space Administration (NASA), and National Institute of Standards and Technology (NIST) – to commission the World Technology Evaluation Center (WTEC) to conduct an assessment of international activities in the field by a panel of SBE&S experts.[2] The panel found that SBE&S is increasingly recognized worldwide as a high priority for national research investment, that the U.S. leadership position in crucial areas of SBE&S is under serious threat, and that other countries have evolved funding strategies and structures that allow their researchers to more effectively compete in a number of areas of SBE&S. The key findings were first presented to sponsors in a workshop held at the NSF on April 25, 2008.[*]

This final workshop – "Research Directions: Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade" – was held over the two-day period April 22-23, 2009 at the National Academies and George Washington University in Washington D.C. The first day consisted of 23 talks by leading SBE&S practitioners and/or advocates from industry, academia, and government and national laboratories. Day two consisted of breakout sessions. Additional input for the workshop was gathered from the SBE&S community at large through a public website (www.sbes-vision.org). This report is the deliverable of the research directions workshop (RDW). Each of the chapters in Parts 2 and 3 of this report are based on breakout sessions that in turn were informed by the talks on day one and expert community input. This report thus represents a distillation of the key findings and recommendations of the SBE&S community, both RDW participants, and virtual contributors. Most chapters were drafted by breakout session chairs, and edited for inclusion in the full report.

As chairs of the RDW, we are grateful to all of the RDW participants for their enthusiastic participation in this important activity. We are buoyed by the unprecedented opportunities for SBE&S research that lay before us and the transformative potential of SBE&S for science, engineering and medicine. The pages of this report contain recommendations from the SBE&S community on new SBE&S programs, strategies, and funding mechanisms that can reinvigorate and continue U.S. leadership in science and engineering while driving the discovery and innovation that will ensure the prosperity and competitiveness of the United States for the coming decade and beyond.

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[*] The final report, available as a download from http://www.wtec.org/sbes, was officially released on April 22, 2009, to coincide with the Research Directions Workshop, the final workshop of the SBE&S study.

Part One: Overview

I. Executive Summary

Simulation-Based Engineering and Science (SBE&S) involves the use of computer modeling and simulation to solve mathematical formulations of physical models of engineered, social, and natural systems. The impacts and uses of SBE&S can be observed in critical industries, such as pharmaceuticals, automotive, medical technologies, and telecommunications. The infrastructure of the nation relies on SBE&S as it enables the efficient construction and design of highways, automobiles and aircraft, buildings and power grids. While these examples are far from exhaustive, it is clear that SBE&S is an integral component of the U.S. research and development (R&D) enterprise, with far-reaching impacts on our lives and national competitiveness.

The computational landscape is changing rapidly with the U.S. invention of many-core computer processors integrated to provide a thousand-to-million-fold increase of computing power over that of today's computer. Remarkable advances in numerical algorithms and solvers for handling complex equations are providing additional many-fold increases in compute power. At the same time, the ability to store unprecedented amounts of digital data continues to grow rapidly. These increases in computational capability will allow simulations that will drive solutions to problems like Alzheimer's and alternative energy, creating unlimited opportunities for tackling the most important issues facing the nation and creating new venues for renewed national and individual prosperity, wealth, and security.

With these advances in computer capabilities, however, comes urgently needed advances in the models, algorithms, and software required to exploit them for scientific discovery and engineering innovation. As SBE&S becomes increasingly intricate, researchers are faced with an enormity of data that must be properly captured, preserved, and mined. In addition, new initiatives in designing dynamic software are needed in order to integrate data into adaptive models. SBE&S is a rapidly evolving field, but many U.S. institutions do not have adequate curricula to provide students with the training and expertise to effectively design, execute, and interpret simulations, or to develop the next generation of scientific and engineering software. There is concern among SBE&S practitioners in academia, government, and industry that the historical leadership of the United States in this field is diminishing as other nations aggressively scale up investments in SBE&S and underlying infrastructure.

To address these challenges, several overarching goals for the next decade have been identified that will guide the growth and development of SBE&S:

- Enable **broad access to** and **adoption** of SBE&S in U.S. industry
- Institutionalize a **life-cycle** culture for **data** from short-term capture and storage to long-term stewardship
- Build the infrastructure needed for the creation, dynamic development and stewardship of **sustainable software**
- Grow, diversify, and strengthen the SBE&S **workforce**, and identify core competencies and new approaches to modern **teaching** and lifelong **learning**

New mechanisms of support for SBE&S are urgently needed to ensure that the United States remains a leader in this critical field and continues to be competitive in the global knowledge economy. The workshop participants propose a multi-tiered national-level investment strategy to ensure that researchers, laboratories, and institutions have sufficient resources to continue to be the global leaders in SBE&S:

- Provide long-term (5+ years) single and small group grants

- Create long-term team grants that support interdisciplinary collaborations among domain scientists, computational scientists, and mathematicians
- Build large-scale virtual institutes/centers tasked with developing and stewarding community codes for specific SBE&S domains
- Provide 10 long-term (10-year) grand challenge public-private partnership grants
- Provide grants for curriculum development and dissemination, and new programs and approaches to foster a highly skilled SBE&S workforce
- Support graduate students and postdoctoral fellows with traineeship grants, including portable awards that support the transition of exceptionally talented individuals to permanent industrial, academic, or government SBE&S research positions
- Establish leveraged investment programs to promote partnerships between academia and industry
- Establish 20+ multi-investigator SBE&S interdisciplinary research institutes, with broad research programs in specific SBE&S problem domains, data and software
- Establish 40+ multi-investigator SBE&S interdisciplinary research centers, with more focused research efforts in SBE&S problem domains, data and software
- Award several hundred innovator grants to individuals or small teams conducting high-risk, high-reward transformative research in data and software

This comprehensive and multi-pronged investment strategy is essential for ensuring that U.S. SBE&S competitiveness is maintained and strengthened. Taking these steps will dramatically alter industry's approach to R&D and decision-making by enabling an efficient, proactive methodology for fostering innovation. The subsequent highly skilled SBE&S workforce, cost savings, and rapid technological deployment will create jobs and provide the nation with a significant competitive advantage in the global knowledge economy.

II. Introduction

> *"In the face of serious global competition and a sobering economic climate, U.S. leadership in high performance computing – in hardware, software, and expertise – stands out as a true national strategic asset. The Council believes that leveraging this leadership to support next-generation innovation and manufacturing is a sure way to advance overall national competitiveness and prosperity."*
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> – "High Performance Computing To Enable Next-Generation Manufacturing," Council on Competitiveness white paper, January 2009. Available at www.compete.org

Simulation-Based Engineering and Science (SBE&S) involves the use of computer modeling and simulation to solve mathematical formulations of physical models of engineered and natural systems. Every field of science or engineering has been advanced by, and in some cases transformed by, SBE&S, with the result that simulation is increasingly regarded as the third pillar of science, along with the traditional pillars of theory and experimentation/observation. In this, the beginning of the fifth century of the telescope,[*] it is appropriate that high-fidelity simulations implemented on the petascale and exascale computers of today and tomorrow are recognized as constituting a "computational multiscope" – a virtual device that allows us to observe simulated complex phenomena in unprecedented detail across all length and time scales. Just as the microscope and the telescope revolutionized science at two opposite ends of a vast spectrum of spatial scales, SBE&S offers the possibility of revolutionizing science and engineering across all scales from quarks to galaxies, and from electrons to enterprise. To borrow a phrase from a *Nature* editorial in the special issue on scientific data,[3] SBE&S is the "**computational intelligence**" needed to understand, predict, and ultimately design and/or control complex natural and man-made systems using computationally solved models and the flood of data coming both from experiments and simulations.

Many future critical technologies cannot be understood, developed, or utilized without SBE&S. Numerous blue-ribbon community-based reports[4- 12] have confirmed repeatedly that SBE&S is a critical capability that enables discovery, design and innovation, and that it is an engine for economic growth and competitiveness. SBE&S is the critical new asset that will enable next generation innovation, design, resource management, and decision support in the full design-to-delivery product lifecycle. When supported as such, it will become an economic and performance differentiator for U.S. industry. Over the next 25 years, those industries that develop and tap the power of SBE&S will be the most competitive and, on a global basis, will be the most able to work with the best in the world, driving global cooperation and competitiveness for economic growth, national security, and social benefit. Indeed, the importance of SBE&S is now recognized worldwide, with many countries actively investing in SBE&S research activities and the high-performance computational infrastructure that supports it as a central piece of their R&D portfolio for economic growth and security.

The recently published study benchmarking U.S. SBE&S activities against similar activities in Europe and Asia[2] confirmed the growing worldwide recognition of the importance of SBE&S, and identified threats to the long-held leadership by the United States in this field. In particular, the "flattening" of the availability of high-performance computing hardware means that competition in SBE&S is increasingly in the realm of software (the codes that run on the hardware) and wetware (human capital). By virtue of being the "first adopter" of leadership-class computing (noting leadership-class is defined at any given point in time), the United States has enjoyed the role of leader, but at the same time has borne the cost of developing the infrastructure (libraries, utilities, operating systems) that are now freely available worldwide.

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[*] 2009 was celebrated as the 400th anniversary of the invention of the telescope by Galileo. See www.400years.org.

The importance of SBE&S in science, engineering and, indeed, in everyday life, grows daily, fueled by advances in computing hardware and software, and through constant human innovation. For the United States to maintain, and in some cases recapture, leadership in SBE&S areas critical to the nation, new investments in SBE&S are required, and the time for action has arrived, a conclusion supported by the Council of Competitiveness.[13]

Why is now the right time for a new, Federal pan-agency investment in SBE&S? Among the threats to U.S. leadership identified in the SBE&S report,[2] two stand out because of their urgency and relevance across all of the Federal agencies: the strategy for increasing the performance of computing hardware is undergoing a paradigm shift from increasing processor clock speed to multiple cores (from uni-processors to multi-core processors), and workforce training in SBE&S is not keeping up with trends. Each is discussed below, followed by recommendations from the RDW for addressing these particular issues, as well as the broader issues raised on the SBE&S report.[2]

The world is facing *a paradigm shift in the technology underlying SBE&S*. For more than 40 years, researchers and users have enjoyed the exponential increase in computing speed promised in Moore's law[14] that has resulted in the doubling of single processor speeds every 18 months largely through increases in clock speed. At the leading edge of SBE&S, researchers have exploited multi-processor parallelism for the most demanding applications; parallel computing has been the realm of relatively few researchers and mostly in science, rather than engineering, and the utilities and libraries to support parallel computing have been a research activity predominantly carried out at the national laboratories and a handful of universities. However, the energy demands associated with increasing clock speeds have resulted in a paradigm shift – clock speeds can no longer increase as they once did due to materials constraints, and Moore's law is now being realized by doubling the number of cores in each processor. Dual-core and now quad-core processors are available, with octa-core on the consumer horizon and a 128-core processor capable of a trillion operations per second has been demonstrated by Intel. Graphics processors used for high-end video games are already multicore chips, each with hundreds of cores in the billion-plus, such processors deployed in laptops, Sony Playstations and X-Boxes worldwide! Suddenly, parallel computing is no longer the exclusive domain or concern of the handful of researchers working at the extreme bleeding edge of SBE&S. Instead, it will be required of every piece of software written for computers already sold today, and those much more powerful to come. However, *the programming paradigm for multicore chips is fundamentally different from that used for traditional parallel or serial computing*. As a result of this sea change in the hardware, extracting maximum computing potential out of multicore architectures will be an enormous software challenge, requiring innovations across SBE&S in areas ranging from programming languages and compilers to underlying mathematical algorithms to simulation methodology.

Paradigm shifts in technology always pose risks for the reigning technology leader. For example, the invention of the assembly line made the United States pre-eminent in car manufacturing, but the diffusion of car manufacturing technology worldwide, plus missteps by the U.S. auto manufacturers themselves, has led to the situation today – leadership and innovation in auto manufacturing resides in Japan. The implication for the United States in SBE&S is striking: the growing pervasiveness of multicore computing means that the United States is vulnerable to relative newcomers into SBE&S who focus on mastering the new architectures. This problem is growing more acute exponentially – at a doubling of cores every 18 months, in six years a single CPU with eight cores today will have 128 cores, which itself will be one of thousands inside a large parallel computer. The methods and skills developed in the United States over the past 40+ years will be of limited benefit in the new competition for success in SBE&S on multicore architectures.

This hardware paradigm shift will require even tighter integration of SBE&S application scientists with computational, computer, and mathematical scientists who develop the underlying algorithms and take into consideration issues such as memory management. In addition, intercore, interprocessor, and internode communication will have large implications for simulation efficiency. For the United States to continue as a leader in SBE&S it will need to fund large interdisciplinary research programs within communities, similar to the long-term, well-funded multidisciplinary projects that have nurtured the development of community-based codes for global climate and molecular biology simulations.

The *sine qua non* of leadership in SBE&S is a highly skilled and productive SBE&S workforce that spans the entire gamut of SBE&S activities: mathematical modeling, algorithm development, coding, interface development, and end-use. A persistent complaint heard around the world, including the U.S, is that the computing skills of students have deteriorated. Where once the ability to code in a serious scientific programming language, such as FORTRAN or C and its variants, was regarded as a necessary skill possessed by all well-educated scientists and engineers, today's scientists and engineers have little to no formal training in computational sciences or programming languages. Yet, scientists today are adept at using domain-specific "black box" codes, usually with a graphical user interface (GUI). The result is that the educational system has created a generation of students who are ill-prepared to create new SBE&S software, let alone optimize or re-invent it for the complex multicore hardware of the future. Furthermore, despite every field of science and engineering relying on SBE&S to some degree, many students today graduate from universities with little to no exposure to the capabilities of modeling and simulation or general computational thinking skills, leaving them ill-prepared to use SBE&S effectively. *Any comprehensive approach to preparing the United States to meet the coming SBE&S challenges must include the education and training of students and postdoctoral researchers in the mathematical, computational, and modeling skills needed to address current and future SBE&S challenges*.

Hence, for the United States to continue to be the world leader in SBE&S, in an increasingly competitive international environment where the cost of computing hardware is no longer an impediment to conducting SBE&S research, the U.S. Federal agencies must invest in SBE&S in a multi-tiered way, as described below. It must also be recognized that SBE&S research – such as the development of better force fields or multiscale algorithms – is increasingly complex and can be painstakingly slow to produce results, and will rarely result in publications in science and medicine's most prestigious journals (though there are notable exceptions); this stands in contrast to, for example, the synthesis of a new material or the discovery of a new signaling pathway. Finally, the paradigm shift of multicore processors, increasing in density by a factor of ten every five years, opens the door for relative newcomers to dominate. Summarizing the recommendations from the individual breakouts of the RDW (see Chapters III-VIII of this report), SBE&S research requires new investments in:

- **Long-term single investigator and small team grants.** Single investigators and small groups remain one of the key engines for innovation in science and engineering. In SBE&S research, the terms of the grants need to be longer (five years versus three), and to have appropriate measures for success (e.g., for those that develop code, number of users vs. number of refereed journal publications). Expected outcome: greater opportunities for computational discoveries; new innovations in how, and to what, SBE&S is applied.
- **Long-term team grants coupling domain application scientists, computational scientists and mathematicians.** Similar to the Department of Energy (DoE) Scientific Discovery by Advanced Computation (SciDAC) program,[15] such projects would be funded by agencies (NSF, DoE, DoD, NIH) in SBE&S fields relevant to their research portfolios. This represents at least an order of magnitude increase in SciDAC-like activities across all of the agencies. Funding should be for a minimum of five years, with renewal for another five years with demonstrated progress and successful collaboration. Even with strong leadership, large collaborations take time to become productive and

must be nurtured. The experience of many veterans of such collaborations (e.g., the NSF four-year Nanoscale Interdisciplinary Research Team grants) is that funding often runs out when the team has become most productive in a synergistic manner that is greater than the sum of the parts. Expected outcome: creation of new SBE&S capabilities that are efficient on emerging computing architectures.

- **Large-scale virtual institutes/centers focused on developing and maintaining community-based codes for specific problem domains.** In fields where the development of community-based codes is an appropriate way of pooling intellectual capital and expertise (e.g. global climate modeling), agencies should fund virtual institutes to capitalize on the skills of a large and diverse group of researchers. National laboratories would be a natural home for these institutes and in the past demonstrated the capability to develop and maintain large codes due to sustained funding and researcher continuity. Community-based codes have benefits that go beyond ease of use by a larger group of people than the few experts in the field. Community-based codes carry with them the validation and verification that the developers have conducted as part the process of putting codes together. Hence, a molecular biologist knows how to evaluate the accuracy of results reported in a publication from a CHARMM, AMBER or NAMD calculation, since the accuracy of these codes and the corresponding force fields (models for the interactions between atoms) is transparent to all. Likewise, the global climate modeling community knows the accuracy to attach to a prediction using a given set of models for ocean circulation and cloud cover – this is part of the collective community wisdom. Such virtual institutes might be the same size as a large SciDAC project, or considerably larger, with a persistence time of a decade or more, and with the expectation that leadership may change over time. Expected outcome: community-based codes will transform subfields of SBE&S, allowing individual SBE&S researchers to contribute their individual expertise to a larger, more powerful capability; end users will have much greater functionality and accuracy in their simulations; validation and verification will be easier to achieve.
- **Grand challenge public-private partnership grants.** Ten 10-year, $50-$100 million-dollar, public-private partnership grants should be established to produce and demonstrate the value propositions for SBE&S discovery-to-market processes. These large projects should be driven by industry and partner together computational and experimental scientists and engineers in industrial, academic, government, and national laboratories to achieve transformative change in the application of SBE&S to technological innovation. Examples of existing public-private partnerships are the $14 million, three-year, systems-biology consortium established in 2008 between Pfizer, Entelos, UC- Santa Barbara, Caltech, MIT, and the University of Massachusetts examining the regulatory mechanisms involved in insulin signaling in fat cells; the £13 million (~$21 million) Unilever Centre for Molecular Science Informatics established by Unilever within the Department of Chemistry at Cambridge University; and the Energy Bioscience Institute, a partnership between UC-Berkeley, University of Illinois, Lawrence Berkeley National Laboratory, and BP, funded for ten years at $50 million per year. The latter is not exclusively an SBE&S endeavor, but includes substantial SBE&S efforts. Expected outcome: best practices in SBE&S will be adopted by more U.S. companies; academic and national laboratory research in SBE&S will be informed by industry's SBE&S needs; SBE&S will expand into new areas relevant to industrial practice.
- **Education excellence grants.** The inherent interdisciplinary nature of SBE&S necessitates a workforce comprised of individuals with deep foundational knowledge both in a core science or engineering discipline as well as in the tools and theoretical underpinnings of scientific computation. Too often, the core competencies of SBE&S fall between the cracks of domain knowledge and traditional computer science, and

students obtain neither the foundational competencies nor the practical skills required for SBE&S. To help universities educate and train the next generation of innovators and practitioners of SBE&S, new programs and approaches are needed that fill this void, and close the gap between today's available SBE&S curricula and the knowledge and skills needed to exploit next-generation architectures for SBE&S. Funding should support the development of new curricula and courses (both formal and informal), the formation of virtual communities engaged in SBE&S education and learning, development or adoption of cyberinfrastructure to facilitate SBE&S education, physical and virtual centers, schools and institutes leveraging faculty expertise across multiple institutions, strategies for broadening participation in SBE&S at all levels and ensuring a continuous pipeline for a diverse and skilled future SBE&S workforce, and research on effective learning strategies for SBE&S. Expected outcome: a world-leading U.S. SBE&S workforce trained in all areas relevant to SBE&S, from conceptualization to implementation to application.

- **Traineeship grants for students and postdoctoral fellows.** Traineeships for graduate students (similar to NIH Training Grants) should be available to students from all of the agencies with a stake in SBE&S. They should be available individually (much like current NSF fellowships) and through traineeship grants made to institutions or virtual institutes. The DoE Computational Science Graduate Fellowship (CSGF) program is an example of an individual-based program; however, the CSGF program is aimed only at DoE research needs, and is far from adequate even for those. In order to create the SBE&S human resources needed in the future, the need for a pan-agency program at least one order of magnitude larger than the DoE CSGF program is envisaged. The traineeships should support students for at least three years of graduate study, recognizing that most students who will engage in SBE&S research do not, today, come equipped with the computational and mathematical skills needed to be productive in SBE&S research at a deep level. Likewise, even with an increase in the numbers of students trained in SBE&S, there will not be enough skilled people to perform SBE&S research. Hence, a pan-agency postdoctoral retraining fellowship program should be instituted that would allow domain scientists with recently awarded PhDs to retrain in the computational and mathematical sciences needed to become productive SBE&S researchers. These postdoctoral positions would be similar to some private foundation programs, such as the Burroughs Wellcome Career Awards at the Scientific Interface (CASI) program[16] that funds promising researchers who wish to bridge from a physical/mathematical/computational sciences background to applications in the biological sciences. Expected outcome: broadening of the SBE&S workforce, shifting scientific and engineering talent from fields of diminished relevance to SBE&S.
- **Transitional grants.** New types of grants should be created that facilitate the transition of exceptionally talented graduate and postdoctoral students in SBE&S to permanent positions in U.S. industry, government and national laboratories, or academia. These awards should be portable, flexible, and tied to the individual, and carry the recipient through the equivalent of tenure.
- **Internship and practicum SBE&S graduate fellowships and corporate postdoctoral fellowships.** A pan-agency program should be created to place computational science and engineering MS and PhD students in industrial, national, and government laboratories and supercomputing centers for 3-6-month periods, and to give recent graduates the opportunity to conduct postdoctoral SBE&S research of great national interest in a corporate setting. Similar to the DoE CSGF program, which places students in national laboratories during their PhD studies, and new ASEE/NSF Corporate Research Postdoctoral Fellowship Program, these programs will also provide additional training opportunities as well as give future employers a first look at potential recruits

and plant seeds for university-industry-lab collaborations. Expected outcome: higher quality training for SBE&S researchers; improved recruitment opportunities for employers of SBE&S researchers and professionals; expedited translation of university-based SBE&S research to U.S. industry.

- **Undergraduate SBE&S fellowships.** A pan-agency program should be established to support undergraduate students to develop expertise in computational and mathematical sciences needed for a career in SBE&S. Research and educational opportunities should be supported that provide foundational learning in modeling, simulation, informatics, software engineering, programming principles, and computational thinking in the context of discovery and innovation. Expected outcome: increase in the number of U.S. students interested in pursuing careers in SBE&S.
- **Interdisciplinary SBE&S research institutes and centers.** To enable interdisciplinary computational discovery in specific SBE&S problem domains, to support long-term research and stewardship/sustainability in data and software, multiple agencies should establish 20+ interdisciplinary SBE&S research institutes, funded at ~$5 million per year for 5 years, with the possibility of renewal for the most successful institutes. These institutes would by their nature be broad with the engagement of multiple disciplines and institutions. For more focused efforts in the same areas, multiple agencies should establish 40+ interdisciplinary SBE&S research centers, funded at ~$1-2 million per year for 5 years, with a possibility of renewal for a second 5-year period. Given the funding levels, centers could be more regional, even located at a single institution, and could, for example, focus on bringing a specific code from research grade to production grade, or develop data curation/dissemination/analysis tools within a specific problem domain. Expected outcome: the institutes and centers will provide the underlying infrastructure needed for long-term progress in SBE&S that will enable the United States to remain at the forefront of the field.
- **SBE&S innovator grants.** Multiple agencies should establish several hundred innovator grants (~$1 million total for 3-5 years) targeting individuals or small teams (2-3 investigators) conducting high-risk, high-reward transformative research in data and software. Expected outcome: these awards should spur innovations leading to breakthroughs in, e.g., sustainable software development and data curation/dissemination/analysis. Innovations and breakthroughs are critical to maintaining U.S. leadership in SBE&S.

In short, to address the global challenges in SBE&S, a pan-agency effort on the scale of the National Nanotechnology Initiative is required. The Council on Competitiveness – a group of CEOs, university presidents and labor leaders focused on U.S. productivity and leadership in world markets – has likewise concluded that it is essential for the United States to capitalize on its existing leadership in high performance computing (HPC) to drive innovation in and deployment of SBE&S in U.S. industry as a means of enabling U.S. industry to be world leaders in their respective fields.[1,13] Case studies[17-24] demonstrating the use of SBE&S and HPC are provided at the Council's website: http://www.compete.org/.

Part Two: Envisioning a Future Enabled by SBE&S

III. Building the National SBE&S Infrastructure for Innovation, Resource Management, and Decision Support

III.1. Vision

Simulation-Based Engineering and Science (SBE&S) represents the technology and applied capability in which computationally-enabled models are the integrating points for data, expertise, decision and discovery and the means of casting data and knowledge into beneficial outcomes.

Globalization along with uncertainties in the availability and cost of energy, security threats to operating facilities, the explosion of information technology, and the relentless pressure of global competition have led to an unprecedented shift in U.S. industries toward the business and economics of change, just-in-time processing, and rapid response. These “forces” push toward an economy of rapid product innovation and design, proactive situational response, and the predictive management of a myriad of supply chain, environmental and energy dynamics. Product, operation, and management transitions must be made faster and faster. The understanding of uncertainty and risk becomes fundamental, especially to ensure optimum economic and environmental operation within safe and responsible operating envelopes. Sustainability, environment, health, and safety become essential performance metrics. For U.S. industry, these forces have translated into a massive push toward new product discovery, product transitions, performance with zero environmental, health, and safety incidents, response to dynamic global supply and energy chains, and a high level of responsibility for the environment.

The United States is at a crossroads. The total solution to these challenges will not be found as a single approach, but in the commitment, application, and assimilation of a model-based, knowledge-enabled environment that encompasses the full spectrum of enterprise product, operational, and management lifecycles. SBE&S, and the knowledge and expertise it embodies, will need to become an integral asset across U.S. industry to become a competitive capability.

SBE&S is emerging as the critical new asset that will enable next generation innovation, design, resource management and decision support.

To be an economic and performance differentiator, SBE&S must be developed, managed, and supported as essential infrastructure and a critical asset that is equal in value to physical and human resources. In this vision, models are integral to the full design-to-delivery lifecycle. They are the means of enabling global cooperation and competitiveness for economic, national security and social benefit. SBE&S models provide new capability in assessing risk and uncertainty with decisions and enable transition into a proactive, preventive, and innovative mode of operation. Over the next few decades, those industries that develop and tap the power *of* knowledge *in* models *and* knowledge *through* models will be the most competitive and will attract the best human resources in the world.

When deployed with robust investment and determination, SBE&S will equip the nation with a renewed global competitiveness and establish a new market paradigm. The development, application, and management of models and their coherent use across an enterprise create new skill-set requirements and new job markets. The innovation borne out of this new market will enable solutions to some of the most complex and pressing challenges facing the nation.

III.2. Summary

The United States is already experiencing the advent of smart industries – Smart Manufacturing, Smart Energy Grids, Smart Water Resources, Smart Equipment, Smart Buildings, Smart Crops, and Smart Cities – all an outgrowth of SBE&S and foundational cyberinfrastructure.

Foundational cyberinfrastructure "…is the coordinated aggregation of software, hardware and other technologies as well as human expertise to support current and future discoveries and to integrate relevant and often disparate resources to provide a useful, usable and enabling computational and data framework characterized by broad access."

- Fran Berman, former Director,
San Diego Supercomputer Center;
Vice President for Research, RPI

These emerging smart industries have begun to embrace various aspects of design, operation, and support. They are beginning to involve the enterprise-wide application of "smart" technologies, tools, and systems coupled with a highly educated workforce to innovate, plan, design, build, operate, maintain, support, and manage products and facilities. SBE&S technology has only just begun to consider smart technologies in full concert with business and manufacturing missions of the enterprise and its supply chains. It has become clear that this integrated approach provides the basis for a sea change toward a fundamentally more predictive mode of decision-making and/or operation with a much swifter and more proactive incident-response capability.

When reviewing the range of new and competitive capabilities, SBE&S plays the pivotal role in prediction, design, experimental support, discovery, and decision support. The value and great potential for SBE&S has been demonstrated. To be transformative in ensuring U.S. competitiveness and job creation and growth, the nation must commit itself to rethinking its culture and infrastructure:

- From investments in facilities to investments in knowledge-embedded facilities and a knowledge-enabled workforce
- From reactive to proactive, understanding probabilities and uncertainties, predicting potential impact and making informed decisions using the best knowledge available
- From response to prevention by understanding, modeling, sensing, and analysis, and from incident mitigation to prevention
- From a culture of compliance to a culture of performance
- From stove piping and isolation to integration and collaboration
- From data-sparse to information-rich understanding and decision making
- From intelligence that is point-to-point to intelligence that is universally connected to the right place, in the right format, at the right time
- From singular functionality to self-awareness that can adapt and ensure a defined role
- From physical discovery to virtual discovery and innovation

SBE&S will fundamentally alter the way people innovate, and will also change the way they think about and enable discovery, decision-making, and design. A substantial investment in SBE&S will foster these outcomes and ensure U.S. competitiveness in the global knowledge economy.

III.3. Goals for the Next Decade

The "smart" industry drives towards zero emissions and zero incidents through proactive, predictive optimization, and management of the enterprise. It ensures safe and health-conscious operations, with full recognition of people as essential resources for success. The smart industry is committed to knowledge, discovery and innovation and the ability to validate and rapidly deploy new developments.

The sea-change transformations described above will require national will, commitment, approach, and investment. The foremost goal for the next decade is to invest in and build the infrastructure, culture, and skilled workforce for SBE&S into a critical asset across all of U.S. industry to be developed, managed, and exploited. As noted, the framework needs to be innovative and transformative and aimed at leapfrogging the United States into the next generation of competitiveness. It must:

- Enable access to integrated and affordable multiscale, multiphysics SBE&S toolkits and facilitate widespread use by U.S. industry

- Disseminate physics-based, holistically integrated models of material behaviors, from manufacturing simulation to electronic structure and materials properties to accurately calculate and predict material performance prior to manufacturing
- Create highly integrated, high fidelity models that unify agent-based, knowledge-based, and mathematical models aimed at supporting decision making, addressing uncertainty and system dynamics, and enabling complex situational response
- Forge cross-industry, academic, and government design-to-delivery SBE&S software frameworks and toolkits
- Foster software that is developed, maintained, validated and managed as a critical industry asset
- Shape universal data and model standards for integration, interoperability, and sharing
- Support not just large organizations, but also small businesses, academic institutions, and government, and involve public-private partnerships between laboratories, universities, and industry

Researchers use SBE&S to inform disaster policy and planning. At one university, researchers use simulations to anticipate the impacts and frequency of large earthquakes. Leaders in the construction industry will rely on the results of these studies to guide investment into building new structures. These design decisions will have a huge impact on new construction, currently valued at about $1 trillion dollars over the next five years. SBE&S provides insight into a range of possible earthquake scenarios by providing the best possible information to policymakers and ensuring that communities are well prepared for natural disasters.

There is a strong recognition that when SBE&S is applied at enterprise levels, is fully integrated into the core value chain and encompasses the full product lifecycle from discovery to delivery, it will provide a competitive advantage. With computing now globally pervasive, all industries in all countries have or will apply computing in niche areas. The leaders in the global knowledge economy will be those countries and their respective industries that invest in the workforce, infrastructure, and practice of SBE&S as a core competitive capability.

With a national investment, in ten years SBE&S should be in wide use for design, prediction, risk assessment, and decision-making. Resource, environment, management, and policy decisions should all be dependent on SBE&S risk and uncertainty analysis. Use of SBE&S, which will include disciplined verification and validation practices, will enable the decision maker to assess the uncertainty and risk of courses of action. Computational time scales will be matched to decision time scales.

III.4. R&D Investment Priorities and Implementation Strategies

The United States has developed and currently leads in the technology and know-how to leverage SBE&S. Implementing a grand scale deployment of SBE&S technology to achieve the vision will require an investment commensurate to the interstate highway system of the 20th century. The essential investment objective should focus on lowering the barriers to entry for the application of SBE&S in U.S. industry core-value chains and enabling broad-based adoption among all industries. Removing barriers will spur the research, development, and industrialization of SBE&S and foster a research, development, and adoption cycle. This is a transformative investment in moving SBE&S from peripheral application and spot value into integrated, holistic application where there can be significant multiplier effects.

Ford Motor Company uses Integrated Computational Materials Engineering (ICME) to develop and design virtual aluminum engine castings in partnership with researchers at several universities. This design process would normally take years to complete on physical engine parts at considerable cost. Instead, ICME ***accelerates the development process by 15-25%*** *and provides an estimated* ***7:1 return on investment*** *through cost avoidance and savings. ICME provides a poignant example of applied SBE&S that is ensuring U.S. competitiveness in the global knowledge economy.*

The RDW proposes a Grand Challenge Pilot

Program comprised of ten, ten-year, $50-$100 million dollar, public-private partnership grants to produce and demonstrate the value propositions for SBE&S discovery-to-market processes. Three investment categories are proposed to lower barriers and encourage industry adoption:

- Establish leveraged investment programs that encourage university, laboratory, and industry (large to small) partnerships
- Establish supply chain partnerships over a range of industry sectors, e.g. materials, energy, sustainability
- Establish collaborative workforce training programs to build a critical mass of skilled workers to increase the probability of successful entry and reduce the investment risk

IV. Revolutionizing Discovery through Simulation-Based Engineering and Science

IV.1. Vision

The vision of the RDW is for SBE&S to be an engine for discovery, with a record of insights rivaling those obtained through experimentation. In order to achieve this, SBE&S must be ubiquitous, widely accessible, truly multiscale (i.e., seamless in allowing increased problem complexity), and validated for relevant domains. Given that discoveries can occur when data (both experimental and computational) is viewed from a different perspective, computationally generated information should be freely accessible in public domain databases in searchable, standard formats.

> *"The whole history of physics proves that a new discovery is quite likely lurking at the next decimal place."*
> — Floyd K. Richtmyer (1881-1939)
> Cornell University physicist
>
> *"The most exciting phrase to hear in science, the one that heralds new discoveries, is not 'Eureka!' ('I found it!') but rather 'hmm....that's funny...' "*
> — Isaac Asimov (1920-1992), author
> and professor of biochemistry
>
> *"There are two possible outcomes: if the result confirms the hypothesis, then you've made a measurement. If the result is contrary to the hypothesis, then you've made a discovery."*
> — Enrico Fermi (1901—1954)

IV.2. Summary

Scientific discovery has typically been achieved through serendipity, through long-term, directed research focused on a specific problem, when an approach or ideas from one scientific discipline are applied to another discipline, or combinations of these. When serendipity plays a role, a scientist or engineer happens upon a new phenomenon or object by accident while in pursuit of a very different goal (e.g., the discovery of X-rays). In order to capitalize on a serendipitous discovery, a researcher may need the ability to pursue a new hitherto unforeseen yet promising research direction without being constrained by questions of funding or applicability; such funding exists today primarily in Europe (e.g., C4 professorships in Germany), Japan, and those countries in which the primary support of research is derived from the federal or state government via the researcher's institution. (See the sidebar on fluctuation theorems for an example of a serendipitous computational discovery that has profound implications.)

Serendipitous discovery is in contrast to directed discovery, which occurs through painstaking, determined, long-term pursuit (e.g. developing an HIV vaccine or the initial sequencing of the human genome), search (e.g. exhaustive astronomical surveys to discover new stars, exoplanets, and other astronomical objects) and the development of a computational simulation code to describe complex phenomena (e.g., global climate models or first principles materials modeling codes). In directed discovery, a researcher or team of researchers needs to have assurance of research funding over a long term to ensure that tangible and rigorous progress is possible. Thus, in both serendipitous and directed inquiry, short-term (three years or less) support at a modest level focused on the solution of a specific problem is often not the *ideal* funding mechanism for promoting discovery. This is especially so for SBE&S research.

> *At the San Diego Supercomputing Center, researchers utilize 10.4 teraflops of computing power to simulate the natural behavior of molecules inside cells. Previously, these systems were studied using x-ray crystallography, which provides a highly detailed, but static picture of molecular interactions. Now, this computationally enabled work allows researchers to realistically model the behavior of drug candidates in a dynamic living system. The results from this work could play a key role in discovering new drugs for treating HIV.*
> – www.nsf.gov/discoveries/disc_summ.jsp?cntn_id=104280

The second law of thermodynamics tells us that entropy is maximized in a closed, constant-energy system. Stated another way, entropy production in such systems is always positive. This concept is strongly tied to irreversibility and the associated idea of "time's arrow." If we see a film in which a stick of dynamite is exploded, we recognize that entropy has increased (dramatically!). We also recognize that a film in which the fragments of an explosion reform to make a stick of dynamite must be running in reverse. At the same time, if we examine the equations that describe a system at the atomic level, there is no "time's arrow" – we can replace time by its negative and everything still works. That is, there is no concept of irreversibility at the atomic level. A theory of how irreversibility emerges – and hence the second law of thermodynamics comes to hold – won Ilya Prigogine the Nobel Prize in Chemistry in 1977. However, there has long been dissatisfaction with this theory.

In the past two decades, our understanding of the way irreversibility emerges at scales in between the atomic and the macroscopic – specifically, at the nanoscale – has been revolutionized by new theoretical understanding of the role of fluctuations (deviations of properties from their average value), encapsulated in the so-called fluctuation theorems (FTs). The FTs are applicable to systems out of equilibrium (see Evans[1-3]), which exhibit negative-entropy-producing states (i.e., violations of the second law of thermodynamics) that are random but with a predictable statistical distribution over time.

The FTs were the end result of more than a decade of computer simulation and theoretical development that began serendipitously with the discovery in 1990 of an anomaly in simulations of small systems in external fields (i.e., in non-equilibrium states). Understanding this observation led Australia's Denis Evans and co-workers on a decades-long quest that resulted in the FTs as we know them today. The FTs have been since verified experimentally in several systems (for an example, see Wang et al.*[25]). The FTs have permitted us to understand for the first time apparently anomalous experimental results at the nanoscale and represent a true computation-enabled scientific discovery.*

The long-term funding situation at the Research School of Chemistry (RSC) in the Institute for Advanced Studies (analogous to German C4 professorships) within the Australian National University undoubtedly contributed to Evans and co-workers being able to pursue this research over the extended period needed to understand it completely.

When an insight or method crosses from one discipline to another, the impact can be immediate. For example, in the early 1980s IBM researcher Scott Kirkpatrick took his Monte Carlo code for finding minimum energy configurations of spin glasses (a fundamental science problem in condensed matter physics) and modified it to predict the optimal layout of integrated circuits (a microprocessor engineering problem), thus introducing the concept of "simulated annealing."[26] Simulated annealing is now recognized as a powerful optimization tool and conceptual approach applied in many industries. Allowing researchers from different disciplinary backgrounds to work in interdisciplinary fashion on the solution of outstanding problems is one of the mechanisms by which discovery can be enabled.

One of the successful recent programs within the United States that funds computational research aimed at scientific discovery is the DoE's SciDAC program. SciDAC teams application-domain scientists with mathematical and computational scientists to develop efficient simulation capabilities on state-of-the-art computational platforms to enable discovery. The funding is in the form of grants as long as five years with levels of funding for some projects reaching up to $5 million per year. One of the most visible successes of SciDAC has been supporting and fostering global climate change modeling,[15] contributing to widespread recognition of the importance of simulation and modeling (the predictions of global climate simulation are informing trillion-dollar policy decisions by the world's governments), and making significant contributions to the reports of the Nobel Prize winning Inter-Governmental Panel on Climate Change.[27]

SBE&S-enabled discovery requires the development of mathematical models and computer algorithms to solve those models. Models and algorithms are prerequisites to software development and data generation – they are "ground zero" for scientific simulation. For many natural and man-made systems modeled at appropriate scales, the equations are known. For example, to describe a single molecule requires principles from quantum mechanics embodied in the Schrödinger equation; for laminar flow through a pipe, the Navier-Stokes equation; and for the diffusion of a nonreacting gas or a liquid in a simple flow field, the convective-diffusion equation. There can be different ways to solve the equations (i.e., different algorithmic approaches), different implementation strategies (how to implement the algorithm on different architectures) and complexities associated with boundary conditions. However, the key point is that the model is known, and the equations are known.

What about problems for which the equations are not yet known (or not correct) – i.e., problems for which the fundamental science is not yet elucidated? One example is high-energy physics, where the "equations" – corresponding to the Standard Model for sub-atomic particles – are awaiting validation by the Large Hadron Collider at CERN. This is an example in which the known equations may turn out to be incorrect, much as the situation was at the turn of the 20th century, when the only known dynamics were classical mechanics – quantum mechanics had yet to be discovered. Another example is turbulence, a field in which the correct formulation of equations is still being debated. Turbulence is a good example of a problem that besets many fields – namely, the equations that are known to be correct at one scale cannot easily be extended to much larger spatial and/or temporal scales. For turbulent flow, at small enough scales, the phenomena can be described by energy, material and momentum balances, or even atomistically if needed; the problem is that one would like to be able to describe turbulence on a scale commensurate with the size of aircraft. A need to solve the Navier-Stokes equation for fluid flow around a Boeing 777 with grid points small enough to describe turbulent flow represents an impossible computational problem. Global climate modelers face the same issue: just how fine a grid is needed to capture all of the phenomena important to ensure an accurate climate model?

Thus, many issues of developing effective models for natural and man-made systems reduce to the following question; Can computational models that self-adaptively span multiple time and length scales be developed? The RDW's vision is that, through a concerted effort of focused research by domain scientists, computational scientists, and mathematicians, the necessary mathematical, algorithmic, and software advances needed to enable seamless, multiscale modeling paradigms for discovery can be achieved.

IV.3. Goals for the Next Decade

- Create an environment in which the opportunities, capabilities, and human resources for computational discovery are broadened (by an order of magnitude) beyond the current scope of such activities today.
- Support computational discovery in fields that today receive little or no support for such approaches, such as medicine at scales between the molecular (biophysics) and the population (statistics).
- Create computational discovery institutes that promote the use of computation as a pathway to discovery.
- Establish a holistic, multitiered approach to computational discovery in which the development of models, algorithms, scale-bridging methodologies, software development, and data generation/mining are systemically supported.

IV.4. R&D Investment Priorities and Implementation Strategies

In view of the above considerations, in order to support serendipitous, directed and/or cross-disciplinary discovery by SBE&S, SBE&S discovery and research should ideally be supported by long-term funding and when appropriate, interdisciplinary teams. Hence the R&D priorities should allow researchers the opportunity to explore in a way that short-term, single-problem-solution grants currently do not allow. Several mechanisms for long-term support were identified:

- Training grants/computational science fellowships for graduate students and postdoctoral researchers, so that these individuals have a degree of discretion in their research focus
- Longer-term (five years or longer) individual and small group investigator grants
- Team grants to facilitate discoveries at the interfaces between disciplines
- Faculty fellow programs
- Opportunities for funding longer-term, high-risk transformative research projects

One of the key recommendations of the Discovery breakout was for a series of national databases, modeled after the Protein Data Bank, to serve as repositories for simulation-generated data. The idea is that the researchers that generate simulation data may not understand, or even be interested in, all of the phenomena and/or relationships present in their data set. In fact, simulations are typically performed by researchers seeking to answer a narrow set of questions, and the results are interrogated to answer those specific questions. SBE&S data institutes would house the raw simulation output (e.g., all of the configurations generated by a heroic molecular dynamics, galactic, or quantum Monte Carlo simulation). They would be freely available through the SBE&S data institutes, which would curate the data and provide tools for data mining. Researchers would then be able to use the data and analyze it in their own way, looking for additional relationships or phenomena. There are past examples of this: for example, the configurations from Rahman and Stillinger's ground-breaking and highly cited simulation of ST2 water[28] were made available as a 9-track tape to interested researchers; quite a few of H.E. Stanley's early papers on water depended crucially on having the data from Rahman and Stillinger's now-historic simulations available to him.[29, 30] Physicists like Stanley have also mined massive amounts of public data from the stock market, and discovered, using SBE&S, new physics-based financial models. Open access to data from all sources will revolutionize SBE&S research.

Opportunities for discovery will also be enhanced when model and algorithm development is supported at sufficient levels to allow complex problems to be solved efficiently on the fastest available computers. Often, models and algorithms developed for one problem may be used for many others, thus there is substantial leveraging of investment. As an example, classical models of liquids developed in the 1960's and 1970's, and the statistical-mechanical based algorithms to solve them, are used today to study problems ranging from protein folding to nanoparticle assembly.

Specific funding mechanisms include:

- Longer-term (five years and longer) individual and small group grants for model and algorithm development
- Discovery institutes focusing on specific classes of algorithms and their application
- Data institutes to curate and disseminate SBE&S-generated data, and to develop analysis tools relevant to the nature of the data

Part Three: Enabling the Future of SBE&S

V. Transforming Data into a Critical National Asset through SBE&S

V.1. Vision

A patient battling cancer for the past ten years enters a hospital reception area. A wave of her medical bracelet over an RFID hot spot serves as her electronic signature for the HIPAA Privacy Rule and initiates her registration process, replacing the need to fill out forms. A few minutes later, she is ushered into the proton therapy room, her scheduled appointment confirmed seamlessly by the hospital IT system from a virtual hand-shake with the reception-desk RFID middleware. Only six months ago, her hospital had acquired the advanced proton source (the cost had come down by a factor of 10 and footprint from the size of a football field to a small adjacent room); now the imaging algorithm targets the new points of tumor growth with minimal damage to the healthy tissues. On her way out of the hospital, she picks up her monthly combo-regimen of several kinase inhibitors complexed with antibodies, the fruits of recent advances in personalized medicine and *in silico* drug design (a decade ago, their molecular entities did not exist in the pharmacopeia but were discovered in a cyber-expedition of ten billion druglike ligands and tailored to her genetic specifications). Later that week she glances at her online bank account and notes that the expected small payment has been automatically deducted from her health-plan savings account.

Is this science fiction? In 2010, certainly. But with the appropriate investments in data infrastructure and SBE&S, rapid advances in biomedical science may very well allow this vision to become a reality within this decade.

V.2. Summary

> *In 2006, 161 billion gigabytes (exabytes) of digital information was created, captured, and replicated. This is about 3 million times more information than in all the books ever written.*
> – www.nitrd.gov/About/Harnessing_Power_Web.pdf

We live in a data-driven world where massive amounts of data are integrated and distilled to guide crucial decisions for individuals, organizations, and nations – with dramatic consequences. Most recently, in the short span of 18 months, the strategic value of massive-scale data management as foundational infrastructure for astute risk management has been demonstrated at the most successful commercial banks. That infrastructure (the network hardware and the software algorithms) originated during the previous decade in the SBE&S activities of the scientific research community. Today, immense new data challenges at the frontiers of SBE&S research are sparking creative innovations to meet those challenges – which will then create new and disruptive technologies that evolve into a data cyberinfrastructure. This will have a profound impact on the broader societal and economic landscape. The recommended R&D investment levels may appear large by traditional measures, but this initial investment is offset when viewed in the context of the historic return on investment for data infrastructure innovations (e.g., the Internet).

V.3. Goals for the Next Decade

- Institutionalize the culture of life-cycle (including data-capture, data-curation, and data-preservation) for the stewardship of data from distributed sources across spatial (geographical), temporal (time series), and social (disciplines) scales
- Meet the challenges – from hardware to algorithms – of managing massively distributed data as it is transitioned to the data cloud

- Create awareness that the dynamic injection of data in SBE&S is a recurring theme, not only for the unification of scientific computation and experimentation, but also as a paradigm for policymakers to address complex socio-economic problems

V.4. R&D Investment Priorities and Implementation Strategies

> *"Researchers need to be obliged to document and manage their data with as much professionalism as they devote to their experiments. And they should receive greater support in this endeavour than they are afforded at present. ….Universities and funding agencies need to provide and support curation facilities, tools and training. ….Above all, data on today's scales require scientific and computational intelligence. ….The future of science depends in part on such cleverness again being applied to data for their own sake, complementing scientific hypotheses as a basis for exploring today's information cornucopia."*
>
> – Editorial, *Nature*, September 4, 2008

The scientific vision and the economic impact pertaining to data issues paint a compelling picture for investments. Here, recommendations pertaining to "data" are presented that highlight R&D priorities and the need for underlying infrastructure. The need for strategic alignment is underscored by the scale of investment, in the hundreds of millions of dollars.

One of the most pressing challenges facing SBE&S is the sheer magnitude of data that researchers are confronting, along with its increasingly distributed nature. This underscores the importance of two data R&D strategies: first, middleware tools are needed to aggregate and integrate distributed and heterogeneous data and metadata to enable their creation, curation, and management. Second, the dynamic nature of the data challenge must be addressed through R&D. R&D will create new tools to integrate distributed data on real-time networks to parsimoniously share only critical data elements. Together, these two capabilities enable new vistas in multiscale modeling and the transformation of data into knowledge, i.e., more rapid knowledge discovery.

Data issues are infrastructure issues. There are two primary infrastructure investments that form foundational, data-related enablers for advances in SBE&S. First, funding should be provided to establish capabilities in data preservation and sharing that conform to standards to improve SBE&S. Second, easily deployed and standardized network transfer protocols for more efficient use and sharing of simulation data are needed. These two infrastructure investments, albeit large, would add value to and leverage many-fold the R&D investments mentioned above and catalyze the transition to the knowledge economy.

A notable and early example of a successful data infrastructure (with support from DoE and NIH), the Protein Data Bank (www.pdb.org) provides the basis for future data infrastructure funding mechanisms. More recently, the NSF Office of Cyberinfrastructure has launched a multi-year plan to establish data preservation centers, Sustainable Digital Data Preservation and Access Network Partners (DataNet). Early and recent examples further inform the recent international benchmarking in SBE&S[2] to recommend the following multiscale approach.

- **Data infrastructure institutes**. The RDW recommends the establishment of 12, large, center-scale institutes funded at a level of $5 million per year for an initial period of 5 years followed by a performance-based renewal term of 5 years. We believe this level of investment is necessary to form the basis for the data infrastructure that will impact a broad spectrum of the SBE&S landscape. Furthermore, the funding mechanism should encourage center-to-center collaborations to foster cross-fertilization of best practices across disciplinary boundaries. The institutes would also be encouraged to collaborate with the data R&D innovators (below).
- **Data R&D innovators**. The RDW recommends the establishment of SBE&S innovator awards in the data R&D category to foster advances in data R&D priorities. These innovator awards ($1 million over three to five years) should be structured to encourage collaborations with other innovators and with the Data Infrastructure Centers. The goal is

to spark new and creative approaches to data, disseminate best data practices across the SBE&S community, and harvest the best ideas into the national infrastructure framework.

Through these investments, critical advances will be achieved in data cyberinfrastructure to transform SBE&S into a critical asset for discovery and innovation.

VI. Ensuring Sustainable Software for Simulation-Based Engineering and Science

VI.1. Vision

The vision of SBE&S is a future where virtual predictions spur American innovation in a global knowledge economy. Such virtual predictions are enabled by software. Scientific and engineering software provides the competitive edge in investments in science, engineering, computing and medicine that transforms knowledge into predictiveness. The United States must provide for sustainable software that can continuously evolve to incorporate new knowledge, data, theories and technologies to fuel innovation and discovery through SBE&S.

The Quiet Crisis of Sustainable Software: U.S. funding for software development fails to support full lifecycle needs, while concerted European and Japanese efforts are leading to a tipping of the competitive balance in some critical SBE&S application areas.

VI.2. Summary

SBE&S enables discovery and design through computation, by creating and testing models of complex phenomena and analyzing vast amounts of data. The computation is enabled by software that involves many layers, from the application layer at the highest level to the language, library and system layers that bridge the application layer to the underlying computing hardware.[2, 31] Software must be continually refined to reflect new advances in the discipline and to adapt to advances in computing hardware.[2, 32] These refinements and extensions should ensure correct results and allow portable implementations that can execute on multiple hardware platforms. Additionally, when faster time to solution provides a competitive edge, software will need to be tuned for increased efficiency of execution on the computing hardware.

In the SBE&S ecosystem of people, software, models, algorithms, data and hardware, *software is the central entity* that constantly needs to evolve in response to changes in the rest of the ecosystem. In turn, advances in software capabilities drive changes in the rest of the ecosystem. The decades-long lifecycle of successful SBE&S software typically spans multiple generations of hardware and requires constant revision for enhanced functionality. For example, software is routinely updated to incorporate new models and methods for sensitivity analysis, optimization and uncertainty quantification. Consequently, *ensuring sustainable software* is critical to the health and well-being of the SBE&S ecosystem and depends on effective management of the full software life-cycle.

However, there is a “quiet crisis” in progress – U.S. funding for software development fails to support full lifecycle needs and concerted European and Japanese efforts are leading to a tipping of the competitive balance in some critical SBE&S application areas.[2] This crisis is further exacerbated by a new era of disruptive computer chip architectures that promise thousand-fold increases in speed. CPU frequency-driven scaling of sequential processor speeds is no longer possible as chips approach thermal limits.[33] Instead, hardware speed will depend on explicit parallelism with multiple cores (processors) on a chip that can execute multiple independent streams (threads) of computation. Today’s commodity quad and oct cores have 16 to 32-way concurrency while the fastest supercomputers are approaching million-way concurrency. The degree of concurrency in commodity multicore chips is expected to double every eighteen months according to Moore’s Law scaling of chip densities.[33] Graphics processors – also multicore – which are driven by a billion-dollar video games industry and can now be used for highly data parallel scientific programming, are increasing in speed even faster. Such architectures are making, e.g., simulations of biological processes possible with molecular resolution.

Consequently, SBE&S software must be designed to scale to exploit increasing levels of concurrency while avoiding sequential and synchronization bottlenecks that can limit achievable speed-ups. Technology trends also indicate greater hardware heterogeneity with highly non-uniform memory hierarchies and accelerators. Additionally, the interplay between hardware and software to manage reliability and fault tolerance will become more complex with increasing soft error rates from increasing chip densities of multicores and decreases in mean time between failures (MTBF) in larger systems[31, 34] due to thermal emergencies and component breakdowns. The confluence of these trends demands complex and specialized tuning to manage performance, energy and reliability trade-offs in order to enable efficient execution of software on multicores.[32]

The software research challenge is clear – developing effective programming abstractions and tools that hide the diversity of multicore chips and features while exploiting their performance for important applications.

While multicore technology compounds the challenges for ensuring sustainable software, it also provides a tremendous opportunity for engaging a broad community of scientists and developers from academia and industry to successfully address the software sustainability challenge while catalyzing the software sector of the IT industry. Until recently, scalable software was the concern of the relatively small number of supercomputing (high performance computing) specialists and SBE&S researchers with large-scale research problems.[2,31] Additionally, the costs of supercomputers are high and the supercomputer market is small, providing little incentive for commercial vendors to invest in software development.[31] The situation is dramatically different now – multicores have made scalable software a major challenge for the over-$450 billion software industry.

The time for strategic investments is now – the United States must seize this opportunity to gain world leadership and an unprecedented level of competitive advantage in the global knowledge economy by addressing the challenges of sustainable software. Providing for sustainable software is a national imperative for leading innovation in a “flat world” of ubiquitous access to computing through transformative SBE&S. The United States should make adequate strategic and long-term investments in R&D to address all aspects of the software lifecycle, spanning all layers of the software stack and addressing new standards and best practices for software stewardship.

*Under pressure to reduce R&D expenditures, the Vice Presidents for R&D at Goodyear chartered a study of alternative product development methods. The study was completed in 1992 and three alternatives were identified: more efficient building and prototype testing, use of predictive testing, and simulation-based engineering and science. SBE&S was ultimately selected as it had the potential to dramatically reduce costs. However, developers soon faced the overwhelming challenge of writing software to successfully model and simulate tire wear. This challenge was overcome through a partnership with Sandia National Laboratories, which lead the creation of high fidelity models and software. This partnership and ongoing development would lead to the Assurance TripleTred, which was Goodyear’s **first product developed entirely using SBE&S** and is the **most successful product introduction in Goodyear’s 110-year history**. Not only had Goodyear **decreased its prototype expenditures by 62%**, but the **product design times were reduced by 67%** from three years to less than one year.*

VI.3. Goals for the Next Decade

Three goals of sustainable software for SBE&S are:

- Create and maintain a world-class R&D program aimed at ensuring and advancing sustainable software for SBE&S
- Facilitate transfer of new SBE&S software innovations into products for economic growth, jobs and public benefit

- Foster educational resources and a skilled workforce for developing sustainable software for SBE&S

VI.4. R&D Investment Priorities and Implementation Strategies

A guiding principle for achieving sustainable software goals concerns determining R&D priorities that are in close concert with the intrinsic characteristics of SBE&S software, its complex lifecycle and the ecosystem in which it operates.

Software is best viewed as a stack of layered abstractions.[2, 31, 35] At the highest level are one or more application layers, followed by one or more middleware layers including compilers, libraries,[36] run-time optimization systems and ending with an operating system layer on which all other software operates to enable computations on the hardware. Standards like TCP/IP and HTML[37] have fuelled the growth of the Internet and more recently, standards such as MPI[38] have resulted in successful middleware development for SBE&S. R&D priorities should focus on articulating layered software architecture standards for SBE&S and supporting development activities at each layer and across layers. Such software architecture specifications could be tailored to the needs of different SBE&S domains such as materials science, chemistry etc. at the higher layers while sharing the specifications for some middleware and lower layers. These specifications will significantly broaden the community of researchers, developers and industry partners who can engage in sustainable software development to fuel innovation and growth. The standards will allow a wide variety of approaches and implementations at layers and across layers that can add greatly to the health and diversity of the SBE&S ecosystem.

Software for SBE&S is sophisticated and tightly coupled to research in simulation models and algorithms, and frequently runs to millions of lines of source code.[2] The lifespan of a successful program is usually measured in decades, requiring adaptations to multiple computer hardware generations. The initial development process is long and software sustainability depends on continued upgrades throughout its decades-long lifecycle. R&D priorities should address the need for long-term funding initiatives for the long-term health of innovation driven SBE&S software. Graduate students, postdoctoral researchers, scientists, and faculty must be supported to conduct innovation-driven research in software prototyping including new algorithms and optimizations, and the hiring of software development professionals for more routine tasks related to full life-cycle maintenance and user support.

There is a lack of students who are adequately trained in SBE&S.[2] Although they are capable of running existing codes, they are typically unable to conceptualize an algorithmic or mathematical framework and the intricacies of concurrency, scalability and computational complexity. They are also not trained in software engineering practices to develop portable extensions and statistical testing for correctness, etc. The limited and short term funding for SBE&S software development as part of Federally-funded research is also leading to reduced production of appropriately trained students, which will threaten the nation's long-run competitive position.[2] SBE&S software education and training must be established as a clear priority with a focus on interdisciplinary degree programs and options that are made readily available both to undergraduate and graduate students.

The RDW proposes an inclusive national organization, where all groups in the SBE&S software community could benefit, either as developers or users. The scope of the research should be on algorithms and software to respond to scientific and engineering challenges across disciplines, to reinvigorate the national community and to promote software stewardship. Selection of proposed software activities should be allocated in response to proposals and based on relevant metrics such as accuracy, time to solution, good software practices, adherence to developing standards, and code usage by the community. A standing committee should be responsible for overall management and review and encourage proposals with an interlocking set of subcommittees in different disciplines and activities. A small permanent staff, consisting of a director and support personnel would coordinate the committee meetings, prepare for reviews, arrange the workshops, and coordinate funding. In addition, there would be a number of competitive, highly recognized national positions for software development to encourage scientific software development as a career path, filled primarily by scientists within a few years of completing their PhD. Interdisciplinary activities will be particularly encouraged, e.g. between the applied math, computer science communities and various scientific disciplines through workshops, and other activities. The education effort, aimed at graduate students, postdoctoral researchers, and faculty, could be modeled along the lines of the recently reconstituted European CECAM, to organize workshops and schools on new algorithms, software development, use and community building.

The RDW recommends the funding of research, development and education in SBE&S software at three scales, in the form of (1) Institutes (2) Centers and (3) Innovator awards to catalyze innovation through SBE&S by reinvigorating and broadening the community. These awards will collectively support a vibrant community of partnerships between academia, government laboratories and industry for the development and stewardship of sustainable SBE&S software to establish U.S. leadership in the global knowledge economy.

- **SBE&S Institutes.** 5-10 large multidisciplinary SBE&S research institutes (at more than $5 million per year for an initial period of 5 years followed by a renewal period of 5 years based on performance in the initial 5 year period, and for the best successes, further 5 year term renewals for sustained community software stewardship). Such institutes will focus on a broad range of R&D including software architecture specification, standards and reference implementations across layers, for one domain or across multiple related domains. These Institutes will bring together a large group of researchers with great breadth and depth, who have a deep understanding and appreciation of many converging disciplines. Some Institutes can leverage investments in computing hardware and industry partnerships to develop end-to-end SBE&S test-beds either in a particular domain or spanning multiple domains to solve, e.g., a grand challenge problem in sustainable energy or brain modeling, self assembly in materials, etc. Such Institutes will also have an integrated program of research, development, education and industrial outreach to promote all key aspects of sustainable SBE&S software. They will also stimulate interaction among all stakeholders through various means including setting of joint research directions and collaborative activities with the international research community and industry partnerships.
- **SBE&S Centers.** 10-20 multi-investigator multidisciplinary SBE&S research centers at $1-2 million per years for an initial period of 5 years followed by a renewal period of 5 years. These centers will bring together a range of expertise to bear on a particular R&D topic. For example, a center could develop a domain-specific application layer or build models of performance that can span multiple software layers to enable metadata and metrics for performance optimizations. They will typically represent efforts to mature and advance results from a small team and individual investigators to serve the broader community. Success as a Center could lay the groundwork for significant expansion in scale and scope through the development of activities that could be funded as an Institute. Centers will be expected to cover a range of research, development and education including, when appropriate, involvement with industry and international efforts.
- **SBE&S Innovators.** Several hundred “Innovator” awards (at less than $1 million total for a period of three-five years) targeting single investigators or small teams of two-three investigators. These awards would spur innovative research that will lead to breakthroughs in sustainable SBE&S software. Efforts could concern the development and testing of new algorithms into a particular software layer for improved modeling or enhanced performance toward faster time to solution or improved accuracy, etc. Funding

of such smaller “Innovator” awards allow the support of a broad range of ideas as well as more high-risk proposals that, if successful, may lead to transformative advances in SBE&S software.

VII. Educating, Training and Diversifying the SBE&S Workforce

VII.1. Vision

The nation's future knowledge workforce must fully exploit the power of computing for discovery and innovation. From manufacturing to medicine, from aerospace to alternative energy, from security to sustainability – the transformative power of SBE&S can only be achieved through a prepared workforce skilled in computational science and engineering. In turn, the foundations of SBE&S – and the appreciation of models and how computers can be used to solve them – is critical for modern science, technology, engineering, and mathematics (STEM) workforce development. Future high-wage jobs and upward mobility career paths that stay in the United States require a new generation of knowledge workers able to harness the power of computing for every aspect of the industrial lifecycle.

The SBE&S workforce must comprise a self-propagating cohort of researchers, students, and practitioners with the necessary breadth of knowledge, depth of understanding, skills and passion to effectively exploit the power of modeling and simulation from laptop to exaflop so as to increase the pace, intensity, and impact of discovery and innovation in science and engineering. Cultivation of this cohort requires a new and different approach to education, training, and broadening participation in SBE&S.

Researchers at Carnegie Mellon University and the University of Pittsburgh are using SBE&S to enhance the quality of life for people with severe disabilities. Using high performance computing, researchers trained in SBE&S are able to build a realistic model of the mobility challenges that face those with disabilities – from opening a refrigerator to answering a phone. New models and simulations allow engineers to design and rapidly prototype assistive robotic devices for enhancing mobility. This process used to be expensive, time consuming, and cumbersome, but thanks to dynamic simulations these assistive technologies can be deployed faster than ever at low cost.

– www.nsf.gov/discoveries/disc_summ.jsp?cntn_id=115433

VII.2. Summary

The inherent interdisciplinary nature of SBE&S necessitates a workforce comprised of individuals with deep foundational knowledge both in a core science or engineering discipline as well as in the tools and theoretical underpinnings of scientific computation. Today's science and engineering students are insufficiently proficient in the latter, often using simulation software as a "black box" without any deep understanding of the underlying algorithms and methods. Many students lack the ability to provide the innovation that would allow that software to be used on new computer architectures to blaze new trails in science, engineering and medicine.

There are many levels on which today's students are ill-prepared to fully exploit the transformative power of SBE&S for discovery and innovation. At the most fundamental level, students are insufficiently exposed to the core competencies of computational science and engineering and its mathematical underpinnings beginning in high school (or even earlier!) and continuing through undergraduate and graduate education and beyond. More and more, universities are eliminating courses in programming and encouraging the use of software packages like Excel and Matlab for problem solving, with the result that incoming graduate students have poor to no programming skills and little understanding of how computers actually work. For those students who somehow learn to program, they then find a persistent and growing gap in the available curriculum at their university between standard introductory courses in supercomputing (such as parallel programming) and what she/he needs to know to use cutting edge computer architectures such as many-core processors.

Standard software "carpentry" – including the practical use of essential tools such as debuggers, profilers and compilers for scientific code development – falls outside of both traditional computer science curricula and domain discipline curricula, and thus is not typically taught as part of any formal curriculum. As a result, students do not learn how to "program for performance" – that is, to fit their problem to the proper computer architecture using the most efficient algorithms and methods in order to fully exploit the power of the machine. Most computational science and engineering students receive no real training in software engineering (how to write sustainable, reusable, robust code), which is critical for a long-lived code, especially open source codes developed by geographically disparate, virtual teams of simulators over a timescale of years or even decades. Computational science and engineering students today receive little training, if any, in uncertainty quantification, validation and verification, risk assessment or decision making, all critical for multiscale simulations that bridge the gap from atoms to enterprise.

Because of this training gap, the United States is not prepared to take advantage of coming hardware breakthroughs being driven largely by U.S. computer companies because the current generation of algorithms and software must be rethought in the context of radically new architectures that few know how to program. Meanwhile, countries such as Brazil, China, Finland, Germany, India, Japan, the Netherlands, and Switzerland now recognize the importance of SBE&S and are reinvesting in their educational infrastructure to create a new generation of computationally-aware workers.[2] In some cases, partnerships among industry, government and academia enable new opportunities for SBE&S training and education abroad.[2]

VII.3. Goals for the Next Decade

Inventing a new America through discovery and innovation requires that U.S. engineers and scientists compete with the broad global science and engineering workforce in SBE&S. For the U.S. workforce to lead all others on timescales of 10, 20, and 30 years, core competencies in computing must be integrated with an appreciation and proficiency in modeling and simulation together with theory and experiment. Although the United States is competitive in theory and experiment, it lags in strategic areas of modeling and simulation; eliminating this gap must be a goal for this decade. In ten years, all students graduating from the nation's universities must have an appreciation of the role of SBE&S in solving the most pressing problems facing the world today, from global healthcare to drinkable water to climate change. A higher fraction of these students must choose to continue on to seek higher degrees and eventually careers in SBE&S. Students of SBE&S must have access to education and training opportunities capable of instilling the expertise and skills to harness the power of high performance computing as architectures and computing capabilities continue to evolve decade after decade. They must also have access to intellectually rewarding, high wage SBE&S jobs. Practitioners of SBE&S must have access to continued learning opportunities in SBE&S long after their traditional formal education and training has ceased. These goals can be achieved if we:

The fruits of SBE&S can be seen in films like Terminator 3: Rise of the Machines, Star Wars: Episode III, and Poseidon. Researchers at Stanford use powerful computational algorithms and high performance computers to simulate realistic 3-D models of fluid dynamics, biomechanics, and computer vision for films like these blockbusters. These SBE&S techniques and the computers that enable them are a driver of the $80 billion dollar U.S. film industry that employs 2.5 million Americans.

– www.nsf.gov/discoveries/disc_summ.jsp?cntn_id=111581
– physbam.stanford.edu/~fedkiw/
– www.mpaa.org/researchStatistics.asp

- Increase, diversify and strengthen the SBE&S workforce, and develop a new cohort of SBE&S workers raised in a culture of sustainable scientific and engineering software development and data stewardship. This workforce must have experience in SBE&S as it relates to discovery, design, prediction, risk assessment and decision-making.

- Identify the core competencies of SBE&S and create sustainable, accessible and modern ways of teaching the knowledge and skills that support these competencies.
- Create an environment for lifelong learning in SBE&S as its tools, applications and uses continue to evolve.
- Create a new breed of computationally-savvy Americans by enriching the understanding of computers and models and how both are used in scientific discovery and in tackling societal and technological problems.

VII.4. Investment Priorities and Implementation Strategies

Investment priorities must address how to rapidly grow the available SBE&S workforce while both deepening knowledge in SBE&S and strengthening skills in HPC and digital data. The nation must take a transformative approach, and seek effective, efficient, and sustainable ways of teaching SBE&S core competencies and tools as they continuously and rapidly evolve – even in the absence of "critical mass" in all aspects of SBE&S at individual institutions.

Achieving these goals will require the creation of a new infrastructure for education and training in SBE&S. The development of new learning resources that take advantage of modern cyberinfrastructure must be encouraged. The RDW recommends a nationally coordinated approach to education and training in SBE&S that fosters both individual and team efforts at many levels and on many fronts simultaneously, all sharing resources and best practices via cyberinfrastructure. Recommended funding mechanisms include:

- **Education excellence grants.** The inherent interdisciplinary nature of SBE&S necessitates a workforce comprised of individuals with deep foundational knowledge both in a core science or engineering discipline as well as in the tools and theoretical underpinnings of scientific computation. Too often, the core competencies of SBE&S fall between the cracks of domain knowledge and traditional computer science, and students obtain neither the foundational competencies nor the practical skills required for SBE&S. To help universities educate and train the next generation of innovators and practitioners of SBE&S, new programs and approaches are needed that fill this void, and close the gap between today's available SBE&S curricula and the knowledge and skills needed to exploit next generation architectures for SBE&S. Funding should support the development of new curricula and courses (both formal and informal), the formation of virtual communities engaged in SBE&S education and learning, development or adoption of cyberinfrastructure to facilitate SBE&S education, physical and virtual centers, schools and institutes leveraging expertise across multiple institutions, strategies for broadening participation in SBE&S at all levels and ensuring a continuous pipeline for a diverse and skilled future SBE&S workforce, and research on effective learning strategies for SBE&S. Funding should be provided on multiple levels, including individual PIs, small teams, large teams, centers and institutes, with activities and coordinated nationally and subsequent products disseminated broadly.
- **Traineeship grants for graduate students.** Traineeships for graduate students should be available to students from all of the agencies with a stake in SBE&S. They should be available individually (much like current NSF fellowships) or through traineeship grants made to institutions or virtual institutes (the equivalent of NIH Training Grants or IGERTs). The DoE Computational Science Graduate Fellowship (CSGF) program is an example of an individual-based program; however, the CSGF program is aimed only at DoE research needs, and is far from adequate even for those. In order to create the SBE&S human resources needed in the future, a pan-agency program at least one order of magnitude larger than the DoE CSGF program is needed. The traineeships should support students for three to five years of graduate study, recognizing that most students who will engage in SBE&S research do not, today, come equipped with the

computational and mathematical skills needed to be productive in SBE&S research at a deep level. Traineeships should include funded onsite experiences (internships, co-ops, workshops, etc.) at national supercomputing centers and at university centers and national laboratories specializing in HPC.

- **Traineeship grants for postdoctoral fellows.** Likewise, even with an increase in the numbers of students trained in SBE&S, there will not be enough skilled people to perform SBE&S research. Hence, a pan-agency postdoctoral re-training fellowship program should be instituted that would allow domain scientists with recently awarded PhDs to retrain in the computational and mathematical sciences needed to become productive SBE&S researchers. These postdoctoral positions would be similar to some private foundation programs, such as the Burroughs Wellcome Career Awards at the Scientific Interface (CASI) program[16] that funds promising researchers who wish to bridge from the physical /mathematical /computational sciences background to applications in the biological sciences. Traineeships should include funded onsite experiences (internships, co-ops, workshops, etc.) at national supercomputing centers and at university centers and national laboratories specializing in HPC.
- **Transitional grants.** New types of grants should be created that facilitate the transition of exceptionally talented graduate and postdoctoral students in SBE&S to permanent positions in U.S. industry, government and national laboratories, or academia. These awards should be portable, flexible, and tied to the individual, and carry the recipient through the equivalent of tenure.
- **Internship and Practicum SBE&S graduate fellowships.** A pan-agency program is recommended to place computational science and engineering MS and PhD students in industrial, national, and government laboratories and supercomputing centers for 3-6 month periods. Similar to the DoE CSGF program, which places students in national laboratories during their PhD, this program will also provide additional training opportunities as well as give future employers a first look at potential recruits and plant seeds for university-industry-lab collaborations.
- **Undergraduate SBE&S fellowships.** A pan-agency program is recommended to support undergraduate students to develop expertise in computational and mathematical sciences needed for a career in SBE&S. These fellowships could be used to obtain a certificate in scientific computing at universities offering such programs, or to obtain knowledge and skills in SBE&S through virtual activities by the Education Excellence Grants. Funds could support participation in computational science REU programs, or to participate in SBE&S research at their home institution. A multi-tiered fellowship program with different sizes of awards is envisioned.
- **Continued learning fellowships.** Fellowships should be provided to academic professionals to assist in costs related to retraining or continued training in SBE&S related competencies. As the core competencies evolve to match rapidly evolving computer architectures, professionals require opportunities to refresh their skills and, in many cases, retrain. A timely example of this is graphics processors, whose use for scientific computing has been demonstrated but the programming paradigm is very different from other paradigms and requires considerable retraining and acquisition of skills. Funds should be made available to support interested faculty, research staff, and other professionals in participating in training workshops developed through the Education Excellence grants, or for extended visits to national supercomputing centers or national laboratories offering hands-on opportunities.

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Appendix

Final Workshop Agenda

Research Directions:
Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade

National Academy of Science Building
2101 Constitution Ave. NW, Washington DC
April 22-23, 2009

Simulation-Based Engineering and Science (SBE&S) is a key element underpinning future progress in science and technology, as has been identified in numerous government, national academy, and other reports. In a recent report,[1] a panel of experts, convened by the World Technology Evaluation Center (WTEC) on behalf of a number of U.S. Federal funding agencies, has highlighted the progress being made in SBE&S worldwide and the growing competitiveness of activities in this area outside the United States. This workshop, facilitated by WTEC, is designed to bring together stakeholders in SBES from academia, government agencies and industry, to address the following questions:

- Why are advances in SBE&S crucial to the future success of U.S. science, engineering, and industry, and how will they contribute to U.S. economic competitiveness?
- What strategic investments in SBE&S are needed in order to achieve the promise of SBE&S?
- How (over what time frame) and in what format can these investments be most productive?

Our goal is to develop a community-driven report on the future of SBE&S research in the United States.[2]

Day one of the workshop will focus on the "why", with presentations from leaders in academia, government agencies, and industry on the present and potential impact of SBE&S. Day two will involve break-out sessions, in which workshop participants will collectively address the question of how research and development in SBE&S can be most effectively advanced in the future. The lessons being learned in other countries, as detailed in the WTEC report,[1] will be particularly relevant to these discussions. On April 24, workshop leaders will convene to draft the report on the workshop, which will summarize the findings.

April 22, 2009, 8:00 AM-6:00 PM
Lecture Room, National Academies Building
2101 Constitution Ave. NW, Washington DC

Theme: Why is SBE&S crucial to the future success of U.S. science, engineering, and industry, and how does it contribute to U.S. economic competitiveness?

7:30 AM Continental breakfast and registration
8:00 AM *Welcome and Introduction to the Workshop*
Peter Cummings, Vanderbilt University and Oak Ridge National Laboratory

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[1] Glotzer, S. C., Kim, S. T., Cummings, P. T., Deshmukh, A., Head-Gordon, M., Karniadakis, G., Petzold, L., Sagui, C. and Shinozuka, M., "International Assessment of R&D in Simulation-Based Engineering and Science," WTEC, 2009 – http://www.wtec.org/sbes.

[2]

8:15 AM	*Objectives and expected outcomes* Phil Westmoreland, National Science Foundation
8:30 AM	*Cyberinfrastructure and Computational Science for Research and Education* Edward Seidel, Director, Office of Cyberinfrastructure, National Science Foundation
9:15 AM	*Revolutionizing Engineering Science through Simulation: Summary of NSF Blue Ribbon Panel Study* J. Tinsley Oden, U. Texas Austin
9:30 AM	*International Assessment of R&D in Simulation-Based Engineering and Science* Sharon C. Glotzer, University of Michigan
10:00 AM	Break (20 min).

Summaries of relevant recent studies & workshops sponsored by US agencies

10:20 AM	*Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security* John Allison, Ford
10:40 AM	*Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security* Horst Simon, LBNL
11:00 AM	*President's Information Technology Advisory Committee Report on Computational Science: Ensuring America's Competitiveness* Daniel A. Reed, Microsoft
11:20 AM	*Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering* John W. Lyons, National Defense University
11:40 AM	*Computation-Based Engineering Summit: Transforming Engineering through Computational Simulation* Arthur C. Ratzel, Sandia Albuquerque
Noon	Lunch: (60 minutes)

Science and Technology Drivers

1:00 PM	*Projections of climate change consequences: A scientific and computational grand challenge* Jim Hack, Oak Ridge National Laboratory
1:20 PM	*Simulating the big one: How we try to anticipate the effects of future earthquakes* Greg Beroza, Stanford University
1:40 PM	*Modeling and simulation of subsurface grand challenges* Mary Wheeler, University of Texas Austin
2:00 PM	*Competitive advantage for industry using simulation-based engineering and science* Loren Miller, Goodyear (ret.)
2:20 PM	*Successes and challenges for simulation and modeling in process systems engineering* Rex Reklaitis, Purdue University
2:40 PM	*Large-scale simulations of complex systems: predicting large economic events* Gene Stanley, Boston University
3:00 PM	Break (20 min)
3:20 PM	*Data explosion and complexity in bioinformatics* Brian Athey, University of Michigan
3:40 PM	*Prospects for simulation-based engineering and science approaches applied to cancer*

Larry Nagahara, National Cancer Institute
4:00 PM *Software requirements and software frameworks for using simulation-based engineering and science*
Phil Colella, Lawrence Berkeley National Laboratory
4:20 PM *Petascale computing: Opportunities in materials and nanoscience*
Thomas Schulthess, Swiss National Supercomputing Center
4:40 PM *Petascale simulations of turbulent combustion*
Jackie Chen, Sandia Livermore
5:00 PM *Challenges in molecular theory, models and simulation*
Teresa Head-Gordon, UC-Berkeley
5:20 PM *The challenge of petascale distributed computing in high energy physics*
Paul Avery, University of Florida
5:40 PM *Summary and charge to breakout sessions*
Peter Cummings, Vanderbilt University and and Oak Ridge National Laboratory
6:00 PM Reception

April 23, 2009, 8:30 AM – 6:00 PM
George Washington University, Marvin Conference Center
800 21st Street, N.W., Washington, DC 20052

Theme: What research directions in SBE&S should be pursued in order to achieve the promise of SBE&S?

Three break-out sessions will be held in the morning and three more in the afternoon. Each session has two moderators who will divide between them the duties of leading the discussions and recording them. Short perspective presentations will serve to stimulate discussion.

MORNING
I. **Creating Software for Creating Models**: *Languages, performance analysis and debugging*
Moderators: Padma Raghavan, Penn State University and Thomas Schulthess, ETH Zurich – **Room 413**
II. **Using the Model-Data Interface**: *Modeling paradigms, domains, simulations that require and/or generate data, especially large data sets.*
Moderators: Brian Athey University of Michigan and Jim Hack, Oak Ridge National Laboratory – **Room 414**
III. **Education, Training and Broadening Participation in Modeling and Simulation**: *Curriculum changes; minors and degree programs, workforce development, virtual communities, gateways, internships*
Moderators: Sharon Glotzer, University of Michigan and Tom Hacker, Purdue University – **Room 411**

AFTERNOON
IV. **Developing, Implementing and Extracting Knowledge from Models**: *New physical models and algorithms. Multiscale Models. Visualization, validation, verification, uncertainty quantification.*
Moderators: Eric Michielssen, University of Michigan and Gerhard Klimeck, Purdue University – **Room 413**
V. **Discovery by Simulation and Modeling**: *Success, future prospects*
Moderators: Peter Cummings, Vanderbilt University and Jack Wells, Oak Ridge National Laboratory – **Room 411**

VI. **Innovation and Engineering Design**: *SBE&S for optimization, design, multiscale time-critical adaptive optimization like supply chain management and optimization*
Moderators: Jim Davis, UCLA and John Allison, Ford – **Room 414**

These breakout sessions will focus on the strategic directions for SBE&S and the scientific infrastructure needed to support those directions. The allocation of the breakouts between morning and afternoon sessions will be finalized at the end of Wednesday.

8:00 AM Continental breakfast and registration
8:30 AM Breakout sessions I-III
9:45 AM Break (15 minutes; participants may move between breakouts)
9:30 AM Breakout sessions I-III (cont’d)
11:00 AM Break (15 minutes)
11:15 AM Plenary session: Summaries of breakout sections I – III by session moderators

12:00 PM Working Lunch (90 minutes)

1:30 PM Breakout sessions IV-VI
2:45 PM Break (15 minutes; participants may move between breakouts)
3:00 PM Breakout sessions IV-VI (cont’d)
4:30 PM Break (15 minutes)
4:45 PM Plenary session: Summaries of breakout sections IV-VI by session moderators
5:15 PM Adjourn

Workshop Participants

John Allison (Ford)
Paul Avery (U. Florida)
Brett Berlin (Berlin Consulting)
Greg Beroza (Stanford U.)
Robert Bohn (NITRD Program)
Tony Chan (NSF)
Jim Chang (AFOSR)
Jacqueline Chen (SNL)
Ken Chong (NSF)
Almadena Chtchelkanova (NSF)
Phil Colella (LBNL)
Clark Cooper (NSF)
Peter Cummings (Vanderbilt U., ORNL)
Frederica Darema (NSF)
Jim Davis (U. California-Los Angeles)
Sharon Glotzer (U. Michigan)
Brian Gopalan (Washington CORE, LLC)
M. Guiton (Cray Inc.)
Jim Hack (ORNL)
Thomas Hacker (Purdue U.)
Jouko Hautamaki (Tekes/Embassy of Finland)
Teresa Head-Gordon (U. California-Berkeley)
Mai Hiroki (Washington CORE, LLC)
Jill Hopper (Cray Inc.)
Eric Itsweire (NSF)
LeLand Jameson (NSF)
David Keyes (Columbia U., King Abdullah U. of Science and Technology)
Gerhard Klimeck (Purdue U.)
Ashok Krishnamurthy (Ohio Supercomputer Center)
Jerry Lee (NCI)
David Levermore (NRC)
Wing-KanLiu (Northwestern U.)
John W. Lyons (National Defense U.)
Ernest McDuffie (NITRD Program)
Cynthia McIntyre (Council on Competitiveness)
Shawn McKee (U. Michigan)
Eric Michielssen (U. Michigan)
Loren Miller (Goodyear, retired)
John Mintmire (NSF)
Raul Miranda (DOE)
Larry Nagahara (NCI)
J. Tinsley Oden (U. Texas at Austin)
Ruth Pachter (AFOSR)
Grace Peng (NIBIB)
Padma Raghavan (The Pennsylvania State U.)
Art Ratzel (SNL)
Daniel A. Reed (Microsoft)
Rex Reklaitis (Purdue U.)
Celeste Rohlfing (NSF)
Celeste Sagui (North Carolina State U.)
Thomas Schulthess (Swiss National Supercomputing Center)
Edward Seidel (NSF)
Horst Simon (LBNL)
H. Eugene Stanley (Boston U.)
Erik Svedberg (NAS)
Suzy Tichenor (ORNL)
James Warren (NIST)
Scott Weidman (NRC)
Jack Wells (ORNL)
Phillip Westmoreland (NSF)
Mary F. Wheeler (U. Texas at Austin)
David Womble (SNL)

WTEC Participants

Michael DeHaemer (WTEC)
Patricia Foland (WTEC)
Geoff Holdridge (NNCO)
Pat Johnson (Johnson Edits)
Halyna Paikoush (NNCO)
Robert Shelton (WTEC)

Acronyms: AFOSR: Air Force Office of Scientific Research; DOE: Department of Energy; LBNL: Lawrence Berkeley National Laboratory; NAS: National Academy of Sciences; NIBIB: National Institute of Biomedical Imaging and Bioengineering; NCI: National Cancer Institute; NIST: National Institute of Standards and Technology; NITRD: Networking and Information Technology Research and Development; NNCO: National Nanotechnology Coordination Office; NRC: National Research Council; NSF: National Science Foundation; ORNL: Oak Ridge National Laboratory; SNL: Sandia National Laboratories; WTEC: World Technology Evaluation Center

WTEC Books:

Brain-computer interfaces: An international assessment of research and development trends. Ted Berger (Ed.) Springer, 2008.

Robotics: State of the art and future challenges. George Bekey (Ed.) Imperial College Press, 2008.

Micromanufacturing: International research and development. Kori Ehmann (Ed.) Springer, 2007.

Systems biology: International research and development. Marvin Cassman (Ed.) Springer, 2007.

Nanotechnology: Societal implications. Mihail Roco and William Bainbridge (Eds.) Springer, 2006. Two volumes.

Biosensing: International research and development. J. Shultz (Ed.) Springer, 2006.

Spin electronics. D.D. Awschalom et al. (Eds.) Kluwer Academic Publishers, 2004.

Converging technologies for improving human performance: Nanotechnology, biotechnology, information technology and cognitive science. Mihail Roco and William Brainbridge (Eds.) Kluwer Academic Publishers, 2004.

Tissue engineering research. Larry McIntire (Ed.) Academic Press, 2003.

Applying molecular and materials modeling. Phillip Westmoreland (Ed.) Kluwer Academic Publishers, 2002

Societal implications of nanoscience and nanotechnology. Mihail Roco and William Brainbridge (Eds.) Kluwer Academic Publishers, 2001.

Nanotechnology research directions. M.C. Roco, R.S. Williams, and P. Alivisatos (Eds.) Kluwer Academic Publishers, 1999. Russian version available.

Nanostructure science and technology: R & D status and trends in nanoparticles, nanostructured materials and nanodevices. R.S. Siegel, E. Hu, and M.C. Roco (Eds.) Kluwer Academic Publishers, 2000.

Advanced software applications in Japan. E. Feigenbaum et al. (Eds.) Noyes Data Corporation, 1995.

Flat-panel display technologies. L.E. Tannas, et al. (Eds.) Noyes Publications, 1995.

Satellite communications systems and technology. B.I. Edelson and J.N. Pelton (Eds.) Noyes Publications, 1995.

Other Selected WTEC Panel Reports:

(Imperial College Press will publish first three reports)

Research and development in simulation-based engineering and science (1/2009)

Research and development in catalysis by nanostructured materials (11/2008)

Research and development in rapid vaccine manufacturing (12/2007)

Research and development in carbon nanotube manufacturing and applications (6/2007)

High-end computing research and development in Japan (12/2004)

Additive/subtractive manufacturing research and development in Europe (11/2004)

Microsystems research in Japan (9/2003)

Environmentally benign manufacturing (4/2001)

Wireless technologies and information networks (7/2000)

Japan’s key technology center program (9/1999)

Future of data storage technologies (6/1999)

Digital information organization in Japan (2/1999)

Selected Workshop Reports Published by WTEC:

International assessment of R&D in stem cells for regenerative medicine and tissue engineering (4/2008)

Manufacturing at the nanoscale (2007)

Building electronic function into nanoscale molecular architectures (6/2007)

Infrastructure needs of systems biology (5/2007)

X-Rays and neutrons: Essential tools for nanoscience research (6/2005)

Sensors for environmental observatories (12/2004)

Nanotechnology in space exploration (8/2004)

Nanoscience research for energy needs (3/2004)

Nanoelectronics, nanophotonics, and nanomagnetics (2/2004)

Nanotechnology: Societal implications (12/2003)

Nanobiotechnology (10/2003)

Regional, state, and local initiatives in nanotechnology (9/2003)

Materials by design (6/2003)

Nanotechnology and the environment: Applications and implications (5/2003)

Nanotechnology research directions (1999)

All WTEC reports are available on the Web at http://www.wtec.org.

On the cover, from the lower left to upper right:

1) Example simulated data for the ATLAS detector of the Large Hadron Collider at CERN, http://cdsweb.cern.ch/record/39448?ln=en
2) Nanowire composed of gold atoms undergoing elongation, courtesy of C.R. Iacovella and P.T. Cummings
3) VMD rendering of Actin cytoskeleton-regulatory complex protein SLA1, pdb:3idw; S.M. Di Pietro, et al. *EMBO J*, 2010 DOI:10.1038/emboj.2010.5
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6) NCAR Mesoscale Model Version 5 model of the winds near a hurricane's eye, from NASA Images http://www.nasaimages.org/luna/servlet/detail/NSVS~3~3~8578~108578:A-Hurricane-Model
7) Global climate model, image courtesy of the National Center for Computational Sciences, Oak Ridge National Laboratory.