Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security An Initiative

The objective of this ten-year vision, which is in line with the Department of Energy's Strategic Goals for Scientific Discovery and Innovation, is to focus the computational science experiences gained over the past ten years on the opportunities introduced with exascale computing to revolutionize our approaches to energy, environmental sustainability and security global challenges.

Executive Summary

The past two decades of national investments in computer science and high-performance computing have placed the DOE at the forefront of many areas of science and engineering. This initiative capitalizes on the significant gains in computational science and boldly positions the DOE to attack global challenges through modeling and simulation. The planned petascale computer systems and the potential for exascale systems shortly provide an unprecedented opportunity for science; one that will make it possible to use computation not only as a critical tool along with theory and experiment in understanding the behavior of the fundamental components of nature but also for fundamental discovery and exploration of the behavior of complex systems with billions of components including those involving humans.

Through modeling and simulation, the DOE is well-positioned to build on its demonstrated and widely-recognized leadership in understanding the fundamental components of nature to be a world-leader in understanding how to assemble these components to address the scientific, technical and societal issues associated with energy, ecology and security on a global scale. For these types of problems, the time-honored, or subsystems, approach in which the forces and the physical environments of a phenomenon are analyzed, is approaching a state of diminishing returns. The approach for the future must be systems based and simulation programs are developed in the context of encoding all known relevant physical laws with engineering practices, production, utilization, distribution and environmental factors.
This new approach will

- *Integrate, not reduce***.** The full suite of physical, chemical, biological, chemical and engineering processes in the context of existing infrastructures and human behavior will be dynamically and realistically linked, rather than focusing on more detailed understanding of smaller and smaller components.

- *Leverage the interdisciplinary approach to computational sciences***.** Current algorithms, approaches and levels of understanding may not be adequate. A key challenge in development of these models will be the creation of a framework and semantics for model interaction that allow the interconnection of discipline models with observational data. At the outset, specialized scientific groups will team with engineers, business experts, ecologists and human behavior specialists to create comprehensive models that incorporate all known phenomena and have the capability to simulate systems characteristics under the full range of uncertainties.

- *Capitalize on developments in data management and validation of ultra-large datasets.* It will develop new approaches to data management, visualization and analysis that can treat the scale and complexity of the data and provide the insight needed for validation of the computations.

This new approach will enable DOE to exploit recent developments in commercially available computer architectures, driven by the implementation of first generation multi-core processors and the introduction of petascale computers within 18 months, and prepare it to take advantage of exascale computers in the next decade. This approach will also guarantee DOE's leadership in applying these computers to critical problems confronting the nation.

Programmatic themes:
The initiative is organized around the following four programmatic themes:

1. **Engage** top scientists and engineers, computer scientists and applied mathematicians in the country to develop the science of complexity as well as new science driven computer architectures and algorithms that will be energy efficient, extremely scalable, and tied to the needs of scientific computing at all scales. Correspondingly, recruit and develop the next generation of computational and mathematical scientists.

2. **Invest** in pioneering large-scale science, modeling and simulation that contribute to advancing energy, ecology and global security.

3. **Develop** scalable analysis algorithms, data systems and storage architectures needed to accelerate discovery from large-scale experiments and enable verification and validation of the results of the pioneering applications. Additionally, develop visualization and data management systems to manage the output of large-scale computational science runs and in new ways to integrate data analysis with modeling and simulation.

4. **Accelerate** the build-out and future development of the DOE open computing facilities to realize the large-scale systems-level science required to advance the energy, ecology and global security program. Develop an integrated network computing environment that couples these facilities to each other, to other large-scale national user facilities and to the emerging international network of high-performance computing systems and facilities.

The success of this fourth effort is built on the first 3 themes because exascale systems are, by themselves, among the most complex systems ever engineered.

Critical Challenges:
This initiative will enable DOE to address critical challenges in areas such as:

Energy- Ensuring global sustainability requires reliable and affordable pathways to low-carbon energy production, e.g. bio-fuels, fusion and fission, and distribution on a massive scale. The existing mix of energy supplies places global security at great risk. Acceptable solutions require rapid and unprecedented scientific and technologic advances. Unfortunately, existing analytical, predictive, control, and design capabilities will not scale. An objective of this initiative is to provide new models and computational tools with the functionality needed to discover and develop complex processes inherent in a new energy economy.

Ecological Sustainability- The effort toward sustainability involves characterizing the conditions for balance in the climate system. In particular, sustainable futures involve understanding and managing the balance of chemicals in the atmosphere and ocean. The ability to fit energy production and industrial emissions within balanced global climate and chemical cycles is the major scientific and technical challenge for this century.

Security- The internet, as well as the instrumentation and control systems for the energy infrastructure, are central to the well-being of our society. There are several potential opportunities relating to accurately modeling these complex systems: understand operational data, identify anomalous behavior to isolate the disturbance and automatically repair any damage.

Introduction

Five years ago, a petascale computing platform seemed beyond our reach. The Earth Simulator in Yokahama, Japan, began operations in the spring of 2002 with a peak speed of 42 teraflops, the fastest in the world, at an enormous cost and complexity. It took the U.S. nearly two years to catch up, both in peak speeds and efficiency and by 2009 scientists, under the auspices of a competitive program, will have access to a one petaflop Cray Baker system at the Leadership Computing Facility at Oak Ridge. Through an accelerated program, we anticipate computers utilizing massive multi-core chips to achieve peak speeds 1,000 times a petaflop, or in these units, an exaflop speed within the next decade as evidenced in the following roadmap:

2008/2009 ⇦ The first petaflop computing resource for open science installed at Leadership Computing Facility at Oak Ridge National Laboratory.

2010/2011 ⇦ 10-25 peak petaflop resources available as a result of DARPA High Productivity Computers Systems (HPCS) program and IBM-LLNL-ANL Blue Gene/PQ research contract.

2011/2012 ⇦ 100-250 peak petaflop systems based on a variety of architectures: multi-core, graphics processor, field programmable gate array, multi-threading, cell processor, etc. Heterogeneous, adaptable systems likely.

2013/2015 ⇦ 500-1000 peak petaflop systems. Possible new architectures including processor-in-memory

Computers at such extreme scales will possess large numbers of processors and an inherent complexity that is a function of both the number of processors and how the processors are interconnected. Past experience has shown that additional system complexity greatly increases the number of unforeseen hardware and integration challenges associated with installing, managing, and using a machines. Experience has also repeatedly demonstrated that each power of two increases in the number of processors reveals unexpected system software behavior.

To exploit this level of parallelism, we must dramatically increase the development infrastructure that will enable writing parallel applications. The majority of scientific applications will need to be scaled to 1,000-node (100,000-CPU) scale, and many of the grand challenge applications to the 10,000-node (1,000,000 CPU) scale. Future leadership applications will need to target the 100,000-node goal and 10,000,000 CPU scale. The current programming paradigms and methodologies will have little chance of achieving such scales. New programming models, advanced system software, and new algorithms will be needed to enable high performance at the application level. At these scales, the entire ecosystem has to be considered and designed as an integral part of the system. This will likely involve a shift from current static approaches to application development and execution to a combination of new software, algorithms and dynamically adaptive method.

We are proposing a strategic initiative to capitalize on the revolutionary opportunities presented by high performance computing systems operating at these extreme scales. As envisioned, this intiative will (a) drive computational sciences to the new domain of complex systems modeling and simulation; (b) foster development of computer architectures that can be exploited for complex sytems simulations; and (c) dynamically integrate mathematics, computer science, computer architectures, network performance, cybersecurity, and application software to establish the computational tapestry needed to attack complex problems at unprecedented scale. Our challenge is to extend the significant gains that the Department of Energy has made in computational science capabilities over the past decade, to increase the breadth of engagement and sustain the U. S. leadership position in technical computing capabilities, systems software, computational science and large-scale computational user facilities.

Initiative Description

The answers to fundamental questions about health, energy security, and the nature of the universe are subtly hidden in the enormous quantities of data generated by large scale simulations and experiments. Scientists and engineers must be able to create the simulations and run them in novel ways on extreme-scale computers, find the key information in the volumes of data generated, and use it to discover fundamental principles that can be used to solve national issues in both validation and application.

This program will push interdisciplinary partnerships beyond traditional models and simulations and focus on the creation of a highly integrated, time-dependent modeling system that encompasses detailed micro-economic models and data in a comprehensive global equilibrium framework. This system will allow for a treatment of the marketplace and all participants, including producers, consumers, and intermediaries, with unprecedented accuracy. It will also allow for the quantitative study of important questions such as the following:

- How will different policy alternatives affect energy supply and demand, the overall economy, the environment, demand for individual products and services, public health, and the vulnerability of the U.S. economy and infrastructure?
- How are answers to these questions influenced by trends such as exurbanization, immigration, outsourcing, modernization in Asia, climate change, behavioral shifts, and increased focus on corporate governance?
- How will the success of potential solutions be affected by technical vs. other factors such as government policy and obstacles to entry for new providers?

These flagship applications will be of real benefit to the government and society. Simulation may be used to inform policy development in the area of emergency planning, health system improvement, management of climate change, and so forth. The development of predictive power in validated models connected to real-time data will provide economic value to businesses that must respond to rapid changes in the operating environment, such as airlines, power companies, and emergency management operations.

To address these issues, this initiative will focus on four broad themes : **Engage** top scientists and engineers, computer scientists and applied mathematicians in the country; **Invest** in pioneering, large-scale science, modeling and simulation; **Develop** scalable analysis algorithms, data systems and storage architectures; and accelerate the build-out and future development of DOE open computing facilities.

Theme 1: Engage an interdisciplinary community

For this project to succeed, we must identify a cadre of computational scientists who can think about the problems in their field in an appropriately computational fashion and are fearless about adopting new technologies. These interdisciplinary teams comprised of county's top scientists and engineers, hardware architects, computer scientists and applied mathematicians must all be engaged from the beginning of the initiative to realize the promise of extreme scale computing. Additionally, proposed activities include the modeling of human behaviors which represents a significant departure from the current practice in traditional computational science communities. Thus, we need to identify sufficient expertise in economics and related disciplines to develop meaningful, efficient, and credible models.

These pioneering interdisciplinary teams will need to:

- Construct a comprehensive suite of models of unprecedented accuracy: some based on existing codes, some entirely new, that successfully bridge the gap to the advanced models used extensively to understand the production, conversion, and consumption of energy products and to study regional and global trends in energy supply, energy demand, and greenhouse gas emissions that are characterized by relatively coarse geographical and temporal resolution and run primary on PCs.
- Undertake basic research into such foundational issues as spatial statistics, modeling of social processes, and relevant micro-economic and scientific coupling issues.
- Assemble and assure the quality control of extensive data collections – much from existing sources, but also from new and unconventional sources.
- Provide a comprehensive and detailed validation of both individual models and model systems.
- Develop novel, robust numerical techniques and high-performance computing approaches to deal with the expected orders-of-magnitude increase in model complexity.
- Study a wide range of applications.

Additionally, direct investments are also needed in the recruitment and development of the next generation of applied mathematics, computer scientists and computational scientists including computational economists. Funding is proposed for new programs at the intersection of mathematics and computer science that would investigate the use of new algorithms for the emerging disciplines related to understanding emergent behavior. Complementary to this effort is the creation of long-term basic research programs at U. S. computer science departments to advance research in algorithms, systems software and computing tools, including multi-core technology with thousands of cores per chip.

Theme 2: Invest in pioneering, large-scale science

Direct support for "leading edge science applications" willing to take on the risks of working with new and emerging languages and tools is an integral initiative component. These pioneer applications will be involved in large-scale science, modeling and simulation that contribute to advancing energy, ecology and global security. Representative examples of such investigations include:

- Improve our understanding of complex biogeochemical (C, N, P, etc.) cycles that underpin global ecosystems functions and control the sustainability of life on Earth. This work will form the foundation to create integrated modeling environments that couple the wealth of observational data and complex models to economic, energy, and resources models that incorporate the human dynamic into large-scale global change analysis. (see Appendix 1)
- Develop and optimize new pathways for renewable energy production and development of long-term secure nuclear energy sources, through computational sciences and physics-based engineering models. (see Appendix 2)
- Enhance our understanding of the roles and functions carried out by microbial life on Earth, and adapt these capabilities for human user, through bioinformatics and computational biology. (see Appendix 3)
- Develop a "cosmic simulator" capability that integrates increasingly complex astrophysical measurements with simulations of growth and evolution of structure in the universe, linking the known laws of microphysics to the macro world. (see Appendix 4)

Several developments in computer science suggest a future paradigm for computational science that is significantly different from the general approach and has the potential to model highly complex systems. In the traditional approach, the forces and physical environment of a phenomenon are analyzed, and then a simulation program is devised that encodes the known relevant physical laws and environmental factors. The pioneering applications will have to not only enable unprecedented precision in our understanding of these micro systems but also enable us to understand the new phenomena that occur when many of these micro systems are linked together. This transition is in many ways like the transition in the 1950s in fusion physics when it became clear that an approach based on the dynamics of single particles was no longer useful and plasma physics emerged as the study of a new state of matter.

Emergent structures have been noted in many natural phenomena, ranging from very large scale phenomena (such as the formation of hurricanes as tropical air passes over heated ocean water) to microscale phenomena (such as the formation of snowflakes as water droplets fall through a subfreezing atmospheric level). The behavior of financial markets is an example of emergence in the field of economics. Investors have knowledge of only a limited number of companies within their portfolio and must follow the regulatory rules of the market, yet their collective behavior determines the fate of national and international economies.

Agent-based modeling is a computational approach that attempts to directly simulate emergent phenomenon by engaging a large number of relatively independent tasks, each of which encodes only a fairly simple set of laws. These schemes attempt to model a complex large-scale phenomenon such as turbulent airflow as an ensemble of millions of very simple entities, which interact only locally and nearest neighbors according to very simple rules. In spite of the low-level rules, the computational ensemble (if constructed properly) exhibits behavior that mimics the real phenomena in convincing detail. Agent-based methods, including cellular automata schemes, tend to be computationally expensive. Fortunately, these schemes are well suited for highly parallel computer systems because they involve literally millions or billions of independent agents that interact exclusively (or at least predominately) with their nearest neighbors.

"Evolutionary computing" refers to the paradigm where the process of biological evolution is mimicked to find an optimal solution or configuration. The most common evolutionary approach is to define a fitness function, which determines overall "goodness" of a potential solution, and then to initiate a population of agents each of which encodes the key details of the design parameters. The control program evaluates all members of the population and identifies a certain fraction as achieving higher-than-average scores. These high-scoring members are then allowed to "mate" with other high-scoring members, in a process that involves some random "mutations." This new population is then scored, and the cycle repeats itself thousands of times. Evolutionary schemes tend to require large amounts of computer time and have weak convergence properties. However, such problems are well suited for very highly parallel computation because every member of the evolving population set can be tested for fitness independently of the others. There are some details that must be attended to in such parallel implementations, but overall the parallel approach has been successful to date

Theme 3: Develop new algorithms, data systems and storage architectures

Future architectures will offer new and different hardware characteristics to achieve high peak performance. However, as systems become more complex, there is a corresponding increase in the number of unforeseen hardware and integration challenges associated with installing, managing, and using these machines. Experience has also repeatedly demonstrated that each power of two increases in the number of processors reveals unexpected system software behavior.

To accelerate development, we must focus investments on the major software, algorithm, and data challenges and build on newly emerging programming environments to develop the infrastructure that will allow applications to scale up to the required levels of parallelism and integrate technologies into complex coupled systems for real-world multidisciplinary modeling and simulation. This will likely involve a shift from current static approaches to application development and execution to a combination of new software tools, algorithms and dynamically adaptive methods. For example, today's software is largely message-passing (MPI) based, with some global view techniques such as Unified Parallel C (UPC) and Co-Array Fortran (CAF). In order to facilitate the utilization of the extreme scale resources, a new "hybrid" programming model must be explored similar to the project initiated by the DARPA High Productivity Computer Systems (HPCS) program. Additionally, we must bring together new developments in system software, data management, analysis, and visualization to allow disparate data sources (both simulation and real-world) to be managed in order to guide research and to directly advance science.

Today algorithms exist for analyzing terabytes of static data stored in a single location, but very few analysis algorithms currently can handle a dynamic data set that is distributed across sites or streamed in live. Feature detection is primitive or nonexistent in many science domains. Human interaction through visualization is today's norm. Major challenges exist in handling the expected data tsunami include dealing with the volume, different formats, transfer rates, analysis, and visualization of massive distributed data sets. In addition, the difference in the rate of increase of performance in computer technology such as memory and processors and storage technology such as magnetic disk and tape will result in the need to achieve unprecedented levels of parallelism to enable the storage systems to keep up with the computers.

Further, a recent workshop held in December, 2006 on Mathematical Research Challenges in Optimization of Complex Systems articulated the challenges presented by modeling complex systems as:

- Effective modeling of heterogeneous, coupled human-made systems with nonlinear interactions that include system components with multiple time and length scales, interacting through complicated feedback mechanisms.
- Analysis and algorithms for a variety of optimization problems involving large systems with a mixture of continuous and discrete variables
- Methods for analyzing and responding to sensitivity in highly nonlinear systems
- Statistical approaches for validating and improving mathematical models of non-physical systems with a limited number of observed data
- Techniques for integrating computational models with real-time data to support decision-making and adaptive control
- Careful analysis of how risk should be incorporated into complex systems models. Risk and uncertainties come from many sources, including economic, social, political, technological and behavior.

Theme 4: Accelerate the build-out of DOE computing facilities for open science.
According to the roadmap, by 2015, interdisciplinary teams may have access to exascale computing resources. To complement the software and application development efforts, we propose to continue the build-out DOE computing facilities for open science. We must invest in truly innovative hardware and commit to building and experimenting with small-scale prototypes for node architecture changes and massively parallel systems for scaling studies. We will continue to invest in research projects partnerships comprised of labs, universities, and end users along with the vendors who will serve be the primary developer.

Challenges include:

- Dealing with future architectures that offer significant flexibility to tailor system characteristics to specific application needs. This will entail strong hardware and software coordination.
- Finding the optimal point between fully general and fully specialized in hardware, software, and algorithms. This technique has proven itself already in many cases.
- Maintaining sufficient system balance to meet application needs. These factors include bandwidth and latency to memory, bandwidth and latency between nodes, bandwidth and latency to storage, memory per node and total memory per system. For example, in order to achieve sustained performance in the 10-20% range on applications such as computational fluid dynamics (direct numerical simulation), high energy physics (quantum chromodynamics), and computational biology (molecular dynamics), our in-depth understanding of today's algorithmic and subsequent communication requirements drive a system balance requiring of the order of 150 GB/s of injection bandwidth, order of 1.5 PB/s global bandwidth, and order of 500 ns latency. These drive the technology requirements in the areas of processor, interconnect, I/O, and storage design. The applications will also require 0.5-2 bytes/flop of memory bandwidth, and we should assume at least 2-4 GB of memory per CPU core.

- Designing future storage architectures as an integral part of the overall system. Currently I/O is an afterthought, which is then “bolted” onto a system. The bandwidth requirements for systems of this size will prohibit this behavior in the future. Efforts to address these issues are already under way, including development of new storage semantics that enable high performance and scalability, the integration of database concepts (relational and object models) into the notions of filesystems and storage models, and the development of effective associative access methods for integrated memory/data systems.

The success of the fourth theme is built on the first 3 themes since exascale systems are, by themselves, among the most complex systems ever engineered.

The improvement in the ability to broadly develop applications for extreme scale parallel systems will have an overall boosting effect to the U.S. software development enterprise, which is currently the most productive by far. It would also help to provide a high-value trajectory for U.S. software development as the lower-value elements are more easily migrated offshore. This would reaffirm the lead once held by the United States in many technological areas where we are no longer considered a competitor.

Appendix 1

Goal: Improve our understanding of complex biogeochemical (C, N, P, etc.) cycles that underpin global ecosystems functions and control the sustainability of life on Earth. This work will form the foundation to create integrated modeling environments that couple the wealth of observational data and complex models to economic, energy, and resources models that incorporate the human dynamic into large-scale global change analysis.

The ability to fit energy production and industrial emissions within balanced global climate and chemical cycles is the major scientific and technical challenge of this century. The effort toward sustainability involves characterizing the conditions for balance in the climate system and in particular, understanding and managing the balance of chemicals in the atmosphere and ocean. Many other aspects of climate change response are strongly influenced by human actors, who will ultimately determine, for example, how supply and demand evolve over time and how and when different mitigation or adaptation solutions are deployed and applied. Only by including these human responses in our climate models can we understand the likely impacts of different technical and policy solutions, and thus how to sustain a prosperous and secure society.

1. What (in broad brush) is feasible or plausible to accomplish in 5-10 years?
Within the next five to ten years, the global modeling framework will be expanded to include biogeochemical cycles of carbon, nitrogen, sulfur, and other chemical species that affect air quality and impact terrestrial ecosystems. By introducing more physically grounded parameterizations at the scales available for modeling on exaflop computers, researchers will be able to couple the biology and chemistry of the planet with physical climate system in a simulation framework.

2. What are the major challenges in the area?
The past decade has seen considerable advances in understanding of important geophysical elements of the climate system, as well as in the micro- and macro-economics, data, modeling methods, and high-performance computing methods required to tackle climate economics. Thus, the building blocks required to undertake this program exist. However, the program will involve a massive, multiple-order-of-magnitude scaleup with major challenges remain including the following.

- Interaction of ecosystems on the global scale with increasing temperatures and increased incidence of extreme events requires advances in modeling techniques and incorporation of complex biogeochemical cycles to gain a predictive understanding of the carbon-climate coupling.

- Cloud physics must be refined to the microscale in order to advance our understanding of this fundamental area of atmospheric science. Several of the long-term observational programs such as the Atmospheric Radiation Measurement Program are starting to have a profound impact on climate science. A new effort to integrate data frameworks for evaluation and improvement of the models into the development process can be expected to yield significant scientific advances. This effort requires advanced data techniques and use of new Earth observations to correctly identify our role in the cycles of carbon, nitrogen, dust, vegetation growth, ocean ecosystem activity, and carbon uptake.

- Characterizing the internal and forced modes of variability of the climate system in their coupling with human-induced forcing, such as the loading of atmospheric greenhouse gases and changing patterns of land use through deforestation, is only partially complete. Improving predictive skill of climate models so that these can be used to explain natural events ,such as extreme seasons and predict near-term likelihoods for adaptation strategies will be important for policy makers. Enhancing the physical basis of climate prediction at the regional scales must go hand in hand with this modeling of the chemical cycles. Correcting physical biases in the climate models to improve internal modes of variability and the balance of processes must be joined with systematic study of the forced modes of the climate system; such an effort will require an increase in resolution for the orographic forcing, as well as advanced grid structures to resolve the moist processes and nonlinear interactions at scales of extreme events such as hurricanes and cyclones. This should be the focus of adaptation efforts to judge probabilities for certain impacts such as the melting of the polar caps.

- Essential for the goal of long-term sustainability is developing greater understanding of equilibrium climate configurations so that mitigation strategies and technology choices can have maximum effectiveness. On the fundamental research side, the location of carbon sources and sinks and the detailed processes in between must be quantified. Aerosol dynamics in the climate system will eliminate a major source of uncertainty in climate change prediction. These advances, together with the enabling mathematical and computer science research that yields improved numerical methods for exaflop computers, will provide a firm foundation for the science of climate prediction.

- Ocean and ice modeling must be improved to correctly identify the likelihood of abrupt climate shifts and alternative stable equilibrium states of the climate system that may be encountered in a greenhouse-warmed world. Mitigation studies should seek to identify possible sustainable climate states and begin mitigation efforts to steer in the right direction.

- Modeling the human response to climate change is a multidimensional, time-dependent problem that encompasses economic relationships between supply and demand; individual choices concerning energy use, energy sources, and occupation; and government policies. It is a multiscale problem, both temporally and spatially. It is a global problem – the strong economic and environmental coupling between different regions means that we cannot study any single region in isolation. Moreover, while vast quantities of relevant data are now available, for instance from satellite imagery, much other relevant data is proprietary or of unknown quality.

3. How would we accelerate development with E^3SGS?

In order to accelerate the development processes, a two-pronged research and development program should be pursued, aimed at adaptation strategies for the near-term effects of climate change, together with a long-term emphasis on mitigation of future climate change through better understanding of the fundamental factors affecting the climate and development of a systematic theory for understanding the uncertainties in the models and experimental data to support game theoretic approaches to mitigation strategies.

A better pipeline of advanced students and young researchers on the development teams is needed; these students need familiarity with the use of supercomputers for computational science investigations and a clear view of the changes to scientific computing methodologies that will result from exascale computers. Advanced computer resources must be readily available to the application development teams. Since analysis tools and better integration of new numerical technologies will play an important role in accelerating the state of the art, a means to incorporate these elements and integrate the development teams with the best research is also needed.

4. What are expected outcomes and impact of acceleration or increased investment (i.e., what problems would we aim to solve or events we would cause to occur)?

The expected outcome of this effort is the ability to ground energy policy with sound carbon-climate science. The discovery of fundamental modes of variability in the coupled climate system will be a hallmark, just as the successful prediction of the ENSO was when ocean and atmosphere coupling was understood. The modes of variability with coupled ocean and biosphere are likely much longer, on the multicentury timescale. Discovering these modes will be of great importance in defining what sustainability means for civilization.

Further, the latest methods in economics, quantitative techniques in behavior and decision theory will be coupled with the development of the expanded global modeling framework to develop a deeper understanding of the technical, economic, political and social issues that underpin the global environmental change challenge,

Appendix 2

Goal: Develop and optimize pathways for renewable energy production and develop secure nuclear energy sources, through computational science and physics-based engineering models.

Ensuring global sustainability requires approaches to energy production with a low- to zero-carbon footprint that are reliable and affordable. The existing suite of energy supplies places global security and prosperity at great risk. Acceptable solutions require rapid and unprecedented scientific and technological advances. Existing analytical, predictive, control, and design capabilities are not up to this task. Clearly needed is a new generation of models and tools that have the functional depth and level of integration across the spatial, temporal, and disciplinary spectra required to discover and develop complex processes inherent in a new generation of energy solutions.

1. What (in broad brush) is feasible or plausible to accomplish in 5-10 years?
Research is being initiated to develop new pathways to fuel and electricity supplies, with major efforts focused on advanced photovoltaic systems, cellulosic biofuels, hydrogen, and advanced nuclear fuel cycles. In the next 5-10 years, an entirely new set of modeling and simulation code development is possible, especially with respect to the performance of nanotechnology building blocks, and by the end of the 10-year period, nanodevice performance with exascale simulation. New classes of biofuels simulation systems should also be possible, including the simulation of plant feedstock performance enhancements, the deconstruction of feedstocks, and new enzymatic pathways for fuels synthesis. In modeling the nuclear fuel cycle, traditional "lumped parameter" models based on empirically calibrated formulas will be replaced by much more fundamental physics simulation. Ultimately, these advances will dramatically reduce the cost and increase the safety of all aspects of the fuel cycle – plant licensing, testing novel design concepts, qualification of new fuels, and so on.

Computational science can revolutionize many renewable energy techniques, from solar photovoltaic cells to photochemical cells that use sunlight to generate chemical fuels. The development of an advanced computational scientific simulation capability could be used to rapidly design more efficient, cost-effective, and innovative solar cells at the nanoscale. Through multi-scale mathematics and algorithms the nanoscale components can be numerically "assembled" and analyzed as a full scale system. With such a capability, several exciting possibilities arise. We could simulate the entire optical-electronic process: from the absorption of sunlight (photon), to the generation of the electron-hole pairs (exciton), to the deassociation of the exciton, to the carrier transport, and finally to the carriers being collected by the electrodes. Advances in mathematical models and algorithms could also transform the field of *ab initio* calculations. For example, insurface passivation, reconstruction, and growth could be simulated directly by using linear-scaling *ab initio* methods. If exascale computing facilities were available, the carrier dynamics could be simulated in conjunction with the atomic dynamics, thus providing an important coupling between these two systems.

2. What are the major challenges in the area?

Computational Science for Revolutionary Photovoltaics

The nation is challenged to develop photovoltaic devices of unprecedented efficiency—greater than 50%, and made from low-cost materials such as self-assembling inorganic or hybrid systems. Optoelectronic properties can be dramatically altered at the nanoscale. For example, the band gap in silicon can be blueshifted from the infrared to the optical region. Exascale computing provides the opportunity to understand and control the complex behavior of such properties at production scale.

Biofuels

Biofuels require an integrated microbial genome database, including the genomes of hundreds of energy-related plants and microbes. Currently, however, genomic analyses are confined to genome structural and functional comparisons. Integration with gene expression and structural biology models is a critical step to developing future biofuels. In addition, efficient large scale processes must be discovered to enable the production of significant amounts of biofuels. There are significant basic research challenges in our understanding of the scalability of production processes as well as evaluations of possible waste streams.

Advanced Nuclear Energy Systems

Experimental research and simulation in support of alternative nuclear fuel cycles has greatly lagged behind the development of multidimensional modeling based on leadership computing capabilities and modern computational science. Central to a sustainable future for nuclear energy is the development of computer modeling and simulation tools for the analysis of all phases of the nuclear power cycle, from fuel fabrication and reactor design, to performance, safety analysis, and waste disposal. A number of areas in computational mathematics and computational science are key to addressing major aspects of the simulation process:

- **Fluid dynamics for multicomponent fluids in complex geometries.** This problem arises in the simulation of the reactor core, in heat and mass transport in the drift tunnels in which nuclear waste is to be stored, and in the macroscale design of separations systems. This area includes the analysis of low-Mach number limits for multicomponent and multiphase fluid mixtures and the design of high-resolution and adaptive discretization methods using cut-cell representations of the geometry.

- **Neutron transport.** Neutron transport is a critical component of the physics in a reactor core. Neutron transport problems are represented by an integro-differential equation in six-dimensional phase space (plus time). The development of S_n and P_n deterministic methods on both structured and unstructured grids with adaptive mesh refinement is ideal for such problems, as well as the use of volume-of-fluid methods for representing the jump relations at interfaces between different materials. Monte Carlo methods are also likely to play a key role in establishing benchmark standards for more idealized (e.g., smaller-geometry) problems.

- **Subsurface flow modeling.** The long-time impact of storing nuclear wastes depends on the transport of contaminants through the soil and rock adjacent to the storage site. Typically, these processes are modeled by porous media equations for multiphase mixtures of contaminants and water. Integrated models do not exist.

- **Full Lifecycle Models.** In addition to these single component models a full lifecycle model of nuclear power must be developed to enable evaluation of the security, energy, and waste disposal challenges associated with different options.

A key aspect of a modern set of nuclear design and analysis tools is a framework-based approach that brings together all code components under one computational umbrella. This approach would enable scientists, reactor designers, and safety analysts who will utilize these codes to map a strategy for common input and output data files, common language interfaces, and common algorithms.

3. How would we accelerate development with E^3SGS ?

Funding research to develop novel algorithms that scale all known relevant physical phenomena from nano-dimensions (i.e. electron-hole transport) to engineered-scale systems will accelerate the discovery-demonstration-implementation cycle. Scientists will be in a position to develop higher-fidelity simulations that could in turn be used within a design cycles to rapidly predict, for example, new solar cells, new biofuels, and alternate nuclear fuel cycles.

4. What are expected outcomes and impact of acceleration or increased investment (i.e. what problems would we aim to solve or events we would cause to occur)?

Increased investment enables the full examination of novel energy production methods, spanning engineering trade-offs, as wells as ecological and societal impacts. Designing solar devices in the range of 50 percent conversion efficiency becomes possible. Smaller investments, yielding 10- or 100-fold increases do not achieve the scale of integration necessary to produce useful results.

Appendix 3

Goal: Enhance our understanding of the roles and functions carried out by microbial life on Earth, and adapt these capabilities for human use, through computational biology

1. What (in broad brush) is feasible or plausible to accomplish in 5-10 years?
An ambitious goal in systems biology is the development of validated capabilities for simulating cells as spatially extended mechanical and chemical systems in a way that accurately represents processes such as cell growth, metabolism, locomotion, and sensing. Two developments render such an effort feasible and timely. The first is the development of first principles-based algorithmic approaches to fully represent the complex spatially heterogeneous, multiscale, and multiphysics processes characteristic of these problems. The second is the wealth of new experimental techniques that can provide the basis for validating the models, including high-throughput methods for acquiring genomics and proteomics data, and high-resolution imaging techniques that can, for example, track the locations of individual molecules in a cell. In fact, the development of simulation models could provide a theoretical framework that will transform these massive data streams into useful scientific insight.

Soon we will be able to sequence representatives of all the culturable prokaryotic species. We could then use these sequences to identify potentially novel proteins and to begin to develop a "universal set" of protein families that will enable us to develop a roadmap for discovering novel biological catalysts. This "universal set" of protein families could be characterized by high-throughput experimental and computational pipelines for discovery of new functions.

In other areas of computational biology, we expect to sequence representatives of most of the known phylogenetic groupings in the single-celled eukaryotes. From these we could develop detailed metabolic reconstructions for their genomes, and begin to develop metabolic reconstructions of microbial communities enabling the linkages of biological activity to the global geochemical cycles. This could advance flux-based modeling to the point where most of the data component of the model are known for most of the genomes. This will allow any group wishing to model a genome to invest significantly less time to achieve a complete representation.

An important element will be to continue to determine which aspects of the complex eukaryotic cells can be mapped to unicellular counterparts. Minimal versions of regulatory mechanisms ranging from control of regulation to proteosome and cell-differentiation could be determined (i.e., the components identified), and work on characterization will interact with what will be done on the complex eukaryotes to inform computational models of critical functions.

We also expect during this time period to be able to characterize microbial populations in many contexts, ranging from complex eukaryotic hosts to extreme environments. This information will be critical to enable computational models to bridge laboratory and field data.

2. What are the major challenges?
Current modeling and simulation capabilities used for self-assembly in molecular biology rely heavily on coarse-grained techniques and empirical approximations for particle-particle interactions. They are also limited in the length of the simulation, which does not capture the

long-time scales of the self-assembly process. Thus, modeling and simulation often provide only a glimpse and a narrow local view of the whole process. With increased investments in mathematics, algorithms, and large-scale computing facilities, we could remove the empirical approximations from the particle-particle interactions, leading to more accurate, reliable, and robust simulations. We could also be able to simulate an entire self-assembly process leading to new scientific insights and discoveries. Combining the higher-fidelity simulations and the longer-time simulations, we might even be able to explore the parameter space (temperature, pressure, different connection and surface capping molecules, etc.) or even use optimization procedures to design new structures with desired properties.

In the area of systems biology, a major challenge is the current lack of practical first-principles models. In principle, systems biology is described by the fundamental laws of physics and chemistry. In practice, the complexity of that level of description (e.g., molecules with hundreds of thousands of atoms) makes its direct use prohibitively expensive. There are as yet no general macroscopic descriptions of cellular dynamics. In addition, because almost nothing can be measured directly, it is necessary to develop cost-effective methods for sensitivity analysis and bifurcation analysis.

Macroscopic complexity is another significant challenge. Mechanically, cells consist of complex combinations of subsystems with varying dimensionalities (point sources and sinks, filaments, membranes, bulk media) each having their own distinct constitutive behavior and mechanisms for transport. Chemical reactions take place at such low concentrations (down to a single molecule for DNA) so that stochastic or hybrid stochastic/deterministic descriptions must be used.

The approach to addressing these two challenges is development of algorithmic and software tools for representing the various macroscopic subsystems, combined with the application of these tools in various combinations to simulate specific problems in systems biology. Both the design of the tools and their application would be done as a collaboration between biologists and mathematicians, with theory and experiments informing the design of models for specific problems and the factorization of the algorithmic tools required into reusable software components. The development of the tools needs to be an ongoing process, as we learn which kinds of macroscopic models provide a robust representation of systems biology across multiple specific problems. For example, we currently have little understanding about how to attack the hybridization of stochastic and deterministic algorithms in a single simulation.

Other major challenges include:

- Getting reasonably accurate sequences of genomes that “cover” most of the diverse taxonomic groupings. Significant computational phylogeny development and real-time data analysis of emerging metagenomes will be important. This is critical and nontrivial.
- Improving the consistency and accuracy of the annotations to accelerate research usage of the data. The development of subsystems that cover almost all of the machinery embodied in these genomes is essential. This will require a much higher level of cooperation between the research community and the teams annotating the genomes than is currently present.

- Advancing modeling to the point where it can produce a steady flow of predictions that are fed into wet-lab operations for functional characterization. We should construct a growing body of models that are continuously calibrated against the growing body of phenotypic data.
- Addressing a growing body of biotechnology applications, many of which will not be predictable (at least, that has been the experience in computer science):

    - ***Energy***: the identification of new proteins and metabolic pathways that can be the starting point for engineering biocatalysis for biofuels is widely recognized as a major application area. Novel approaches such as biofuel-cells and direct solar conversion to liquid fuels are also interesting.

    - ***Enviromental remediation***: the ability to engineer individual organisms to more effectively transform unwanted compounds to harmless metabolites, as well as the ability to engineering multispecies communities for efficient functional purposes.

    - ***Industrial use of microorganisms***: the ability to produce recipes of mutations that transform wild strains to production strains (for production of fine chemicals, pharmaceuticals and next generation green feedstocks) has become feasible. For it to become widespread, we need to lower the cost of sequencing, and develop complete metabolic and functional models.

3. How would we accelerate development with E^3SGS?
Several steps could be undertaken to accelerate development:

- Produce well-annotated genomes for thousands of single-celled organisms. This part is well understood and based on existing computational tools.

- Develop the computational framework to accelerate modeling and characterization of novel biochemistry. This, too, is becoming well understood.

- Build computational frameworks for maintaining a growing body of “kernel” complete genomes (that are well annotated and maintained) to support characterization of massive amounts of metagenomics data.

- Build a computational environment to drive the large-scale characterization of protein function determination from the kernel databases.

- Characterize the regulons in a growing subset of the kernel genomes. These will need to be coupled to descriptions of “states of the cell” represented by differing types of data (most notably microarray data). We also need to build a library of representative genomes for which the regulons are largely characterized.

- Develop predictive tools to aid in the screening of new genomes for novel protein functions.

4. What are expected outcomes and impact of acceleration or increased investment (i.e. what problems would we aim to solve or events we would cause to occur)?

One expected outcome is development of computational models that correspond with phenotypic data in a set of representative organisms. These will support engineering of industrial strains, characterization of novel biochemistry, and understanding of host-pathogen relationships.

We also anticipate a dramatic acceleration of the global inventory of known microbial protein functions and known microbial interactions and associations, as well as a starting point for connecting genes and genomes to ecosystems.

Another expected outcome is rapid advance in the connection of mechanisms in complex eukaryotes to simpler context, which would accelerate our understanding of these systems.

Appendix 4

Goal: Develop a "cosmic simulator" capability that integrates increasingly complex astrophysical measurements with simulations of the growth and evolution of structure in the universe, linking the known laws of microphysics to the macro world. Develop large-scale, special-purpose computing devices and support breakthroughs in algorithm development to achieve this goal.

1. What (in broad brush) is feasible or plausible to accomplish in 5-10 years?
Astrophysics is undergoing an extraordinary transition from a data-starved to a data-swamped discipline. New technologies are enabling the detection, transmission, storage, and analysis of data of hitherto unimaginable quantity and quality. From maps of the entire microwave sky at unprecedented resolution, to surveys encompassing millions of galaxy redshifts, to a supernova "factory," to the prospect of the first detection of gravity waves, the observational data obtained in the next decade alone will supercede everything accumulated over the preceding 4.000 years of astronomy. These advances will enable us to address a number of the questions in the "Connecting Quarks to Cosmos" report from the National Academies. Examples of the important questions include:

- **What Is Dark Matter?**
- **What Is the Nature of Dark Energy?**
- **How Did the Universe Begin?**
- **Did Einstein Have the Last Word on Gravity?**
- **What Are the Masses of the Neutrinos, and**
- **How Have They Shaped the Evolution of the Universe?**
- **How Do Cosmic Accelerators Work and What Are They Accelerating?**
- **What Are the New States of Matter at Exceedingly High Density and Temperature?**
- **How Were the Elements from Iron to Uranium Made?**

Realizing the full scientific potential of these observations will require correspondingly precise predictions from our theoretical models. Given the physical complexity of the systems involved, obtaining such predictions necessarily requires ever more detailed numerical modeling, which couples more and more individual components with their own length and time scales, and simultaneously generates an equivalent quantity of simulation-data. Computational astrophysics has an essential role to play in providing the point of contact between theory and observation. From the detailed theoretical predictions made possible by complex simulations, to the precise reference points obtained from painstaking analyses of the new observations, the development of astrophysics in the new millennium will be regulated by our computational capability and our ability to develop trusted techniques for validating our models and comparing simulation data to observations.

2. What are the major challenges in the area?
The nearly century-long quest to measure the half dozen or so cosmological parameters that describe the shape, matter-energy contents, and expansion history of our universe has been accomplished. Recent observations of the cosmic microwave background, high redshift supernovae, and galaxy clusters have yielded a concordant set of parameters with a precision of about 10%. The next-generation cosmology experiments will push these measurements to a precision of 1%. At this level systematic uncertainties dominate over the statistical ones, and we

become dependent on simulations to reveal the true nature of the universe. Historically there has been a need to simplify simulated astrophysical systems to make then computationally tractable. The result has been a series of disjoint classes of simulations each dominated by a particular class of physical processes. As the quality and quantity of our observational data increase, these simplifications compromise both the accuracy and the scope of the simulations' predictions, and we are pushed to explore the boundaries between these classes. Likewise we are compelled to improve the veracity of the initial conditions used as input to a simulation and to rigorously test its reliability through the validation of the end state it outputs; both of these needs are also met by coupling simulations across their traditional boundaries. Our understanding of the coupling of these complex systems is in its early stages, as evidenced by the recent discovery that Type Ia supernovas explode asymmetrically. In the past state of the art simulations were required to explore just one component. The promise of being able to do integrated simulations will drive astrophysics in the future, provided we can develop the mathematical and computer science tools to understand and validate the results from these models.

3. How would we accelerate development with E^{3}SGS?

To meet these challenges, we must lay the basis for a "cosmic simulator" – a computational framework within which we can couple individual astrophysical simulations until they span the entire history of the universe. This basis must include the underlying mathematical methods to simulate the coupled systems, validate the results and extract scientific insight from the combined observational and simulation data. The dynamic range in both time and space for typical astrophysical simulations can be enormous – easily spanning 10 to 15 orders of magnitude. In addition, many astrophysical problems involve a broad range of physical processes, from nuclear reactions to general relativity, not all of which can be captured by a single closed set of evolution equations.

4. What are expected outcomes and impact of acceleration or increased investment (i.e. what problems would we aim to solve or events we would cause to occur)?

The ultimate goals of a cosmic simulator program are to provide a science-based story that details the history of the universe and how that history and its products are dependent on the cosmological parameters and basic fundamental physics. The resultant data sets and visualizations of the universe at various epochs will then be directly comparable to observations (see the figure below). The E^{3}SGS program will allow us to build this framework and make the first pass at an end-to-end simulation of the universe.