Scientific Grand Challenges

Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale

May 11-12, 2009 | Washington D.C.

U.S. DEPARTMENT OF ENERGY

Sponsored by:

The Office of Nuclear Energy

The Office of Advanced Scientific Computing Research

Table of Contents

1. Executive Summary 1

2. Introduction 3
   2.1. Focus Areas: 5
   2.2. Panel Proceedings: 6

3. Final Whitepaper - Integrated Performance and Safety Codes Panel 8
   3.1. Introduction 8
   3.2. Striving Toward Predictive Capability in Modeling and Simulation for Nuclear Energy 8
   3.3. Panel Findings, Challenges, and A Summary of Research Priorities 11
   3.4. Conclusions 30

4. Final Whitepaper - Materials Behavior Panel 32
   4.1. Introduction 32
   4.2. Toward Predictive Performance Models 33
   4.3. Priority Research Directions 38
   4.4. Summary 47

5. Final Whitepaper - Verification, Validation and Uncertainty Quantification Panel 49
   5.1. Introduction 49
   5.2. Background on Modeling Nuclear Energy Systems 49
   5.3. An Overview of the Key Elements for Verification and Validation and Uncertainty Quantification 51
   5.4. Key Issues and Challenges in V&V and UQ 56
   5.5. The Treatment of Nonlinear, Coupled, Multi-Scale Physics Systems 57
   5.6. Summary of Recommended VU Research Priorities 62

6. Final Whitepaper - Systems Integration Panel 64
   6.1. Introduction 64
   6.2. A Critical Review of Available Models 68
   6.3. Recommendations: A Path Forward 73
   6.4. Immediate next steps 76

7. Conclusions and Recommendations 77
   7.1. Introduction 77
   7.2. Integrated Performance and Safety Codes Panel: 77
   7.3. Materials Behavior Panel 79
   7.4. Verification, Validation and Uncertainty Quantification Panel 80
   7.5. System Integration Panel: 82
   7.6. Overall Workshop Conclusions: 83

Appendix A: Charge for the Workshop 85

Appendix B: Workshop Agenda 88

Appendix C: Workshop Attendees 90

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On the cover: The IBM Blue Gene/P supercomputer at Argonne National Laboratory. Visualization inset: A 19-pin fuel bundle computed using the large eddy simulation code NEK5000. Image courtesy of Paul Fischer, Argonne National Laboratory.

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1. Executive Summary

On May 11th and 12th, 2009, the Department of Energy's Office of Science and Office of Nuclear Energy held a joint workshop to explore critical science issues related to the use of fission nuclear energy and the role of extreme computing. The purpose of this workshop was to examine how the implementation of a "science-based" approach might improve the way industry and government address nuclear energy technology issues.

The open workshop was attended by over 75 participants, representing 16 American universities, 8 DOE national laboratories, the nuclear and computer industries, and international collaborators (France and Russia). Approximately two thirds of the representatives at the workshop were drawn from the nuclear engineering and nuclear energy community.

The workshop was not intended to address the full range of science issues involved with advanced modeling and simulation nuclear energy systems. Instead, it focused on several areas that are high priorities:

- **Performance Issues Surrounding Integrated Nuclear Energy Systems.** These issues include, but are not restricted to, reactor core and safety simulations, nuclear fuel performance simulations, separations and safeguard simulations, waste forms and repository simulations, and materials simulations.
- **Materials Behavior.** These issues include understanding the behavior of the materials in existing reactors that have been exposed to hostile conditions. This area also considers how to create advanced materials that can be part of future systems. These materials would confer these systems with improved behavior.
- **Verification, Validation, and Uncertainty and Risk Quantification**: This area explores the challenges of verification, validation and uncertainty quantification for the advanced modeling and simulation of fission nuclear energy systems. It examines possible methods to understand the contribution to overall risk quantification of nuclear energy systems.
- **Systems Integration.** The use of modeling and simulation to understand the interactions between complex nuclear systems from the energy source itself up to and including the entire fuel cycle.

Advances in modeling and simulation enabled by the availability of advanced high performance computing systems underlie the potential for progress in each of these topic areas. Previous successes at the Department of Energy illustrate this potential. In recent months, the DOE has introduced petaFLOP/s computers at both Los Alamos and Oak Ridge National Laboratories. These are helping scientists create new levels of understanding of complex systems.

The workshop was organized into a series of panels that focused on the technical issues identified above. Prior to the workshop, whitepapers were prepared to be used as "starting points" for the panel's discussions. During the workshop panelists provided

comments, additions, and suggestions to improve the whitepaper. These were subsequently incorporated into final versions of the white paper that appear in this report.

Each white paper also included important conclusions and recommendations summarized below:

- **Integrated Performance and Safety Codes:** The use of extreme computing is likely to improve the modeling and design of nuclear energy systems significantly. Nuclear energy science and engineering simulations will drive the need for exaFLOP/s-scale, computing power to create robust, predictive simulations that have quantifiable uncertainties. The creation of IPSCs faces considerable technical challenges that range from improvements in software engineering and numerical methods, to the development of more fully-integrated physics models.

- **Material Behaviors:** Materials scientists face a tremendous challenge: to develop transuranic-bearing nuclear fuels, fuel cladding and structural components for advanced nuclear reactors that withstand ultra-high fuel burnups, neutron doses and temperature extremes. Meeting this challenge will require these scientists to push the limits of high performance computational materials modeling.

- **Verification, Validation and Uncertainty Quantification**: For nuclear energy systems, there are two motivations to perfect Verification, Validation and Uncertainty Quantification (VU). The most obvious is to improve the confidence users have in simulations' predictive responses and our understanding of prediction uncertainties in simulations. Additionally, scientists must also perform VU for nuclear energy systems because the U.S. Nuclear Regulatory Commission, the licensing body, requires it. This is based on the premise that an extensive experimental database can provide important insights about system attributes.

- **Systems Integration:** The Systems Integration Whitepaper outlined the weaknesses common to most, if not all, of today's energy system models and underscored the issues we believe are of greatest concern. And yet, having a robust energy system analysis capability is critical to providing sound analysis of important policy decisions. The panel recommends taking a new approach to developing a modeling tool for the U.S. energy system that takes advantage of recent developments in software engineering and computer science.

2. Introduction

On May 11th and 12th, 2009, the Department of Energy's Office of Science and Office of Nuclear Energy held a joint workshop to explore critical science issues related to the use of fission nuclear energy and the role of extreme computing. The purpose of this workshop was to examine how the implementation of a "science-based" approach might improve the way industry and government address nuclear energy technology issues.

The open workshop was attended by over 75 participants, representing 16 American universities, 8 DOE national laboratories, the nuclear and computer industries, and international collaborators (France and Russia). Approximately two thirds of the representatives at the workshop were drawn from the nuclear engineering and nuclear energy community.

This workshop was held in an environment of great concern over our nation's energy future. Over the last several years, energy issues and the energy security of the United States have risen in importance as political and economic issues. Our nation faces a need to ensure its energy security. Although we might define this in many ways, if we consider how it impacts our nation, it encompasses:

- **National Security** – a dependence on unreliable sources that require protection
- **Economic Security** – a need for assured supplies at affordable prices
- **Environmental Security** – obtaining energy in ways that does not harm the environment

Over the last five decades, the U.S. and global nuclear energy industry has demonstrated that nuclear power can be a safe, reliable and a carbon free source of assured supplies of energy. To improve U.S. energy security and to meet prudent greenhouse gas emission goals, our nation might significantly expand its use of nuclear energy, along with renewable sources, carbon dioxide sequestration, and energy conservation.

Nevertheless, safely and reliably expanding our nation's use of nuclear energy poses significant technical challenges. These are associated with the need to:

- Extending the life of existing nuclear reactor plants
- Building and operating new reactors with advanced designs
- Developing innovative uses for nuclear energy (e.g. producing hydrogen)
- Closing the nuclear fuel cycle and responsibly dealing with long term waste

If our nation is to overcome these challenges, we must obtain a greatly improved scientific understanding of the processes involved with nuclear fuels, reactors, safeguarding separations processes, and long term waste disposal sites. To achieve this, we must develop new insights into the basic science of the underlying physical processes and apply them to the physical systems that we need to support actions listed above.

The development of new nuclear energy technologies and their associated analytical tools is an expensive, multi-decadal proposition. We need to embark on program development expeditiously, if we are to meet the needs in a timely way. The questions posed for this workshop are:

1. What are the critical issues that need to be addressed before our nation can accelerate the development and deployment of these new reactors, fuel and fuel cycle technologies?
2. Might advanced modeling and simulation at the extreme scale play a key role?
3. What are the DOE program requirements for developing and implementing the essential tools?

The aim of the workshop was to play a seminal role in understanding the issues and possible solutions.

Over the past decade, the Department of Energy has used advanced modeling and simulation to apply a first principles science-based understanding to large, complex, tightly coupled systems that are as diverse as the operation of nuclear weapons, the behavior of materials in hostile environments, and automobiles' fluid dynamic turbulence.

DOE's hopes for this workshop were to build on this experience as well as the results of three previous workshops held in 2006 on nuclear energy modeling and simulation. These workshops developed recommendations about how DOE might apply this experience to the technical challenges related to an expanded use of nuclear energy.

The goal for this workshop was to identify the scientific and engineering challenges that must be met before our nation might increase the use of nuclear energy systems to improve U.S. energy security. It included a consideration of how advanced modeling and simulation employing extreme computing might contribute to meeting these challenges.

The workshop's participants proposed a series of recommendations to help the Offices of Science and Nuclear Energy consider how extreme computing might reshape their research and development agendas.

The workshop's participants examined how taking a "science-based" approach might speed the development of technologies needed to advance the safe and environmentally conscious use of nuclear energy and contribute to the nation's shift to energy sources that have lower levels of carbon emissions. The participants also considered how such an approach might improve the chances that major improvements in timeliness and creativity could alter the position of nuclear energy in our economy as compared to the traditional "empirical or test-based" approach that was the mainstay of nuclear energy technology development, when the current technologies were developed in the 1960s and 1970s.

The participants also considered how the introduction of advanced modeling and

simulation using extreme levels of computing might promote a shift to a "science-based" approach. They also explored whether advanced computing together with more sophisticated modeling and simulation, plus combined with theory and advanced experimental techniques might create a new, more detailed understanding not only of the end results of physical processes, but also of the processes themselves. Participants also evaluated whether the use of a "science-based" approach might permit scientists to develop technologies faster, thus, increasing the innovation cycle, and at lower cost, thereby reducing the need for time consuming and expensive testing. They also considered whether a "science-based" approach would produce better end results, thus reducing risks and optimizing operations.

The participants' deliberations took into account the fact that most of today's nuclear energy models derive from models that were first developed twenty years ago. At that time, the fastest computers were a million times slower than current high performance computers. Over the last fifteen years, the Department of Energy's Scientific Discovery through Advanced Computing and NNSA Advanced Scientific Computing programs have produced considerable improvements in the utility and fidelity of physical system models through three-dimensional, highly-resolved simulations. These programs have also advanced the frontier for predictive science. An additional goal of this workshop is to define actions to leverage these investments and produce significant advances in the state-of-the art in nuclear energy and fuel cycle system modeling and simulation.

2.1. Focus Areas:

The workshop was not intended to address the full range of science issues involved with nuclear energy systems. Instead, it focused on several areas that are high priorities:

- **Performance Issues Surrounding Integrated Nuclear Energy Systems.** These issues include, but are not restricted to, reactor core and safety simulations, nuclear fuel performance simulations, separations and safeguard simulations, waste forms and repository simulations, and materials simulations.
- **Materials Behavior.** These issues include understanding the behavior of the materials in existing reactors that have been exposed to hostile conditions. This area also considers how to create advanced materials that can be part of future systems. These materials would confer these systems with improved behavior.
- **Verification, Validation, and Uncertainty and Risk Quantification**: This area explores the challenges of verification, validation and uncertainty quantification for the advanced modeling and simulation of fission nuclear energy systems. It examines possible methods to understand the contribution to overall risk quantification of nuclear energy systems.
- **Systems Integration.** The use of modeling and simulation to understand the interactions between complex nuclear systems from the energy source itself up to and including the entire fuel cycle.

Advances in modeling and simulation enabled by the availability of advanced high performance computing systems underlie the potential for progress in each of these topic areas. Previous successes at the Department of Energy illustrate this potential. In recent months, the DOE has introduced petaFLOP/s computers at both Los Alamos and Oak Ridge National Laboratories. These are helping scientists create new levels of understanding of complex systems.

The growth of computing power should continue over the next decade. It is realistic to expect at least exaFLOP/s levels of power. The workshop's recommendations are framed in light of the technical and scientific challenges that might be addressed with such expanded levels of computing power. Also, where appropriate, the workshop considered a range of issues and opportunities related to utilizing exascale[1] computing and evolving exascale architectures and programming models for nuclear energy simulations.

2.2. Panel Proceedings:

To make the most efficient use of people's time at the workshop, a series of whitepapers were written for each panel session. During the workshop, each panel reviewed the whitepapers and used them to launch their discussions. The panels then prepared summary presentations which were presented to the entire workshop. After the workshop, the panels commissioned authors who used the pre-workshop whitepapers as starting points and then added or deleted material to create a product that reflected the panel's conclusions and recommendations.

The following were the charters given for each panel and the questions they were asked to address.

Session	Purpose
1. Integrated Performance and Safety Simulations of Nuclear Energy System	This session will discuss issues that include, but are not restricted to, reactor core and safety, nuclear fuel performance, separations and safeguard, waste forms and repository. Questions for this session will include: • What are the key technological challenges in each area • What are the research priorities for development of key and missing simulation capability for addressing these challenges?
2. Advanced Material Behavior Modeling	This session will discuss the understanding of behavior of the materials in existing reactors that have undergone exposure to hostile conditions. Also, this area will cover the ability to create advanced materials that can be used in future systems with improved behavior properties. Questions for this session will include:

[1] A definition of exascale computing would be helpful here or in the text. [NEED TO FINALIZE]

Session	Purpose
	• What physics is unknown that will be required for the modeling of materials needed for advanced nuclear energy systems? • What research is required into the lower length scale modeling approaches (e.g. molecular dynamics, quantum mechanics) needed for advanced material behavior modeling? • What opportunities will advanced petaFLOP/s and exaFLOP/s systems offer for this element of nuclear energy modeling and simulation?
3. Verification, Validation and Uncertainty Quantification for Nuclear Energy Simulations	This area will discuss the challenges of verification, validation and uncertainty quantification for the advanced modeling and simulation of fission nuclear energy systems. It will explore possible methods for understanding the contribution to overall risk quantification of nuclear energy systems. Questions for this area will include: • What V&V and UQ approaches should be used for nuclear energy systems modeling and simulation? • What research in complex mathematics is needed to deal with the V&V and UQ of simulations operating with millions of lines of code on millions of computing thread? • What experimental capabilities will be needed to support the V&V and UQ of nuclear energy advanced modeling and simulation capabilities? • The role of predictive modeling that is well-validated and underpinned by a robust quality assessment and QU methodology in the NRC licensing process
4. Nuclear Energy System Integration	This session will discuss the use of modeling and simulation to understand the interactions between complex nuclear systems from the energy source itself up to and including the entire fuel cycle. Questions for this area will include: • What are the important nuclear energy systems relationships that will drive the systems analysis? • Are the current generation of system analysis tools sufficient to capture the complexity of nuclear energy and if not, what areas of research are needed? • Will systems analysis require the use of high performance computing systems?

3. Final Whitepaper - Integrated Performance and Safety Codes Panel

3.1. Introduction

Over the next decade, experts anticipate that significant, transformational advances in computing result in at least an order of magnitude increase in the power available to run many scientific applications. This will be a dramatic improvement over previous computing systems. As a result, scientists should be able to solve critical issues that might substantially improve nuclear energy's chances of having a positive impact on our nation's energy future. Before these breakthroughs in performance can occur, however, scientists must create new suites of application codes, Integrated Performance and Safety Codes (IPSCs) that incorporate innovative numerical methods, software engineering, and integrated uncertainty quantification.

Integrated Performance and Safety Codes (IPSCs) encompass nuclear energy's integrated experimental data, state-of-the-art physics models, computer science, computational tools, and engineering experience. Since these codes include a wide range of features, to emerge as a new suite of application tools, they must first overcome a series of technical challenges. Among these are solving scientific unknowns, improving the fidelity of numerical and geometric simulations, developing improved physics models, integrating multiple physics scales and time domains, and advancing software engineering.

A comprehensive review of the challenges and research priorities is beyond the scope of this document. Nevertheless, the IPSC panel of the Nuclear Energy Workshop provided scientists and engineers with an opportunity to discuss relevant issues and exchange ideas about what key research areas they should pursue. Some issues did arise around how to unleash adequate computing horsepower and create new computer science capabilities that might have an impact on the nation's energy agenda.

3.2. Striving Toward Predictive Capability in Modeling and Simulation for Nuclear Energy

There are four main reasons to use nuclear energy simulations: 1) to speed the discovery, design and engineering iteration cycle in order to optimize existing and new nuclear energy applications; 2) to reduce design uncertainties through characterization, understanding, and discovery; 3) to shorten the licensing process; and 4) to reduce construction costs. In accelerating the discovery of new nuclear energy applications and the design and engineering iteration cycle, simulations analyze normal and off-normal operations for fuels, reactors, waste disposal, separation plants, and other related nuclear energy technologies and processes. To find new discoveries, scientists must remove simulation empiricism, combine multiple length-scales and time-scales in single

simulations, and reduce design uncertainties by integrating simulations with validating experiments that in some cases can reduce the need for validating efforts. One aim of these efforts is to demonstrate that high fidelity simulations can depict the behavior of existing generation reactors so accurately that licensing agencies will reduce the time required to license a new facility. This would reduce construction costs and enhance the economic viability of nuclear power. The IPSC panel estimated that if operators used such simulations, they could save at least a 20 percent of their construction costs, or about $3 billion of the $15 billion cost of a large-scale, nuclear plant. Ultimately, simulations should be able to increase operating margins and reduce uncertainty in existing reactors, provide a rapid mechanism for the insertion of new technologies (i.e., fuels) in existing reactors, and create model-based design and licensing procedures for new reactors, repositories, and related nuclear energy technologies.

The move to predictive modeling emphasizes the reduction of uncertainties in simulations. The best way to achieve this is to improve: 1) geometric fidelity (i.e., use 3-D and better coverage of the domain of interest); 2) numerical fidelity (by using finer resolution, higher-order schemes, and/or higher precision schemes); and 3) application performance (i.e., the speed of producing results) and physics fidelity (by resolving scientific unknowns through improved models, for example, using transport instead of diffusion models and large-eddy simulation (LES) instead of k-epsilon, etc). In the area of geometric fidelity, some improvements include predicting how nuclear waste evolves in a geochemical, repository environment or the rate of radionuclide migration in highly-inhomogeneous, geological media. Improvements in numerical fidelity might include better uncertainty quantification methods for models and simulations, as well as the elimination of homogenization. This advance would permit an explicit up-scaling of macro-scale to meso-scale models and computational methods. Improvements in numerical fidelity and speed would allow scientists to model the simulated evolution of pin assembly and deformation in fuels, of detailed peak fuel pin fluxes and temperatures to a 1 percent uncertainty level, of reactor transient conditions with loss of flow, and of the up-scaling of bench-level technologies to the plant level. With improved physics, scientists could predict material thermo-mechanical responses, damage, and, ultimately, failure under extreme conditions in fuels, cladding material, pin assemblies, and reactor vessels, a key objective of any reactor simulation.

Application codes are at the core of these enhanced capabilities. They would help solve a range of scientific questions. These codes are suitable for many applications and encompass a wide range of characteristics. *Integrated codes* are production design codes that are used for the design and performance evaluation of engineering-scale plants, processes, and technologies (e.g., fuels, reactors, separations, etc.). These codes are usually large, complex, integrated multi-scale and multi-physics codes. *Material property codes* are science codes are commonly used to develop material libraries and compositional models that integrated codes (e.g., nuclear data, equations of state, and chemistry, etc) use. *Specialized codes* permit scientists to explore physical phenomena and numerical algorithms, future paths forward for science and technology, new computing architectures, and numerical methodologies, as well as frontiers in uncertainty

quantification and validation. *Specialized codes* include atomistic, turbulence, and molecular dynamics codes.

Experience from other areas[2] where high-level modeling and simulation tools are used in the discovery, design, engineering, and iteration cycle, suggests that there are many driving factors and computational risks. For example, efforts to estimate uncertainty more accurately -- with the purpose of reducing the time needed to license nuclear plants and obtain certification -- are likely to require thousands of simulations using uncertainty quantification techniques. Resolving scientific unknowns and bridging length and time scales is likely to require 100 times improvement in standard-resolution, 3-D simulations. It is essential that scientists develop "ultra" resolution simulations to confirm that high-resolution simulations are sufficiently converged and include validation experiments. This will require computer platforms at the exaFLOP/s level and synergy between exascale computing and advanced numerical methods.

Figure 1 provides a vision of this future.

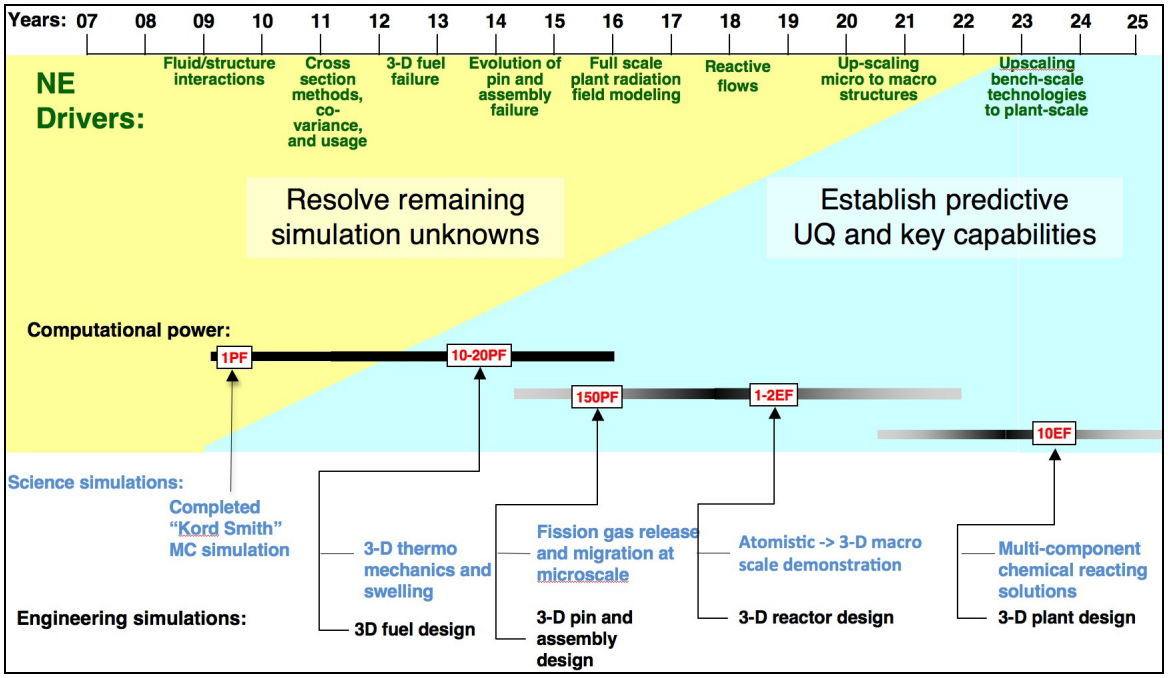

Figure 1: Advancing nuclear energy as an element in the nation's energy portfolio requires scientific, computer science, and large-scale computing advances along a particular timeline and trajectory. The main abbreviations in this figure are PF for petaFLOP/s and EF for exaFLOP/s. The current state of the art is 1 petaFLOP/s of sustained performance[3].

[2] This includes the nuclear weapons program, the aerospace industry, and the Department of Energy's Accelerated Strategic Computing Initiative's (ASCI's) experiences at national laboratories and universities, etc.

[3] The Roadrunner supercomputer at Los Alamos that the nuclear weapons program designed and purchased has achieved sustained performance levels greater than one petaFLOP/s in May, 2008. The Jaguar supercomputer that the DOE Office of Science purchased for Oak Ridge National Laboratory broke the petaFLOP/s barrier in November 2008.

The timeline in Figure 1 includes nuclear energy drivers (in green below the timeline), science simulations to resolve science unknowns, and engineering simulations that use integrated codes. The timeline shows how much computing is likely to be required – from today's petaFLOP/s computing[2] to 10 exaFLOP/s in 2024. We estimate that it will take nearly 15 years to resolve many of the scientific questions identified in Figure 1 and to establish fully-predictive, integrated codes that can quantify uncertainties.

3.3. Panel Findings, Challenges, and a Summary of Research Priorities

The panel analyzed and discussed technical challenges and research directions in five major areas:

- Nuclear fuels
- Nuclear Reactors
- Waste forms
- Fuel reprocessing
- Balance-of-plant (reactor plant systems analysis)

We discuss each of these areas in detail after a brief introductory discussion of software engineering and coupling issues. These latter issues are significant for any IPSC initiatives.

At the workshop, the panel created the following table to summarize *some* of the issues in the five technical areas identified above. This list is meant to be representative, not exhaustive.

Fuel	**Reactors**	**Waste Forms**	**Reprocessing**	**Balance-of-Plant**
Properties (i.e., thermal conductivity)	Neutronics: Power distribution; Neutron spectra for depletions; Improved models for cross sections leading to improved nuclear data – *a priori* cross section prediction	Chemical and mechanical degradation	Physical dissolution models (first-principles based models)	Plant response to extreme motions and conditions (Cascade modes)
Fission gas and other fission product release and migration	Structural mechanics Degradation of materials; core expansion; seismic response; core degradation and relocation; fluid/structure interaction	Transport and near-field environments (higher dimensionality), migration in geological media	Multi-component chemical reacting solutions or gas chemistry	Construction costs
Response and failure 3-D thermo-mechanics;	Thermal hydraulics Multiphase, critical heat flux; coupling CFD and system codes; improved	Geochemistry and volcanisms	Risk reduction for full scale plant (up-scaling	Materials accountability and control

swelling; plastic flow	wire-wrapped designs		technologies)	
Isotopics	Physical chemistry best estimate prediction of thermal chemical behaviors; coupling chemical sources and kinetics	Different options for waste forms	Proliferation	Coupling and up-scaling, new ideas for current and future plants

Table 1: A brief summary of research directions and technical issues for each major area

Software Engineering

Often overlooked, the software engineering challenges of creating a suite of IPSC tools are central to advancing our state-of-the-art understanding and achieving innovative, conceptual breakthroughs to support advances in nuclear energy. IPSCs facilitate passing from improved scientific concepts to practical advances in the field. These codes are pertinent to the development of new nuclear fuels for an existing reactor, improvements in an existing reactor's operating margin, the adoption of new sensor technology for materials' accountability, and using controls in a separations plant.

For example, when we consider a nuclear reactor, there are multiple challenges in modeling design, performance, and safety. Figure 2 illustrates the multi-scale physical challenges that a nuclear reactor faces in size (length) and time.

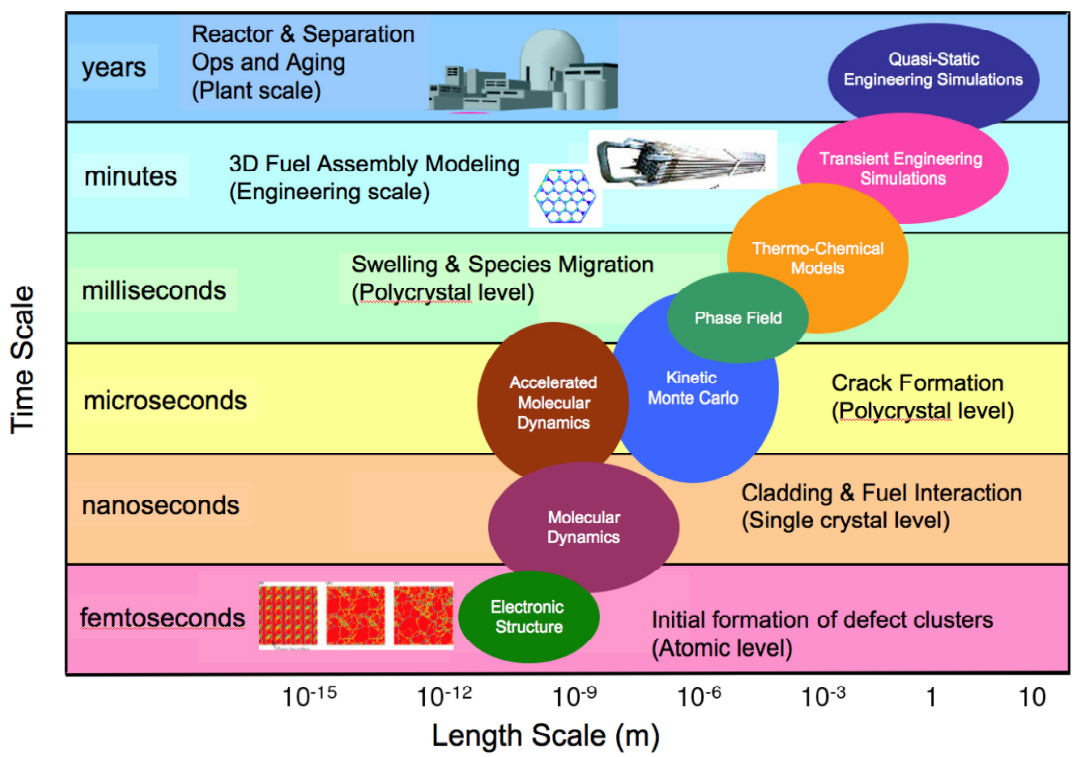

Figure 2: Individual simulation tools and IPSCs involve different physical phenomena at varying scales of interest.

Figure 2 highlights physics issues and the challenges involved in coupling two different scales. Over time, IPSCs will provide scientists with the ability to model fuel performance at the micron level, either for the entire reactor or the plant. In coupling these length and time scales in software, scientists face a significant conceptual challenge in the design of all IPSCs involved in the nuclear energy environment. There are also important numerical and algorithmic challenges in coupling individual physical phenomena. The discussion that follows addresses these challenges where appropriate, but we want to underscore the seriousness of the software challenges in coupling phenomena since they are often not given adequate emphasis.

When scientists adopt new computing technologies and architectures, software engineering and computing approaches change in significant ways. Recent developments in computing software and hardware suggest that promising innovations are possible in multi-scale, multi-physics integrated solutions for many areas of interest (including nuclear energy) linked to heterogeneous computing, such as mixed processing types and architectures in a single integrated system. The current petaFLOP/s system at Los Alamos (the Roadrunner system) is an interesting example that mixes Opteron and Cell processors. In the future, scientists are likely to speed up computing by using field programmable gate arrays (FPGAs) and graphical processing units (GPUs). FPGAs already provide software developers with a means to build hardware tailored to specific computing tasks, making it possible for such hardware to perform far better than general-purpose processors. This performance enhancement comes from exploiting fine-grain parallelism through loop-body pipelining that exploits "deep" parallelism and the instantiation of multiple execution units that exploit "wide" parallelism. With AMD and Intel adding support for accelerators, next-generation, high-performance computing systems are likely to include acceleration technologies. Since these emerging technologies will advance long-term, large-scale modeling and simulation, they should be incorporated into any efforts to enhance the algorithmic and simulation components, from atomic scale simulations and computational fluid dynamics (CFD) to neutronics and reactor physics. Research and development in computer science to support new techniques and integrated codes on the latest architectures should be a priority, especially as they are central to physics integration and software engineering issues.

Nuclear Fuels

Despite significant advances in modeling, scientists continue to rely upon empirical correlations to characterize how irradiation affects fuel and cladding. Developers are modifying codes such as FRAPCON (for light water reactors, or LWRs) to address this issue. Given widespread use of empirical correlations, research into state-of-the-art, nuclear fuels should focus on two levels — an intermediate-level and atomic-scale level. The intermediate level should take a science-based approach, while the atomic level should aim for a much more fundamental simulation capability. In fission gas production, coated-particle fuels (Tristructural-isotropic, or TRISO) are a major factor in either pebble bed or prismatic design for high-temperature gas reactors (HTGRs). Fission gas release plays an important role in TRISO fuel performance because accumulations of

fission gas inside the TRISO kernel and buffer layer can cause structural changes that magnify mechanical interactions between the pyrolytic carbon (IPyC and OPyC) layers and the silicon carbide (SiC) layer.

New simulations to evaluate nuclear fuels must be first-principle based, multi-physics, and multi-dimensional simulations, within the limits of available computing power. Several features should be part of advanced fuel modeling and simulation: 1) fission product and fission gas production; 2) gas transport and the formation of void or bubbles; 3) temperature distribution and void transport; 4) the impact of irradiation, and 5) the thermo-mechanical response. At an intermediate level, these processes can be modeled using continuum approaches. Nevertheless, accurate and robust science-based models based on a continuum approach are still few in number. Today, most advanced codes rely on a *mechanistic approach* that uses a broad set of microscopic parameters to characterize the radiation effects governing transport equations (fission products and void/bubble transport, temperature distribution, etc). Since they are physical in nature, these parameters are usually fixed after scientists analyze the available experimental data. Then the values are used in simulations without any additional fine tuning. One foreseeable advance is that scientists would determine these parameters from lower-length-scale simulations of microscopic phenomena, using high-performance computing. One result of improved computing power could be micro-scale representations of materials and physics to support system-level simulations via meso-scale codes.

The scientific and computing challenge is to develop multi-scale and multi-physics models to illustrate how irradiation affects fuel behavior. This will improve design, performance, and safety, and offer a way to integrate such improved models into IPSC tools. New models will span micro-meso-engineering scales and IPSCs will provide complete descriptions of 3-D, assembly-level fuel performance, deformation, and fluid/structure interactive simulations. To properly simulate the behavior of nuclear fuels, scientists need to develop analytic capabilities that span highly disparate length and time scales. As shown in Figure 2, fuels have important physical phenomena that occur at each part of the scale and modeling techniques must be applicable to such segments in the scale. Figure 3, by contrast, focuses on what scientists need to model in a fuel-centric IPSC. The figure is based on a metal fuel and illustrates how modeling can include the typical inputs, outputs, and phenomena associated with a fuel.

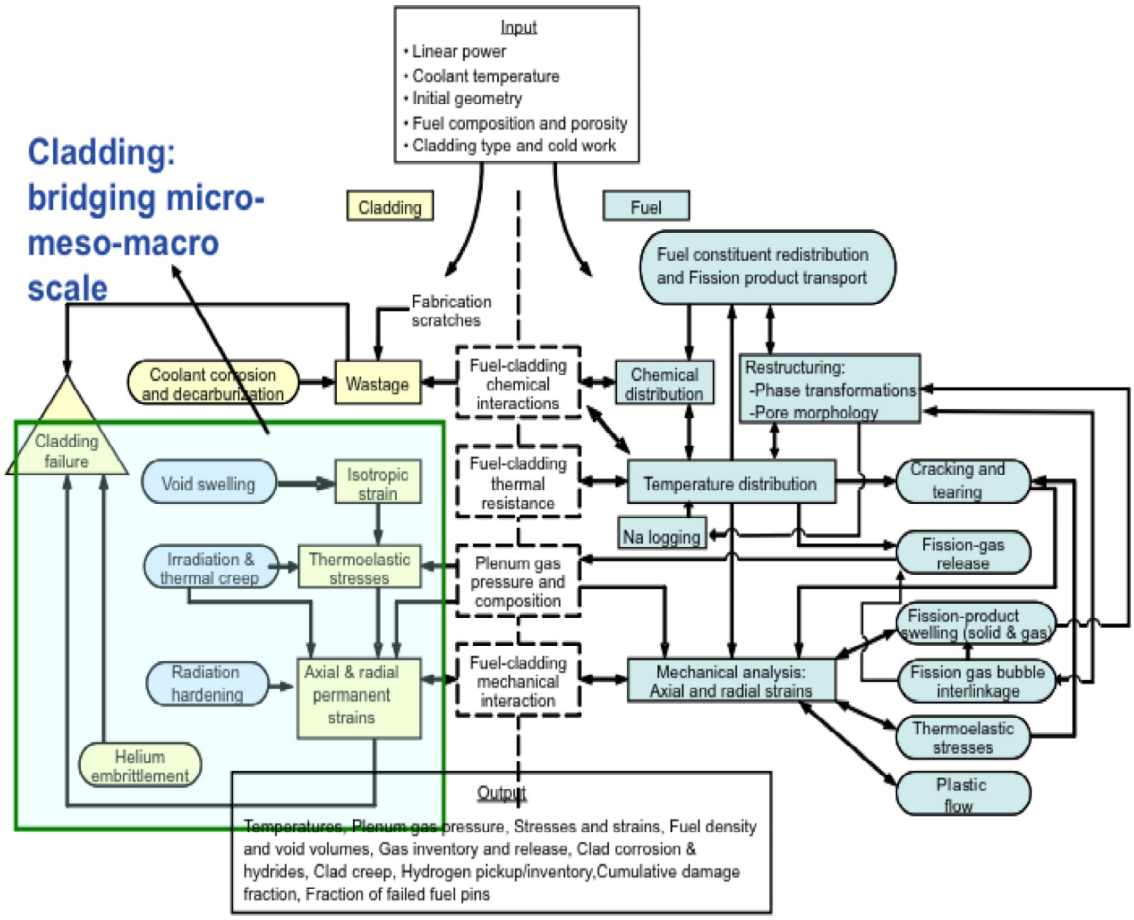

Figure 3: An IPSC to model the behavior of a metal fuel, including inputs and outputs.

In the past, scientists created first principles, lower-length-scale (i.e., less than engineering scale) models of how fuel behaves under irradiation, but insufficient computing power limited their efforts to develop a comprehensive, mechanistic model informed by atomistic, molecular, and meso-scale insights. As a result, scientists have not explored many of the fundamental atomic-scale concepts that control fuel performance.

Improved computing power should permit IPSCs to bridge time and length scales and support higher length-scale models with lower length-scale insights, a major advance over earlier simulations. The resulting multi-scale simulations should be based upon accurate atomic scale physics, an improvement on today's fuel performance codes. Furthermore, once an IPSC uses accurate fundamental phenomena, it should be able to predict changes across a wide range of fuel compositions and reactor conditions. Advances in computing power will contribute significantly to efforts to develop such first principles-informed, mechanistic models. As a result, system-level simulations will be built upon reliable micro-scale representations of materials and physics.

To succeed in this area, scientists will need to use algorithmic research that bridges multiple scales, solvers, physics-based preconditioners, and coupled physics methods. The algorithms will need to scale from *ab initio* to molecular dynamics to continuum

scales, and map different mesh types and physics (and, in some cases, cover the generation of the computational meshes).

Once scientists create predictive fuel IPSCs, innovative designs will increase burn-ups in existing reactors, reduce qualification time, lower the cost of new fuels (since fewer experiments will be needed), speed the creation of new fuels with a broader exploration of possible designs, and enhance the safety of nuclear power.

Nuclear Reactors

Science-based IPSCs will not only facilitate the design of new technologies and lessen our reliance on prototyping, saving time and money, but also impact life-extension issues and the operations of existing reactors. The scientific and computing challenge that scientists face is to create IPSC tools that integrate the physics of time and length scales with methods that insure that predictions are reliable. This will require full physics, high-resolution, 3-D, steady-state and transient simulations. On one level, this implies a robustness and scalability in multi-physics solutions that is not attainable today. To achieve the needed innovations, scientists will have to borrow and refine techniques from other fields and reduce their current reliance on empirical estimates with simulation tools that can quantify error margins and understand the source and nature of uncertainties. If new IPSCs result in simulations that speed up licensing, expand design space, and give rise to reliable, new designs, they will increase our nation's use of nuclear energy. New IPSCs will also very likely improve operating margins and the economics of existing reactors, extend the lives of existing reactors, and increase confidence in the safety of existing reactors and plants.

The following sections discuss nuclear reactors' neutron transport, thermal hydraulics, and uncertainty quantification. These are factors of considerable importance to improving nuclear reactor design and performance.

Nuclear Reactors: Neutron Transport

The requirements for neutron transport calculations are more rigorous than those for changes to models in other physics components. Even traditional approaches to simulate whole-core nuclear reactors require faster computers and better numerical methods and algorithms. When the need to more tightly and accurately couple neutronics to other physics, both at larger- and smaller-scale, is added to these requirements, it is clear that the need for methods research and large-scale computing has never been greater. For instance, a first-principles treatment of neutron and gamma-ray transport to solve the linear Boltzmann transport equation (BTE) demands enormous computing resources because the solution must embrace seven dimensions: three in space, two in direction, and one each in energy and time. Traditional, whole-core reactor simulations to solve neutronics (neutron plus gamma rays) for a steady-state reactor utilize symmetry and rely on homogenization methods and strategies. These simulations must pre-calculate detailed

pin and sub-assembly cross-sections that are embedded in the whole-core simulation without sacrificing its accuracy. Other physics models of isotopic changes, thermo-hydraulics, and material models have only been loosely coupled to neutronics via models. Given the need to more tightly and accurately couple neutronics to other physics, both at larger- and smaller-scale, the demand for methods research and large-scale computing has never been greater.

There are different ways to solve the BTE. *Monte Carlo* methods can solve the BTE stochastically with computational particles representing neutrons and gamma rays. *Deterministic* methods, such as the S_N, or discrete-ordinates method, discretize the equation in each independent variable and solve the coupled, partial differential equations. Both methods play a fundamental role in reactor modeling and simulation, but Monte Carlo methods have the advantage of representing energy- and angle-dependence in a continuous manner. At least for static geometries, we can model space almost exactly. Statistical uncertainty is the most noticeable error when scientists use traditional Monte Carlo methods to model neutronics. Deterministic methods have discretization errors in each independent variable that get smaller as resolution increases, although this depends on the numerical scheme. Monte Carlo codes are often used to benchmark deterministic codes that are then used for engineering analysis. Hybrid methods combine deterministic methods with Monte Carlo methods and can increase the speed of Monte Carlo calculations. Even with few statistical and discretization errors, the uncertainty of available nuclear data will determine the uncertainty of precise methods.

There are several existing, applicable, neutronics codes. Some of the more prominent ones are:

- Monte Carlo codes
    - MCNP (Los Alamos National Laboratory or LANL), a general-purpose, continuous-energy Monte Carlo code used worldwide as the accepted neutronics benchmark.
    - SCALE (Oak Ridge National Laboratory or ORNL), a nuclear analysis code suite, containing the KENO and MONACO codes. These codes provide continuous-energy and multi-group Monte Carlo solutions for a wide range of applications.

- Deterministic codes
    - PARTISN (LANL) is a general geometry, massively parallel S_N code used widely for detector, shielding, and criticality calculations for massively parallel architectures.
    - UNIC (Argonne National Laboratory or ANL) is a massively parallel, second-order, even parity code.
    - SCALE (ORNL) contains the massively parallel Denovo S_N code that utilizes structured meshes for both reactor and shielding applications.

- Hybrid codes
    - ADVANTAGE (ORNL) is an integration of the Denovo code with MCNP (LANL). It is currently used for shielding applications, but NC State University is extending it to include reactor applications.
    - SCALE (ORNL) contains the MAVRIC sequence that integrates MONACO with Denovo for shielding applications.

Monte Carlo Codes

Monte Carlo codes model the nuclear system in detail and solve any part of the modeled system stochastically. They are built upon first-principles, nuclear reactions and, as a result, provide greater accuracy and efficient parallel algorithms to track particles when models run using extreme computing. They also face significant challenges. For reactor applications, scientists have extensive experience using Monte Carlo codes to calculate integral parameters like the effective multiplication factor or a reactor's reactivity coefficient, even when they model every geometric detail of the individual fuel pins in a fuel assembly. However, when Monte Carlo codes demand more fine-level detail, such as measuring the local power density in a fuel pin's small regions axially and/or radially, it is difficult for them to produce acceptable results, for instance a statistically-significant standard deviation, during a computing run that is not very lengthy. Monte Carlo codes have an even more difficult time when they must tally a large number of results, as when they must estimate the local power densities in all of a reactor's fuel pins, subdivided by a number of axial and, possibly, radial regions.

In an invited lecture at the American Nuclear Society's Nuclear Mathematical and Computational Sciences conference in 2003, Kord Smith[4] formulated the challenge facing future Monte Carlo simulations of burn-up calculations, including how to estimate the local power required by every fuel pin in a fuel assembly that is subdivided into 100 axial and 10 radial zones. There are about 300 fuel pins in the fuel assembly of a pressurized water reactor (PWR) core and around 200 fuel assemblies in a reactor core, so this adds up to around 60 million tallies. For an acceptable result, Smith estimated that the standard deviation in each local power region would have to be 1 percent or less. In addition, Smith specified that the reaction rate needed to consider 100 different nuclides. This would bring the total number of tallies to 6 billion. This huge number of tallies not only poses a problem for CPU time, but also stretches the limits of computer memory. Smith estimated that, using Moore's law, it would take until 2030 before such a full core Monte Carlo calculation could be done in less than one hour on a single CPU. William Martin[5] analyzed the situation in detail in his invited lecture at the Nuclear Mathematical

[4] Kord Smith, "Reactor Core Methods," American Nuclear Society, Mathematics and Computation Division, 2003 Topical Meeting on "Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew," Invited Keynote Address, April 2003, Gatlinburg, Tennessee.

and Computational Sciences 2007 conference. Assuming that Moore's law manifests itself only as more cores in a desktop computer, Martin estimated that it would be 2019 before scientists could perform a full reactor core calculation with 40,000 fuel pins and 100 axial regions and achieve 1 percent statistical accuracy for local power region estimates. These are only a few reasons why improvements in full core Monte Carlo reactor calculations could turn out to be more difficult to achieve than we have estimated.

It is important to note that both Smith's and Martin's analysis and computer performance predictions are based on a "business-as-usual" approach. This means that a nuclear engineer runs does all these computations on a single, dedicated computer or using computers scaled according to Moore's law. This fails to take into account today's large-scale computer systems and emerging, heterogeneous technologies. In fact, the world's two best reactor design laboratories, the Knolls Atomic Power Laboratory (KAPL) and the Bettis Atomic Power Lab (BAPL), have used supercomputers to run large-scale, detailed Monte Carlo calculations to evaluate reactor performance since the early 1990s. They designed Monte Carlo code systems to solve large-scale problems using parallel calculations on large, dedicated clusters. It is likely that such calculations can be run for commercial PWR and Boiling Water Reactor (BWR) systems (the "Kord Smith Challenge") using today's terascale and petascale clusters and conventional Monte Carlo models. Some improvements may be necessary to facilitate model setup and the handling of results data for such large-scale applications. In addition, Smith's and Martin's predictions for 2019 and 2030 may be overly pessimistic. Given the importance of Monte Carlo techniques in this area, and possibility that extreme computing will provide scientists with far greater power, further work is needed to help accelerate the performance of Monte Carlo models.

MCNP Monte Carlo Code

LANL developed the MCNP Monte Carlo code in the 1970s. Work has continued to extend this code's usefulness and support its operation. The code uses quite precise, 3-D, geometric modeling and the best-available, continuous-energy, nuclear data and physics models to provide accurate, detailed solutions for reactor core neutronics calculations. Since the code is generally considered the "gold standard" for such calculations, the reactor physics community makes extensive use of it to validate less elegant, deterministic methods. It is the choice to analyze almost every advanced reactor system concept today, either to evaluate reactor design or to verify and validate faster deterministic solvers. MCNP Monte Carlo codes have also has been used with large-scale, parallel clusters. In some calculations, they have drawn on the power of thousands of processors.

[5] William Martin, "Advances in Monte Carlo Methods for Global Reactor Analysis," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications, April 17, 2007, Monterrey, CA.

Deterministic Methods

For large problems, deterministic transport methods may be an expensive way to use computing power. Although high performance computing has reduced the computing power they require, deterministic methods have faced problems scaling parallel algorithms to solve transport problems because of limitations with the source iteration techniques they use to solve equations. Source iteration itself can be unreasonably slow during the convergence of transport solutions, but Los Alamos National Laboratory (LANL) resolved this issue when it developed Diffusion Synthetic Acceleration (DSA).

At the present time, there are several notable, state-of-the-art, deterministic codes that we will describe here. We will also examine what directions research needs to take.

SCALE-6 Nuclear Analysis Suite

In the next 5to 10 years, Monte Carlo methods could be used as a hybrid tool that couples multi-physics to deterministic neutronics and thermal hydraulics codes. ORNL's work to develop the SCALE-6 nuclear analysis suite is a promising effort in hybrid deterministic and Monte Carlo methods. The MA VRIC sequence in SCALE-6 incorporates a new, three-dimensional, discrete ordinates (S_N) transport code, Denovo, with a modern Monte Carlo transport solver, Monaco. The release version of MA VRIC is designed for nuclear shielding and radiation dose assessments, but its ongoing development includes the extension of Denovo for reactor simulation applications. ORNL scientists have been able to get Denovo to scale to 40,000 processors of XT5 (ORNL) when they simulated an entire PWR facility. This run required just over an hour of computing time, including the setup and I/O. The simulation included over 1 billion spatial elements, 27 energy groups, and 624 directions or 1.7×10^{13} degrees of freedom.

PARTISN

Another deterministic transport method, LANL's PARTISN (PARallel, Time-dependent S_N) code, and its DANSYS predecessors, have been used in nuclear engineering applications since the 1960s. Its first-order, discrete ordinates algorithm has been an accurate and efficient solution for reactor engineering applications over many decades. PARTISN is production-level software, with an extensive pedigree and rigorous software quality engineering, verification, and documentation that is routinely chosen to run design calculations to evaluate reactor shielding on thousands of processors. In addition, considerable efforts have helped optimize its computational performance (i.e., as measured by cache hit rates, FLOP rates, communications bandwidth and/or latency tradeoffs) and algorithmic performance, including its source iteration. While DSA has resolved the known, slow convergence of source iteration methods, it also demonstrated that this algorithm must have a highly efficient diffusion solver. PARTISN uses a parallel Conjugate Gradient method, and combines it with a variety of pre-conditioners (including a geometric multi-grid) for optimum solution times. Through the "KBA" [knowledge-base agency] algorithm, PARTISN has been successfully parallelized and, as a result, KBA has become the standard for first-order S_N solvers. With this algorithm, PARTISN

has moved from machines such as the Connection Machine of the early 90's to today's massively parallel processing (MPP) platforms. Efforts are now underway to adapt it to run on heterogeneous platforms such as Roadrunner. When Roadrunner can use tens to hundreds of thousands of processors, PARTISN will be even more useful.

Scientists continue to rely upon PARTISN to develop and test new physics for reactor engineering. Recent additions include: 1) an option to use a chi matrix instead of the traditional chi vector to describe the fission spectrum; and 2) temperature-dependent, cross sections where the temperature can vary as a function of both individual spatial cells and time. In addition, PARTISN has a transport methods interface that lets users embed the entire code as a module that is callable from FORTRAN or C++ codes in applications such as fluid flow, heat transfer, etc. This facilitates using reactor simulations to model detailed, complex, feedback loops between physics packages. PARTISN is also able to run structured or block-structured, that is, with adaptive mesh refinement, i.e., orthogonal meshes in 1, 2, or 3 dimensions with Cartesian, cylindrical, and spherical coordinates. These meshes usually require more spatial cells than unstructured meshes because they need to resolve non-orthogonal geometries accurately. An increase in the spatial cell count is often offset by reduced computing complexity that allows structured mesh codes to run as fast as or faster than unstructured mesh codes.

ULTIMATE NEUTRONIC INVESTIGATION CODE or UNIC

Argonne National Laboratory's (ANL's) initiatives with the UNIC code also address solutions for reactor applications that rely on advanced Boltzmann solvers. ANL is developing UNIC to solve large-scale nuclear reactor core problems that the Boltzmann equation describes. These solutions include seven dimensions: three in space; two in angle; one in energy; and one in time. ANL's efforts plans to reduce uncertainties and biases in reactor design calculations by replacing existing, multi-level, averaging (homogenization) techniques with more direct solutions. At the present time, UNIC has two solvers for the neutron transport equation that use a second-order, even-parity, transport equation with spherical harmonics and have discrete ordinates approximation techniques to estimate angles. A third solver uses first-order characteristics to create more efficient, explicit, geometry modeling.

UNIC uses an unstructured mesh. In order to represent the complex geometry of the reactor core, it employs billions of spatial elements, hundreds of angles, and thousands of energy groups. This leads to problems with scalability and petascale degrees of freedom. Such calculations can easily exhaust the memory resources of current and even next-generation computing architectures. ANL has evaluated the performance of UNIC and the potential impact of higher-fidelity methods for two representative fast-reactor problems, PHENIX and ZPR-6, using Argonne's and ORNL's advanced computing platforms. In both cases, UNIC showed it could scale modestly, with 80 percent scaling on up to 163,840 cores of BlueGene/P (Argonne) and 131,072 cores of XT5 (ORNL). Ongoing research efforts will try to improve per-processor performance and maintain the highly-parallel efficiency that better algorithms, for instance, spatial p-refinement, multilevel preconditioners and weighted partitioning for load balancing, can provide.

Transport Methods Research

Both deterministic and stochastic methods will play an important role in the near-term and long-term development of high-fidelity, nuclear-reactor physics simulations. There must be bigger research efforts – these deserve special attention -- if extreme computing is to improve the usefulness of these methods. To achieve maximum, parallel performance, scientists must develop new algorithms for deterministic methods that are vastly different. They also need to insure that these algorithms cover a reactor core's seven dimensions. Today's adaptive techniques generally apply only to spatial adaptation, but their extension to angle and improved energy discretization techniques is necessary if they are to perform with the greater efficiency on the best computing platforms. Such enhancements would make it possible for scientists to solve a number of intractable problems. With Monte Carlo methods, further extension of hybrid deterministic or Monte Carlo algorithms is important if we want to compute the spatial distribution of neutrons throughout a reactor's geometry on a non-orthogonal grid of cells more efficiently, particularly in support of multi-physics coupling. The use of Monte Carlo methods for reactor applications will also require work on how to achieve tighter integration of reactor depletion and kinetics. In addition, research must identify algorithms that can convey uncertainties in the nuclear data as well as statistical uncertainties throughout the reactor depletion/kinetics process.

Nuclear reactor simulation efforts might also benefit from methods R&D, advanced computer architectures, and large-scale componentized software that are part of the National Nuclear Security Administration's (NNSA's) Advanced Simulating & Computing (ASC) program. One of the ASC program's themes is software quality. The lessons learned in this area in the creation of new reactor codes. Many of ASC's advances have been in modeling thermal x-ray transport for high energy-density physics applications. This modeling places enormous demands on computing that are equal to the demands of long-term simulations of nuclear reactor behavior. For example, LANL's Jayenne and Capsaicin Projects for thermal x-ray transport utilize object-oriented designs that allow for extensive unit and regression testing. These are indispensible features for assuring verified software and methods development. In the Monte Carlo simulation of thermal X-rays, the spatial mesh parameters will not fit in the memory of one processor or node. Parallelism via spatial decomposition as used in deterministic methods is problematic for Monte Carlo transport simulations because it requires asynchronous transport schemes to manage the transport of particles and insure simultaneous communication between processors. LANL's Jayenne Project created a special, event-loop, asynchronous, transport scheme. It has improved this scheme so that it has now become the standard domain-decomposed, asynchronous, transport scheme for thermal x-ray and linear transport. As nuclear reactor simulations become more detailed and more tightly coupled with other physics, scientists will need an asynchronous transport scheme similar to the one the Jayenne Project developed because spatial representations can't fit on a single processor.

Nuclear Reactors: Thermal Hydraulics

Thermal hydraulic (TH) analyses are critical for optimizing reactor design and evaluating safety. These analyses must have a detailed understanding of heat transfers and mixing processes if they are to predict hot spots, identify detailed temperature distributions, and perform a wide range of full-scale plant analyses related to safety. They also must describe localized phenomena, such as thermal striping, fretting, and flow-induced vibration. Next-generation TH simulations will help optimize the design of new reactors and open opportunities for new design features not seen in today's reactors, a significant benefit.

In general, scientists cannot perform first-principles, direct numerical simulations (DNS) of the Navier-Stokes equation across the entire domain of a nuclear reactor using today's high-end computers. There are limitations such as the range of fluid phenomena -mixing in the upper plenum, stratified pipe flow, and heat exchanger analysis, etc. Probably the most canonical, important example is heat transfer in a rod bundle. Since a typical per-channel Reynolds Number is in the range 10,000-100,000, a DNS of just a single channel can challenge the capabilities of today's supercomputers.

For example, a typical fast-reactor design calls for sodium-cooled rod bundles arrayed in a triangular pitch within hexagonal subassemblies of 217 pins. Each subassembly is hydro-dynamically isolated by subassembly walls with the fuel pins separated by either wire wrap spacers or spacer grids. Spacer design influences how pressure drops and heat transfers occur in the core. It also affects how coolant mixing influences peak fuel pin temperatures. Therefore, understanding these flows is important in estimating pumping power and power output. In normal operation, coolant flows through the channels between pins as well as between the pins and the walls. The wire-wrap spacers direct flows between adjacent channels and enhance the cooling of isolated hot pins. While the majority of the flow is in interior channels, the bypass and perimeter swirl flows through the edge channels and can significantly impact overall cooling. As a result, alternative channel configurations are of special interest, such as pins with oppositely-directed wire wraps. In fact, the influence of the edge channels prevents the direct extrapolation of low pin-count test results, numerical or experimental, to higher pin count situations.

These complexities preclude the use of DNS or even large-eddy simulations (LES) for a full 217-pin subassembly. Consequently, scientists construct advanced TH simulations on a hierarchy of simulation capabilities, each operating at differing scales. DNS and LES compute fine-scale turbulence in relatively simple geometries with a minimum of turbulence modeling assumptions (none, in the case of DNS). With lower computing requirements, Reynolds-averaged Navier-Stokes (RANS) simulations can compute mean flow effects in more complex domains. A key area for research on using extreme computing should be the integration of RANS and LES methods with the corresponding codes used in different portions of the reactor. This will probably require a software platform for the efficient, highly-parallel, and stable transfer of needed information at different codes' domain boundaries. Stanford's ASC Center's CHIMPS package for

integrated, numerical simulation of a gas turbine engine is an example of such an integrated software platform.

TH analysis faces another bottleneck in modeling boiling and multi-phase processes. This analysis typically relies quite heavily on empirical correlations. One illustration of the barriers to progress is the notable example of scientists' inability to model critical heat flux using science-based models. Similarly, two-phase flow models also depend on correlations and parameters that scientists need to determine empirically. In spite of significant advances in commercial CFD modeling, CFD models for nuclear issues has not received the same attention that they have received in the aerospace, chemical, and semiconductor industries. This occurred in spite of the fact that CFD problems in some of industries were more daunting than the nuclear industry's single-phase flow problems. Nuclear energy problems were not addressed adequately because of the dormant state of the industry while other sectors were expanding rapidly.

A modeling and simulation initiative to improve nuclear power plant design and licensing would have to address problems specific to nuclear energy, such as boiling, two-phase flow, and critical heat flux. Recent attempts to use Lattice-Boltzmann (LB) techniques to solve fluid mechanics problems show promise. There is a possibility that the LB approach will provide better and easier coupling with particle-based radiation transport codes. The complex process of nucleation, bubble growth and detachment, phase transition, moving boundaries, and breakup and coalescence of bubbles suggest that only a multi-scale, multi-physics modeling approach where simulations at different levels are fed into more encompassing, general CFD simulations can adequately address the problems reviewed here. At the same time, work is needed to refine the global set of multi-phase flow equations. These equations must provide a way to measure parameters with more precision and to include distinguishing flow characteristics and flow regimes.

Nuclear Reactors: Uncertainty Quantification

Although a first-principles treatment of radiation transport and DNS flow simulations are visually captivating, there are basic uncertainties that reduce their accuracy. As a consequence, a substantial research effort is needed to estimate the effect of random factors, such as manufacturing tolerances, material compositions, nuclear cross section uncertainty, etc., on the solutions to radiation transport, thermal-hydraulics, and other physics simulations. This would provide greater insights into how much resolution each physics solver must achieve. If these uncertainties are have small relative to the solvers' computing errors, scientists probably need to make greater efforts in software and algorithm development. As the resolution of the solvers improves, however, error in random factor uncertainties may mask additional improvements to the solvers.

Today's solvers do not employ rigorous methods that can carry forward large uncertainties and evaluate the sensitivity of high-resolution solutions because of inherent uncertainties. To solve this problem, scientists will need to develop solvers that reach forward and adjoint solutions. Such an undertaking would be substantial, because few

codes execute in this manner. For instance, the current, multi-level approach to radiation transport cannot evaluate computing errors because it includes several levels of homogenization. Also, most continuous-energy, Monte Carlo codes cannot provide adjoint solutions due to the way they store data and how they evaluate first-principles, nuclear scattering. Therefore, a substantial effort is needed to enable radiation transport, thermal-hydraulics, and coupled-physics solvers to provide both forward and adjoint solutions. This would be one way to provide the information needed to estimate sensitivities and to create better criteria for halting software development.

Waste Forms

Modern modeling and simulation (M&S) techniques can improve how scientists develop and qualify waste forms and waste treatment processes in closed fuel cycles. In fact, to predict the performance of waste forms over geologic time scales, scientists rely on validated models and simulations augmented with naturally occurring analogs and accelerated aging techniques. A panel of experts developed a list of M&S needs and priorities for waste forms and Peters *et al.*[6] have documented them.

Among the three primary objectives for waste-form M&S are: 1) developing next generation waste-form processes using modern materials design processes; 2) predicting waste form behavior, such as chemical and structural changes, along with interactions with their environment over very long time periods; and 3) simulating fundamental chemical and physical processes that are central to the processing and/or formation of waste forms with desired properties. Meeting these objectives requires a clear understanding of material behavior based upon theory, experimentation, and modeling in many related areas. These areas include:

- The structure and chemistry of radionuclide-bearing phases in waste forms and their corrosion products.
- The corrosion and alteration of nuclear materials, some of which are so durable as to require new techniques to study the corrosion mechanisms and measure extremely low release rates.
- The measurement and prediction of thermo-chemical parameters for nuclear materials and an extended thermodynamic and kinetic database for modeling the long-term behavior of nuclear waste forms in the environment. Such models must consider property changes that occur at multiple spatial scales (especially the nanoscale) and the thermodynamics of surface and interface reactions.
- The development of theories, models, and in-situ experimental techniques that can help scientists understand the atomic-scale behavior of solid-liquid-vapor interfaces, particularly interfaces that control the synthesis and long-term corrosion behavior of nuclear waste forms.

[6] Mark T. Peters, Rodney C. Ewing, and Carl I. Steefel, "GNEP Waste Form Campaign Science & Technology and Modeling & Simulation Program: Roadmap with Rationale & Recommendations," U.S. Department of Energy, Global Nuclear Energy Partnership Waste Form Campaign, Washington, D.C., March 14, 2008.

- The development of theory, models, and data to understand the effect of radiation and radiolysis on materials and the long-term behavior of materials following their disposal.
- Further development of theory, models, and data to predict the migration of radionuclides under certain geochemistry and geological conditions.
- The use of advanced modeling and simulation within an IPSC to integrate all the data and insights about waste forms and systems.

A central challenge to developing new waste forms is how to integrate four different activities — design, development, synthesis, and performance — with material properties and disposal strategies. Modeling and simulation can help unify our understanding of full-scale performance over a range of conditions. More specifically, challenges in this area include: 1) creating simulations that span broad ranges in time and distance scales, from ns and Å through millions of years and kilometer scales; 2) concurrently developing theoretical and experimental data as well as models to predict materials' behavior under a schedule that will meet project needs; and 3) improving the M&S of interfaces, especially those between solids-liquids-gases, between grains of waste forms, etc., where most materials' properties change and where they also control processes that are central to the successful creation of waste forms. The highest priorities for research are: 1) developing advanced waste forms with reduced costs and lower environmental impacts; and 2) optimizing disposal strategies via risk-based approaches.

A waste forms' IPSC should serve as an integrated suite for the computer modeling and simulation of waste forms' performance in engineered near- and far-field environments in waste storage or disposal repositories. The suite should include first-principles codes for property characterization and high-fidelity modeling of coupled transport phenomena. It ought to contain efficient surrogate models of verifiable accuracy to conduct performance assessments in well-specified regimes. A key challenge will be to develop constitutive models from sub-grid scale computer studies and experimental data. This probably will require new up-scaling techniques and/or ways to implement multi-scale methods. In addition, if scientists rigorously apply model abstraction techniques and uncertainty quantification methods, higher fidelity models can be used to create surrogate models.

A waste forms IPSC should be designed to include optimization and uncertainty quantification. In that way, it can support verification and validation, sensitivity analyses, and predictive information. Besides a "best estimate plus" uncertainty extracted from a cumulative distribution function for a suite of simulations, any predictive information should treat "unknown unknowns," conceivably through safety factors, peer review, and an evaluation of the robustness of simulations. The ultimate goal is simulations that can predict quantifiable events in support of science-based, risk-informed decision making that helps manage nuclear waste, now and in the future.

Fuel reprocessing

If scientists can model and simulate the range of steps in fuel reprocessing, it will improve the analysis of fuel cycles. Although the entire process needs to be modeled based on first principles, the state-of-the-art is not very advanced. Scientists need to develop a number of sub-models before they can create a well-integrated, multi-physics, multi-scale model for the entire process. For example, a first principle-based dissolution model for spent fuels does not exist. In addition, scientists have not created improved models for unit operations, distillation columns, mixing, off-gas recovery, and other processes. They also need a well-integrated, dynamic model of the entire range of fuel reprocessing operations, including logistics. Finally, new technologies and data assimilation techniques for sensors could help improve safeguards and regulate proliferation.

Balance-of-Plant: Reactor Plant Systems Analysis

Over several decades, fully-integrated, "whole-plant," systems' analysis codes have been indispensable tools for performing systems' level calculations to evaluate designs and safety. From an engineering standpoint, a robust analysis of a whole plant system's response can be as important to the design and licensing of a new power plant as individual high-fidelity component analyses.

A nuclear power plant's safe and efficient operation ultimately depends on whether different system components interact properly during normal, off-normal, and potential, accident-driven, operating conditions. Many systems and subsystems play vital roles in overall reactor system behavior, including many in-vessel components and subsystems, as well as ex-vessel subsystems and components. Among the latter are the pumps, control valves, turbines, heat exchangers, electrical systems, secondary and tertiary coolant systems, and reactor containment systems that are examples of ex-vessel subsystems and components. A reactor systems code considers all the components and physical processes, such as in-vessel, ex-vessel, and balance of plant, but a model's fidelity is balanced against computing costs when using today's most powerful computers.

Systems-level, analytic tools are typically used to explore "design space" or "accident space." They perform a large number of calculations that vary according to changes in the way scientists specify potential problems. For example, the Probabilistic Risk Assessment (PRA) analysis a new nuclear power plant needs to pass in order to gain its license may require many thousands of runs to estimate the uncertainty of its risk profile. The runs must analyze all potential "internal" (i.e., a major pipe break) and "external" (i.e., an earthquake of given seismic load level) initiating events. They must also consider any potential effects of malevolent physical attacks, including scenarios for aircraft crashes. In addition, evaluators of a new nuclear plant must perform all of these calculations in a timely manner and insure that the results are robust and well-documented, so that they can be easily reproduced.

These requirements, combined with previous limits on computing power, have severely hindered scientists' pursuit of models that can accurately depict reactor performance and

geometric complexity. Such models need to be accurate enough to be incorporated into systems-level codes. A new generation of tools will provide greatly improved fidelity, facilitate the 3-D representation of many key components, and insure that models provide the framework necessary to apply advanced techniques for uncertainty quantification. In sum, the application and use of advanced computing (hardware, software, solvers, etc.) are likely to prove to be just as important to systems-level modeling as they are for detailed first-principles analytic codes that concentrate on the coupled physics that occurs in specific components.

To cite just one example, we can examine some of the simulation requirements and challenges for a sodium-cooled, fast reactor plant that could be included in a future closed fuel cycle. A license application for the proposed new plant would require a rigorous analysis of how the system responds to a wide range of potential off-normal accident scenarios, including "beyond-design-basis accidents," such as an unprotected loss of flow (ULOF). During a ULOF sequence, a simulation must assume that all primary and secondary coolant pumps lose power and the reactor scram systems fail to activate. In evaluating the response, a simulation estimates the coupled neutronic, thermal-hydraulic, and thermal-mechanical performance characteristics of the system and assesses whether maximum temperatures in fuel and fuel cladding could result in system failures. At the highest scale, a simulation must model the secondary coolant system's thermal hydraulic response as the pumps shut down and evaluate natural circulation and heat transfer through the passively-activated, direct reactor auxiliary coolant system (DRACS). Within the reactor vessel, transient, liquid-sodium flow through the reactor core and through the heat exchangers changes from a turbulent forced convection to laminar/turbulent, natural convection regimes with a highly complex, 3-D geometry. As the core region heats up, the reactor assemblies expand both radially and axially, changing shape according to carefully engineered constraints that predispose the assemblies to "bow" in a particular manner. Such small geometric changes significantly lower power demands, since they directly affect neutronically-driven fission heating in fuel rods, largely through increased leakage. The size scales that are of interest here range from sub-millimeter, in the potentially thousands of fuel rods and cladding, to the tens of meters associated with the highly-complex, 3-D geometry of the piping, pumps, and other systems that are external to the reactor vessel. While the overall transient response time is usually measured in hours, characteristic times for fluid flow and neutronics fluctuations may be in the sub-microsecond range. The vast majority of equations governing these diverse physical processes are coupled and nonlinear. Any report must identify the predicted maximum cladding temperatures and quantify the uncertainty range that considers all of the uncertainties in physical properties, geometric variations, boundary conditions, and the numerical models used in the calculation.

Earthquakes are an important, externally-initiated event that has been considered crucial to the design of nuclear power plants. Extensive probabilistic studies of how earthquakes might contribute to reactor core damage[7] have shown that seismic loading is a large, and

[7] U.S. Nuclear Regulatory Commission, Office of Nuclear Regulatory Research, "Severe Accident Risks: An Assessment for Five U.S. Nuclear Power Plants," Final Summary Report, Staff Report NUREG-1150,

often dominant, contributor to the annual potential for reactor core damage, after all other possible internal and external events are considered. This concern is of paramount importance in the eastern United States as well as in the West.

In recent years, professionals have employed a seismic design approach to evaluate different types of structures, including large bridges and buildings. This approach relies upon measures like Performance-Based Design standards, where an objective estimate of structural performance is defined at different levels of excitation. In this approach, the structure is designed to remain elastic under more frequent events, such as frequently-occurring, small earthquakes, while controlled inelastic behavior can occur during very infrequent, large events, such as rare, large-magnitude earthquakes. Designs that employ performance-based approaches can reduce costs significantly and create engineering designs that perform more predictably during extreme events.

The key to performance-based design is the accurate prediction of system performance and the forecasting of damage levels for different levels of excitation. Typically, performance-based designs must be able to simulate a nonlinear system response at specified levels of excitation. As a consequence, over the past 10 to15 years, a great deal of research has gone into designing advanced, nonlinear, simulation models for different types of infrastructure. The nuclear power industry has started to adopt design standards based upon the Department of Energy's[8] performance-based standards for nuclear facilities. Even with these advances, computer models that incorporate modern tools and algorithms have been unable to simulate the full, nonlinear response of a nuclear power plant's systems. In order for modern, performance-based approaches to improve nuclear plant design, scientists need to create high-fidelity, three-dimensional, computer models that can accurately incorporate nonlinearity effects (e.g., steel yielding, concrete cracking and strength degradation) and depict the behavior of nuclear power plant systems.

Since nuclear power plants are massive structures that are part of the supporting soil, plant-level computer models must consider soil-structure interactions, an additional level of complexity. As a result, computer models for plants must include not only the plant superstructure but also the surrounding "soil-island" and nonlinear soil characteristics. This drives the need for very large computer models that run on high performance computers and for efficient nonlinear solutions.

To achieve more fundamental insights into system performance and develop cost-effective designs that can survive extreme events, scientists need to formulate realistic structure and soil nonlinear models for nuclear plant systems. This is an opportunity to see if new sensor technologies might simulations by monitoring plants in real time. While such efforts could draw upon existing simulations and models, they might also demand computing features that are custom designed for nuclear plants. One example of more-

December 1990. http://www.nrc.gov/reading-rm/doc-collections/nuregs/staff/sr1150/v1/sr1150v1-intro-and-part-1.pdf

[8] U.S. Department of Energy, "Natural Phenomena Hazards Design and Evaluation Criteria for Department of Energy Facilities," DOE Standard, Report DOE-STD-1020, January 2002. http://www.hss.doe.gov/nuclearsafety/ns/techstds/standard/std1020/STD-10202002.pdf

focused modeling might be accurate, nonlinear response models for massively reinforced concrete shear walls, a notable feature of nuclear power plant construction. Only with such new, advanced, computer models can performance-based designs demonstrate their benefits for massive and costly nuclear power systems.

In summary, a nuclear power plant contains many engineered systems, components, and buildings. To simulate a reactor plant system, scientists need to create comprehensive models of all of these facilities so that they can produce overall assessments of safety and risk. A plant's physical infrastructure is an essential safety system; they offer protection when extreme natural events, such as earthquakes and windstorms, and extreme man-made events occur and are important in the event of malevolent physical attacks. Advanced balance-of-plant designs, supported by high-performance computing, offer a way to reduce costs, speed plant construction, and improve estimates of safety margins during extreme events. In addition, computer science and new technologies offer an opportunity to explore how new sensors and data collection techniques might monitor the "health" of a plant on a continuing basis.

3.4. Conclusions

The use of extreme computing is likely to improve the modeling and design of nuclear energy systems significantly. Nuclear energy science and engineering simulations will drive the need for exaflop-scale, computing power to create robust, predictive simulations that have quantifiable uncertainties. The creation of IPSCs faces considerable technical challenges that range from improvements in software engineering and numerical methods, to the development of more fully-integrated physics models. Given the increase in computing power and the scientific issues that should be addressed in this area, the following research and development subjects require attention and additional analysis:

- Multi-scale methods that allow direct up-scaling of micro-scale science simulations to meso-scale simulations (in both length and time, perhaps even in the same source code, in some cases);
    - Atomic-scale physics in IPSC for nuclear fuels;
    - First-principles informed mechanistic models; and
    - Algorithms that support scaling from *ab initio*, to molecular dynamics, to continuum.
- Advances in computer science to support new techniques, algorithms, and integrated codes on emerging architectures;
- Solvers and physics-based preconditoners;
- New models for understanding fission gas production, gas transportation and formation, void migration, and bubble detachment;
- Advanced uncertainty quantification and validation methods;
- Acceleration methods for Monte Carlo transport algorithms at the extreme scale;

- Hybrid, deterministic and Monte Carlo transport methods, particularly in support of IPSC multi-physics coupling;
- Advanced Boltzmann solvers that can replace the homogenization techniques that are in common use today;
- Spatial p-refinement, multilevel preconditioners and weighted partitioning for load balancing in deterministic transport solvers;
- Adaptive deterministic methods that solve all seven dimensions of the Boltzmann transport equation;
- Methods that achieve a tighter integration of reactor depletion and kinetics;
- Asynchronous transport schemes;
- The development of advanced, adjoint radiation transport, thermal hydraulics, and coupled-physics solutions;
- An integration of RANS, LES, and DNS methods;
- Software platforms that facilitate the development of new methodologies and the integration of multi-physics;
- Improved boiling, two-phase flow and critical heat flux methods;
- The structure and chemistry of waste forms' radionuclide-bearing phases and their corrosion products;
- The measurement and prediction of thermo-chemical parameters for nuclear materials and an extended thermodynamic and kinetic database;
- Theory, models, and data to predict the migration of radionuclides under various geochemical and geologic conditions;
- New dissolution models for spent fuels;
- Improved models of unit operations, distillation columns, mixing, and off-gas recovery in fuel reprocessing operations;
- 3-D models that accurately incorporate nonlinearities, such as steel yielding, concrete cracking, and strength degradation specific to a nuclear power plant;
- Material damage and failure models scaled up to a plant level;
- Sensor technologies and data acquisition techniques.

4. Final Whitepaper - Materials Behavior Panel

4.1. Introduction

This review explores how high performance computing at the petascale or exascale level can address some of the basic materials challenges facing nuclear energy. It also identifies some of the important advances that are likely to be achieved through the use of simulations. The development of transuranic-bearing nuclear fuels, fuel cladding and structural components for advanced nuclear reactors that can withstand ultra-high fuel burnups, neutron doses and temperature extremes is a tremendous challenge that will require new computational techniques that are likely to push the limits of high performance computing and create important innovations in chemical modeling. Several recent reports have focused on the materials challenges for advanced nuclear energy systems,[9] the emergence of computational materials engineering[10] and simulation-based engineering science,[11] as well as the impact of high-performance capability computing in selected areas (not materials).[12] But much less attention has been paid to how high-performance computing might accelerate the deployment of advanced nuclear energy systems.[13] While simulation at extreme scales may not be applicable to every important materials challenge facing nuclear energy,[14] this chapter provides a timely examination of the essential advances that such simulations[15] will probably enable. In doing so, it

[9] "Materials Challenges for Advanced Nuclear Energy Systems," *MRS Bulletin*, January 2009, vol. 43, no. 1, and U.S. Department of Energy, Office of Science, "Basic Research Needs for Advanced Nuclear Energy Systems: Report of the Basic Sciences Workshop on Basic Research Needs for Advanced Nuclear Energy Systems," 2006. http://www.science.doe.gov/bes/reports/files/ANES_rpt.pdf

[10] National Research Council, Committee on Integrated Computational Materials Engineering, *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, Washington, D.C.: The National Academies Press, 2008. http://www.nap.edu/catalog/12199.html

[11] Sharon C. Glotzer, Sangtae Kim and others, "International Assessment of Research and Development in Simulation-Based Engineering Science," World Technology Evaluation Center, WTEC Panel Report, 2009. http://www.wtec.org/sbes/SBES-GlobalFinalReport_BW.pdf

[12] National Research Council, Committee on the Potential Impact of High-End Computing on Illustrative Fields of Science and Engineering, *The Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering*, Washington, D.C.: The National Academies Press, 2008. http://www.nap.edu/catalog/12451.html

[13] U.S. Department of Energy, Office of Science, Office of Nuclear Energy, Science and Technology, "Workshop Report on Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors," 2004. http://www.er.doe.gov/bes/reports/files/ACMS_rpt.pdf.
U.S. Department of Energy, Office of Advanced Scientific Computing Research, Office of Nuclear Energy, "Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems," 2006. http://www.er.doe.gov/ascr/Misc/gnep06-final.pdf.
U.S. Department of Energy, Office of Science, "The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles," 2005. http://www.er.doe.gov/bes/reports/files/PSNE_rpt.pdf.

[14] "Materials Challenges for Advanced Nuclear Energy Systems," and U.S. Department of Energy, Office of Science.

[15] National Research Council, Committee on the Potential Impact of High-End Computing on Illustrative Fields of Science and Engineering.

illustrates the power of theory and the importance of far larger scale simulations than have been possible before.[16]

The development and testing of nuclear fuels, cladding, and structural components have traditionally required decades-long testing and examination. Such long lead times are a result of the lengthy process during which nuclear test reactor radiations create micro-structural and material property changes. These processes are needed if we want to have materials that can survive as reactors are pressed into very lengthy service lifetimes. Several factors are responsible for pushing reactors to endure such long material service lifetimes and a deep burn of fuels. They include economic and national security issues and the fuel utilization gains that are a byproduct of keeping reactors in lengthy service. This demand for long service lifetimes is likely to increase in the future. In the past, material scientists have relied upon reactor radiation analysis for materials design, development, and qualification because it was impossible to reproduce the degradation of materials observed in reactors outside of such environments. In addition, these scientists could not credibly utilize the results of accelerated out-of-pile materials experiments to develop reliable forecasts of in-pile performance. This problem is a challenge facing primary materials theory, modeling and simulation. If exascale computing can help materials science to solve this challenge, the solution would enable materials scientists to resolve major bottlenecks that stand in the way of more intelligent management of nuclear energy.

The promise of high-fidelity, predictive, performance models is not only to predict the lifetime and failure of fuels and components in a wide variety of advanced nuclear energy systems, but also to facilitate the design of new materials tailored for such aggressive environments. In addition, such models would need to illustrate how materials and chemical systems perform throughout the nuclear cycle including the design of separation systems and of containers for waste repositories. Materials scientists expect that high-fidelity predictive performance models will explicitly incorporate all the relevant physical mechanisms controlling material behavior that is revealed by sub-scale physics modeling, parameterized by targeted laboratory experiments, and validated by full scale test reactor irradiations. Once scientists have developed models that depict in high fidelity the performance of physically-based nuclear materials, they will safely increase the burnup and performance of nuclear fuels in a wide range of reactor designs. As a result, this will improve the licensing process and waste stewardship, as well as decrease the time necessary for new materials insertion.

4.2. Toward Predictive Performance Models

The development of better predictive models will require a more comprehensive understanding of nuclear fuels that is built upon greater knowledge of the microstructure of multi-component oxides, nitrides, carbides, and alloys containing uranium, neptunium, plutonium, americium, and curium. New models will need to depict the performance of

[16] National Research Council, Committee on Integrated Computational Materials Engineering. Glotzer, Kim and others.

these actinide elements and also include the in-growth of fission products such as xenon, cesium, strontium, helium, iodine, and technetium. Reactor cores, fuels, cladding, and structural materials (pressure vessels, pipes, ducts, etc.) are subjected to severe radiation, as well as chemical and thermo-mechanical environments that continuously alter their physical properties. The physics and chemistry of such materials becomes more complex as reactor exposure increases. Research has shown[17] that ceramic fuels develop radial and angular cracks and that the severity of the structural damage increases with burnup. Root cause analysis of clad failures indicates that the predominant cause of rupture is the degradation of fracture properties that are the result of complex micro-structural changes. The micro-structural changes are due to exposure to high-energy neutron radiation that violently displaces atoms from their lattice sites repeatedly, while also altering the material's chemistry.

Irradiation's effect on materials is a classic example of an inherently multi-scale phenomenon (See Figure 1). The added complexity that radiation effects introduce in materials is the overarching concern for advanced nuclear energy systems. This takes top rank, although the initial material state and thermo-mechanical loading need to be considered significant in all materials performance-limited engineering applications. The pertinent processes that must be modeled span more than 10 orders of magnitude in size from the sub-atomic nuclear to the structural component level, and span 22 orders of magnitude in time, from the sub-picosecond level of nuclear collisions to decade-long component service lifetimes.[18] Many variables are needed to describe the mix of nano- or micro-structural features that are formed when irradiation degrades the physical and mechanical properties of nuclear fuels, cladding and structural materials. The most important ones are the initial material composition and microstructure, the thermo-mechanical loads, and the irradiation history.

At the smallest scale, radiation damage is continually occurring when energetic primary knock-on atoms (PKA) form, primarily through elastic collisions of reactor materials with high-energy neutrons. At the same time, radiation generates high concentrations of fission products in fuels and trans-mutants in cladding and structural materials that can profoundly alter the overall chemistry of materials, especially at high burnup. The PKAs as well as recoiling fission products and trans-mutant nuclei quickly lose kinetic energy through electronic excitations that are not generally thought to produce atomic defects and as a result of a chain of atomic collision displacements that produce a cascade of vacancy and self-interstitial defects. High-energy displacement cascades occur over very short time spans of 100 picoseconds or less, and in small volumes, covering a size of about 50 nm or less in length. They can be modeled using molecular dynamics (MD) simulations if accurate potentials are available.

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[17] D. R. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements," U.S. Department of Energy, June 1976. Report TID-26711-P1.

[18] G. R. Odette, B. D. Wirth, D. J. Bacon and N. M. Ghoneim, "Multiscale-Multiphysics Modeling of Radiation-Damaged Materials: Embrittlement of Pressure Vessel Steels", *MRS Bulletin*, vol. 26, 2001, p. 176.

B.D. Wirth, G.R. Odette, J. Marian, L. Ventelon, J.A. Young and L.A. Zepeda-Ruiz, "Multiscale Modeling of Radiation Damage in Fe-based Alloys in the Fusion Environment," *Journal of Nuclear Materials,* vols. 329-333, part 1, 2004, pp. 103-111. Proceedings of the 11th International Conference on Fusion Reactor Materials (ICFRM-11).

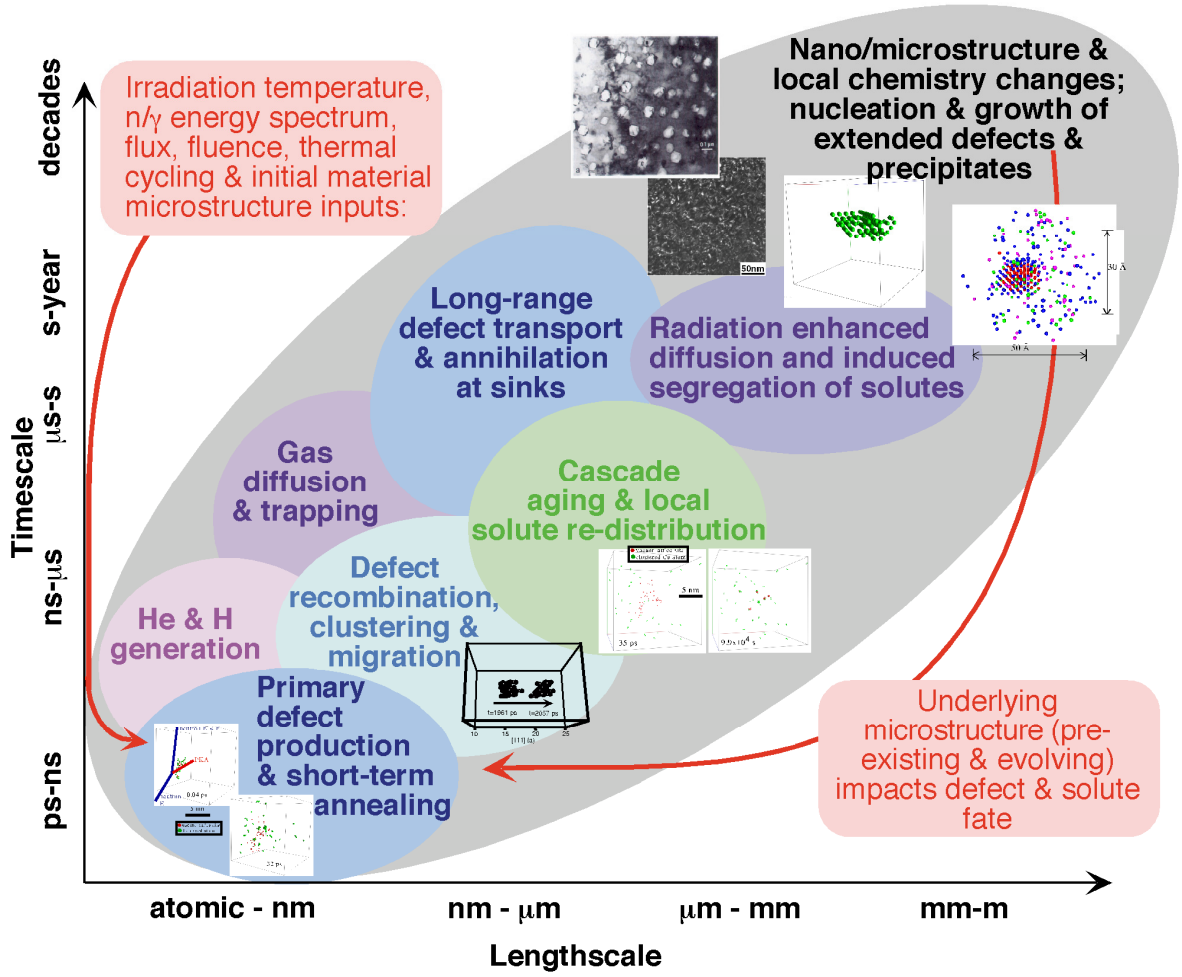

Figure 1 –The multi-scale processes responsible for micro-structural changes in irradiated materials that are categorized by size and the duration of radiation exposure. (See LAMMPS [Large-scale Atomic/Molecular Massively Parallel Simulator] Web site. http://lammps.sandia.gov/bench.html).

Materials scientists who have studied the physics of primary damage production in high-energy displacement cascades using MD simulations[19] have found that:

1) The intra-cascade recombination of vacancies and self-interstitial atoms (SIAs) results in ~30% of the defect production expected from displacement theory;
2) Many-body collision effects produce a spatial correlation (separation) of the vacancy and SIA defects;

[19] A. F. Calder and D. J. Bacon, *Journal of Nuclear Materials*, vol. 207, 1993, p. 25.
W.J. Phythian, R.E. Stoller, A.J.E. Foreman, A.F. Calder, and D.J. Bacon, "A Comparison of Displacement Cascades in Copper and Iron by Molecular-Dynamics and Its Application to Microstructural Evolution," *Journal of Nuclear Materials*, vol. 223, 1995, pp. 245-261.

3) Substantial clustering of the SIAs and to a lesser extent, the vacancies, occurs within the cascade volume; and
4) High-energy displacement cascades tend to break up into lobes or sub-cascades that may also enhance recombination.[20]

Research has concluded, however, that the subsequent diffusional transport and evolution of the defects produced during displacement cascades are the primary cause of radiation effects in materials and changes in material microstructure,[21] in addition to solutes and transmutant impurities. Displacement cascades begin by having important spatial impacts at small scales that continue to play a significant role over much larger scales, as do processes that include defect recombination, clustering, migration, as well as gas and solute diffusion and trapping. Consequently, changes in the underlying materials structure reflect the time and temperature kinetics of diffusive and reactive processes, although they are strongly influenced by spatial correlations associated with the microstructure and the continuous production of new radiation damage.

Since there is such a wide range of time scales and a "rare-event" nature characteristic of controlling mechanisms, efforts to model the effects of radiation on materials are extremely challenging and it is often difficult to obtain even tentative characterizations of the processes. Indeed, materials scientists have been unable to create accurate models of microstructure evolution during service that consider point defects, dislocations, and grain boundaries.

Today, materials scientists face a substantial challenge: to discover the processes that control how nuclear materials perform and use them to model this behavior. To create what we would regard as high fidelity models, scientists would need to develop a more profound understanding of irradiation effects and microstructure evolution through a combination of experimentation, theoretical analysis, and computation. Exascale computing can enable such breakthroughs through discovery-class simulations, although scientists would need to assess how accurately models can describe critical physical phenomena. If they could overcome some of the important limitations in current knowledge about the kinetic processes that control defect cluster and microstructure evolution, as well as materials degradation and failure modes, it would open the way to include accurate descriptions of key controlling processes in high fidelity models and reduce errors currently due to in-service surprises.

In summary, the challenges that materials scientists face in developing high fidelity nuclear materials performance models are many. They include:

1. Bridging the inherently multi-scale time and size scales that characterize materials degradation in nuclear environments;

[20] Calder and Bacon. Phythian, Stoller, Foreman, Calder, and Bacon.
[21] Odette, Wirth, Bacon, and Ghoneim. Wirth, Odette, Marian, Ventelon, Young, and Zepeda-Ruiz.

2. Dealing with the complexity of multi-component materials systems, including those in which the chemical composition is continuing to evolve as a result of nuclear fission and transmutation;
3. Discovering the controlling factors that are key to materials performance and including them in models; this would reduce the likelihood of technical surprises;
4. Transcending ideal materials systems to engineering materials and components; and
5. Incorporating error assessments within each modeling scale and propagating the error through the scales to determine the appropriate confidence bounds on performance predictions.

If materials scientists can successfully meet these challenges, they will create nuclear materials performance models that can predict the properties, performance and lifetime of nuclear fuels, cladding and components in a variety of nuclear reactor types. They will be able to describe events throughout the entire reactor life cycle, and provide a scientific basis for the computational-based design of new, advanced materials. High performance computing at the petascale and exascale levels and beyond is a necessary and critical tool in resolving these challenges. Nevertheless, it is important to realize that exascale computing on its own will not be sufficient. This is demonstrated if we consider the computational degrees of freedom in a molecular dynamics simulation. If we assume that reliable, multi-component, inter-atomic potentials exist for actinide-bearing nuclear fuels and that a constant time-step of $2x10^{-15}$ seconds would sufficiently capture the physics of high-energy atomic collisions and conserve energy, then to simulate a single day's evolution of a 1 centimeter tall and 1 centimeter in diameter fuel pellet would require ~$6x10^{22}$ atoms for ~$4x10^{19}$ time-steps. By comparison, the LAMPPS molecular dynamics code using classical force fields has been benchmarked with 40 billion atoms ($4x10^{10}$) and 100 time-steps on 10,000 processors of the RedStorm at Sandia National Laboratory with a wall clock time of 980 seconds and on 64,000 processors of the BlueGene Light at Lawrence Livermore National Laboratory with a wall clock time of 585 seconds [8a] Thus, even if we assume optimistic scaling and parallelization, a brute force atomistic molecular dynamics simulation of the first full power-day that a nuclear fuel pellet experiences in a reactor is likely to remain well beyond the reach of high performance computing capabilities for the next decade.

With these challenges to the development of a high fidelity nuclear materials performance models in mind, we recommend four primary research directions that we will discuss in greater detail in the section that follows. These recommendations include developing the ability to:

1. Understand and predict micro-structural evolution in irradiated nuclear materials;
2. Perform electronic structure calculations of the fundamental mechanisms within either solid or liquid nuclear materials reliably and accurately;
3. Predict the macroscopic properties and performance of non-equilibrium and evolving micro-structures; and
4. Predict the degradation due to coupled extreme environments, e.g., involving corrosion, high temperature, thermo-mechanical cycling and irradiation.

4.3. Priority Research Directions

The theory and simulation of complex systems in materials science and condensed matter physics employs a hierarchy of models that include: macro-scale continuum mechanics, meso-scale models of defect evolution, molecular scale models based on classical mechanics, and various techniques that represent quantum-mechanical effects. In Figure 2, these models are classified according to the spatial and temporal scales that they describe. Figure 2 also identifies individual modeling techniques that are described as a series of linked process circles that overlap in parts of the length scale and time scales. The modeling approaches are: *ab initio* electronic structure calculations, molecular dynamics (MD); accelerated molecular dynamics; kinetic Monte Carlo (KMC); phase field equations or rate theory simulations with thermodynamics; and kinetics by passing information about the controlling physical mechanisms between modeling techniques over the relevant length and time scales. The objective of this approach is to track the fate of solutes, impurities and defects during irradiation and provide modeling techniques that predict micro-structural evolution.

In short, detailed micro-structural information is the basis for modeling the mechanical behavior through meso-scale, i.e., kinetic Monte Carlo, dislocation dynamics, and phase field methods, and continuum scale models. The latter models must be incorporated into constitutive models at the continuum finite element modeling scale in order to predict performance limits on both the test coupons and components.

Multi-scale simulation provides the means to span length and temporal scales. In Figure 2, arrows illustrate how information passes between the scales, so that lower length scale modeling provides constitutive properties to higher length scale, continuum level simulations, while higher length scale simulations provide boundary conditions to the lower length scale models. Higher length scale simulations also contribute information about the accuracy or/validity of the predicted constitutive properties.

Due to the current limits of simulations to describe materials evolution over long periods of time, materials scientists are restricted in their ability to describe slow processes (e.g., phase transitions) or rare events, both of which will play an important role in harsh nuclear environments. At present, there is no way to link single-scale methods into a multi-scale simulation that incorporates error control across the scales in a reliable manner. Models can introduce errors when they pass information from fine grained to coarse grained models because this typically means there is a loss of physical detail. Multi-scale simulations are computationally intensive even when they do not include error controls. Massively parallel computation can provide a way to overcome most length-scale constraints because computers configured as clusters or grids can run simulations that focus on different spatial regions in parallel.

The same approach cannot resolve time scale constraints since, with a few exceptions,[22] models that analyze time scale events must run sequentially and are not suitable for parallel processing. Molecular dynamics simulations that model realistic forces calculated from electronic structure theory[23] can reliably simulate ~50 picoseconds of evolution, while similar simulations employing more simplified assumptions about empirical force fields can reliably simulate hundreds of nanoseconds but cannot describe bond breaking or charge transfers. Thus, as previously discussed, molecular dynamics simulations alone will be unable to simulate the dynamic behavior of nuclear materials over long periods of time. Recently developed accelerated molecular dynamics,[24] meta-dynamics,[25] or adaptive kinetic Monte Carlo methods[26] can extend time scales out to microseconds and beyond when high performance computing is used and limits are placed on system size.

[22] A.F. Voter, "Parallel Replica Method for Dynamics of Infrequent Events," *Physical Review* B vol. 57, 1998, p. 13985.

[23] R. Car and M. Parrinello. "Unified Approach for Molecular Dynamics and Density-Functional Theory," *Physical Review Letter,* vol. 55, 1985, pp. 2471–2474.

[24] B.P. Uberuaga, F. Montalenti, T. C. Germann, and A. F. Voter, "Accelerated Molecular Dynamics Methods," p. 629 in Sidney Yip, editor, *Handbook of Materials Modeling,* Volume 1, Part A—Methods. Dordrecht, Berlin, Heidelberg, New York: Springer, 2005.

[25] A. Laio and M. Parrinello, "Escaping Free-Energy Minima", *Proceedings of the National Academy of Sciences*, vol. 99, 2002, p. 12562.

A. Kushima, X. Lin, J. Li, J. Eapen, J. C. Mauro,X. Qian, P. Diep, and S. Yip, "Computing the Viscosity of Supercooled Liquids", *Journal of Chemical Physics*, vol. 130, 2009, p. 224505.

[26] G. Henkelman, and H. Jonsson, "Long Time Scale Kinetic Monte Carlo Simulations without Lattice Table," *Journal of Chemical Physics,* vol. 115, 2001, p. 9657.

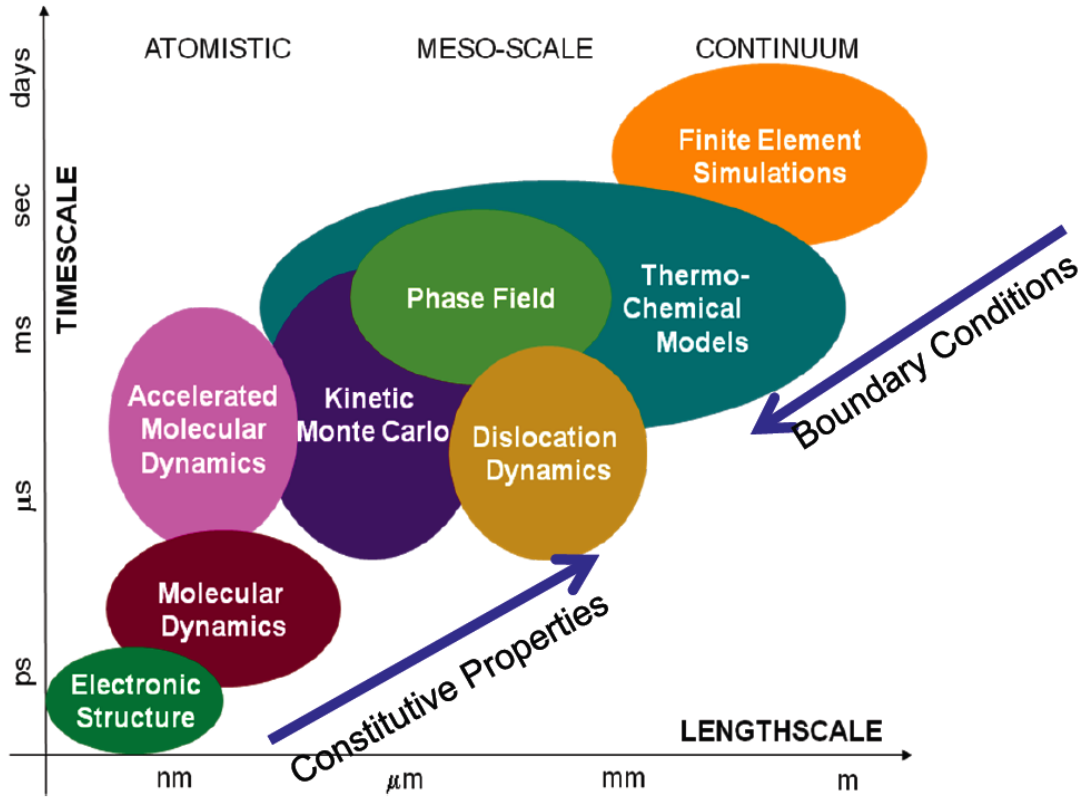

Figure 2 – Multi-scale materials modeling paradigms, showing simulation techniques that address events at specific length scale (size) and time scales. When hierarchical modeling is used, lower length (size) scale models provide constitutive properties that are used in larger length scale methods, while boundary conditions are provided by continuum simulations (reproduced from W.J. Phythian, R.E. Stoller, A.J.E. Foreman, A.F. Calder, and D.J. Bacon, "A Comparison of Displacement Cascades in Copper and Iron by Molecular-Dynamics and Its Application to Microstructural Evolution," *Journal of Nuclear Materials*, vol. 223**,** 1995, pp. 245-261.)**.**

In conclusion, the central challenge is to develop a predictive capability that allows scientists to model how radiation affects concentrated alloys with complex, realistic micro-structures. This will require further development of predictive theories of kinetics, nucleation and coarsening. Such advances assume that scientists will achieve a level of predictive capability where multi-scale models will accurately describe macro-scale properties that include detailed depictions of microstructure evolution. Such a predictive capability implies that key coarse-grained order parameters (or collective variables) can be transferred from the lower scale models and incorporated into engineering calculations, for example, into continuum finite-element-type models.

Materials scientists also face a series of challenges in other aspects of modeling. First, there is an urgent need for efficient and accurate predictive modeling of thermally activated unit mechanisms. This should cover both atomistic and meso-scopic scales, and

couple dislocation processes with alloy chemistry, diffusion and precipitation. It should also include voids, dislocation loops and point defect clusters, grain growth, and other relevant phenomena. Second, although there has been progress modeling phase nucleation and stability involving alloy chemistry under irradiation,[27] this is a long-standing scientific problem and much still remains to be done. Third, another challenge is the need to combine multiple concurrent processes into a comprehensive computational model to provide accurate descriptions of the co-evolution of various interacting elements of microstructure—dislocations, grain boundaries, radiation defects, and alloy phases—to yield the required net thermo-mechanical response. If hierarchical, multi-scale simulation is to become a useful and reliable tool for material design, insertion, and certification, models at every single-scale level will have to be computationally efficient. That is, they will need to allow not only for error propagation and quantification-margin-uncertainty analysis but also for a thorough exploration of the relevant parameter space in order to identify most the informative validation experiments.

Reliable/Accurate Electronic Structure Predictions of Fundamental Mechanisms

To model and simulate advanced nuclear energy systems, scientists must be able to predict the electronic structure of chemicals and materials with accuracy. This would let them obtain accurate information about the thermodynamics of such systems and the kinetics of critical reactions and processes that are crucial to the modeling and simulation of advanced nuclear energy systems. Several caveats must be noted for these models. One is that compounds containing heavy elements require a proper treatment of relativity that includes both scalar relativistic and spin-orbit components. For instance, actinide and lanthanide bearing molecules and materials with open *4f* and *5f* shells exhibit strongly correlated electron behavior, a feature that has prevented reliable prediction of their physical properties with current electronic structure methods. As a consequence, there is a need to develop new approaches to describe molecular behavior and the solid state so that models can accurately incorporate strong electron correlations, spin-orbit coupling, relativistic effects, and multiplet complexity. Some new approaches that are promising include: improved density functional theory (DFT), exchange-correlation functionals, dynamic mean field theories; quantum Monte Carlo methods; and new, highly-correlated, molecular orbital theory approaches.

To improve electronic structure predictions, the new theories, their algorithmic implementation, and application need to focus on accurately predicting physical properties. This need not include empirical parameters and uncontrolled approximations. Since nuclear transmutation of fuels results in the development of complex mixed actinide/lanthanide solids and there is also a potential for the formation of many phases that can influence critical physical properties, such as thermal conductivity, new *ab initio* electronic structure results must be integrated with available thermodynamic databases to facilitate the prediction of phase equilibria and oxidation states that contain fission products that may be generated in a reactor core or mixed into fresh fuel. Theoretical

[27] Odette, Wirth, Bacon and Ghoneim.

development will drive innovations in physical property measurement techniques that can be used for validation and to quantify uncertainty better. In addition, transferring quantitative measurement of the propagation of uncertainties in physical property models to uncertainties in system performance must be formalized.

Such new electronic structure approaches also need to be able to quantify the defect properties of multi-component actinide fuel/fission product systems (including conventional fuel compositions and advanced fuel forms such as inert matrix fuels). For example, the quantitative modeling of redox reactions, critical for the interpretation of speciation, requires the ability to treat different numbers of *f* electrons with substantially improved calculation accuracy. For solids, a new underlying theory is needed to compute fundamental defect properties such as the formation and migration energies in both pure metals and compounds (oxides, nitrides, carbides) that involve mixed actinides and lanthanides. To predict the transport properties (thermal, mechanical, mass) of these materials, scientists need to calculate the defect physics accurately. Furthermore, the presence of persistent non-equilibrium defect/solute densities and fluxes from irradiation may alter phase equilibria and enhance transport properties.

The dynamics of many of the processes that generate nuclear fuels and are used to separate spent fuel for recycling or waste involve complex reaction coordinates, not just simple bond breaking or formation, and control the selectivity and efficiency of separations processes. The vast majority of such processes occur in solutions or at interfaces. Weak, anharmonic, coupled interactions that dominate solution behavior, such as hydrogen bonds and van der Waals interactions, and stronger interactions, such as ion-ion interactions and bonds between ligands and metal atoms, play crucial roles in separations or radiolytic processes. But since the common density functional methods currently used by the broad scientific community do not treat such weak interactions well, advances in the development of accurate reactive force fields for classical molecular dynamics (MD) simulations of solutions in which solute and solvent polarization occur are needed. In addition, new sampling and time integration algorithms are required to enable the simulation of rare events using MD. Such advances would permit scientists to investigate large systems and provide initial structures for more accurate computations at the electronic structure level. Besides these advances, new techniques are needed to predict the effects of radiolysis, which introduces trace species with cascading chemical effects that result in surface and materials damage and to reactions in solution. At the present time, it is extremely difficult if not impossible to predict the reaction rates of radicals in solution. This is especially true of fast reactions. Predictability is even worse for reactions of highly excited states formed from the interaction of radiation and molecules.

New techniques to optimize and sample large realms of parameter space need to be developed if scientists are to create new solvent systems (e.g., ionic liquids) to minimize environmental concerns. To improve current solution models for thermodynamics, scientists would need to move beyond the parameterized, self-consistent, reaction field approaches that are employed to predict the properties that depend on temperature, pressure, pH, and ionic strength. Innovations are also needed in the methods used to

predict the properties of alternate media, such as molten salts, ionic liquids, or supercritical fluids. Improved computational techniques are required to characterize long-duration dynamic events that include processes like diffusion, self assembly, self healing/repair, and rare-event kinetics. Additional innovations are needed to improve the methods currently used to study nucleation phenomena and reactions leading to colloid formation. All of these new capabilities will facilitate the prediction, management, and control of entropic processes.

As a result of the innovations and advances described above, scientists would achieve a far better predictive capability (e.g., chemical accuracy for equilibrium constants and rate constants) to model solutions and interfacial phenomena for actinide-containing systems under extreme conditions of pressure, temperature, pH, and high radiation fields for aqueous media as well as other solvents and other media such as molten salts and ionic liquids. Such advances will give scientists the ability to predict how nuclear materials behave under "real" irradiated conditions and to enhance the design of separation systems for current and future fuel cycles, as well as materials used for waste management. As a consequence of having improved input data for large-scale simulations of nuclear plants and separation plants, designers will provide better construction designs, more optimal operating conditions, and better control over catastrophic events. In order to attain these advances, scientists must develop new modeling techniques and will need to exploit petascale and exascale or higher scale computing resources. The results could have a substantial impact on the design of fuels, separations systems for current and future fuel cycles, and waste systems.

Predict Macroscopic Properties and the Performance of Non-equilibrium Evolving Micro-structures

While materials scientists and engineers routinely manipulate the microstructures of materials by controlling the manufacturing processes needed to create required properties, the complexity of modern engineering materials and the multitude of micro-structural mechanisms that can contribute to the macroscopic performance of materials make the prediction of chemical properties from evolving microstructures a grand challenge in materials theory, modeling and simulation. As a consequence, scientists are turning away from the centuries-old approach of creating engineering materials that can be improved by empirical experimentation. For example, in the past, the hardness of steels with the same chemical composition has been improved by an order of magnitude during processing with the resulting parts easily hardened to bear significant loads. In practice, the optimization of new manufacturing processes has been done largely through empirical adjustments. For example, actinide-bearing fuels and wastes often contain significant concentrations of a dozen or more elements. Cladding and containment vessels are similar in their chemical complexity. In the case of fuels, this chemical complexity develops naturally during burnup and increases with increasing burnup. In structural materials, the chemistry is complicated by design to improve the in-core properties and life limits of these materials. While materials scientists and engineers can, as demonstrated in the past, empirically design processes to optimize microstructures of

fresh fuels and structural materials, these microstructures may not endure through the service life of the fuels and wastes, as discussed in the first Priority Research Direction

The prediction of properties and performance from microstructures at the end of nuclear reactor service life is most critical and challenging. To break the current experimental bottleneck associated with the aging of materials in test reactors, materials scientists need a robust theory, modeling and simulation effort to predict the physical properties that result from irradiated microstructures. This new approach would overcome the difficulty scientists currently have when they try to reproduce the microstructures observed inside reactor cores or waste repositories in an accelerated laboratory setting. One step in this direction is that high-fidelity performance models can be benchmarked to a wider variety of microstructures and external loadings (mechanical, thermal, and irradiation-based) in a laboratory setting than is possible in a reactor. These models provide a way to analyze the energy and kinetics of multiple competing physical mechanisms relevant to a reactor setting so that each mechanism can be investigated separately, parameterized, and explicitly included in the model. Using this approach, integral reactor material irradiations can be used for validation, to show that the relevant mechanisms have been appropriately included and properly parameterized. Through this targeted focus on individual mechanisms and their cooperation and competition in the manifestation of macroscopic properties, theory, modeling, and simulation will serve as the basis for the creation of truly predictive tools.

The most important macroscopic material properties in advanced nuclear energy systems are (in no particular order): 1) thermal conductivity; 2) fracture toughness; 3) mechanical strength; 4) creep resistance; 5) swelling resistance; 6) corrosion resistance; and 7) chemical species diffusivity. The external factors that alter these properties include a broad spectrum of neutron irradiation dose rates, high temperatures, high heat fluxes, and mechanical loading. In parallel with the way that multiple length (size) scales play a role in the outcome of the micro-structural evolution of materials in nuclear energy system environments, multiple length (size) scales are simultaneously involved in manifesting the macroscopic properties of materials. For example, creep resistance may be controlled by bulk diffusion processes (Nabarro-Herring), dislocation climb, and/or grain boundary diffusion (Coble). Each of these processes operates on a different length scale, and each has its own micro-structural variables with its own distinct kinetic equations.

Furthermore, not only can the microstructure dictate which mechanism dominates, but the thermal, irradiation, and mechanical loading conditions can also determine the dominant mechanism. Similarly, predicting the thermal conductivity of a material at the atomic level includes both electronic and ionic contributions to the thermal conductivity of bulk material, and, and at larger length scales, the influence of scattering from solute atoms, second phase precipitates, dislocations, and grain boundaries. To create credible predictions of macroscopic properties under a wide variety of conditions, meso-scale simulations must simultaneously incorporate all of the known unit mechanisms together to transcribe the discrete defect dynamics at the atomic level to the coarsened engineering behavior of materials. These meso-scale simulations typically employ phase field methods, rate theory, and discrete defect dynamics so that they can incorporate the

competing unit mechanisms from which macro-scale properties are derived. Such simulations will very likely continue to push the limits of future massively parallel computing platforms. Spatial discretization of competing unit mechanisms operating at different length (size) scales may require on the order of a trillion mesh points yielding $1/10^4$ resolution in each dimension spanning 10 nanometers to 100 micrometers. Likewise the temporal discretization may require a resolution of $1/10^{10}$ with the fastest kinetic processes operating at microsecond timescales and incorporate macro-properties that evolve over a span of days. While spatial fidelity maps well into anticipated advancements in high performance computing hardware, temporal fidelity requirements do not. Improvements in time integration may need to await algorithmic breakthroughs.

The co-integration of competing unit mechanisms to predict the macro-scale properties of materials from their micro-structural foundations can only be as good as the database of unit mechanisms included in the integral simulations. Materials scientists need to carry out high-resolution electronic structure and atomistic simulations and accelerated bench top experiments to identify these unit mechanisms. Nevertheless, there remains an inherent danger that the relevant mechanisms that control macro-scale properties will operate on timescales longer than those that can be evaluated using these methods. As a consequence, "rare event" sampling algorithms need to be developed to extend the timescales of these simulations so that in-service surprises caused by unknown mechanisms do not occur. This may be the greatest risk to the program, and can only truly be resolved by resorting to test reactor validations of radiation effects.

Predict Coupled Environmental Degradation (Irradiation, Corrosion, and Thermal-mechanical) Mechanisms

Advanced nuclear energy systems will require materials that can perform in aggressive environments for extended lifetimes under conditions that are close to safe operating limits. Some examples of such materials are: materials for high temperature gas-cooled reactor systems; high temperature, liquid metal or supercritical fluid systems; and advanced light-water reactor systems. In this context, special attention should be paid to a range of materials degradation phenomena that range from general surface dissolution to localized corrosion, such as pitting, stress corrosion cracking and hydrogen or liquid metal embrittlement. Such degradation occurs in the presence of intense radiation, high temperature, and mechanical stress, and includes a common underlying element, the interaction of an interface between a base material, often a metal alloy, and a gaseous or liquid environment. Figure 3 illustrates such an interaction between the interface layer and its environmental surroundings that results in the formation of local pits that subsequently concentrate stress and break inter-atomic bonds, resulting in materials degradation. This is a plausible explanation of how trans-granular and/or inter-granular cracks can be initiated and propagated, but it has not been confirmed in quantitative testing. The fracture or compromise of the protective layer also provides a route for the transport of "embrittling" factors such as oxygen and/or anions, such as chloride, to new reactive zones. The evolution of thermal, micro-structural and stress environments further aggravate the creation of such transport opportunities. Thus, at the molecular scale, stress

corrosion phenomena have their origins in the action of aggressive elements and anions in the interface layer with their environmental surroundings.

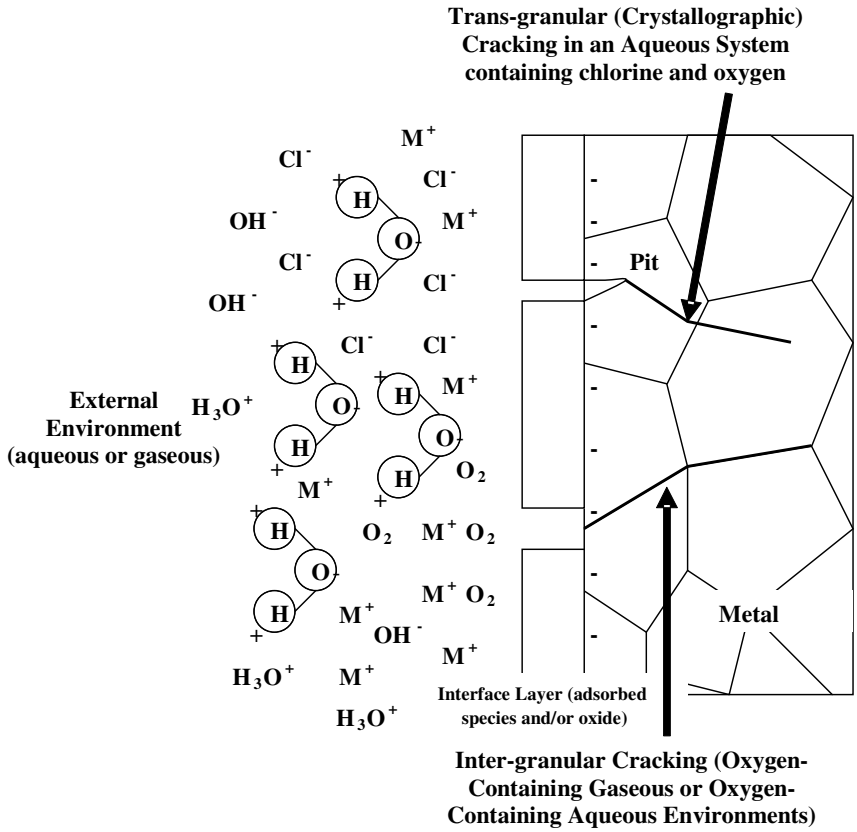

Fig. 3. The formation and destabilization of an interface layer as a result of environmental degradation, leading to trans-granular and inter-granular cracking (Source: R. G. Ballinger, Private communication with S. Yip, Massachusetts Institute of Technology, 2006.)

We can illustrate the issues that require additional study by considering two related baseline problems. One involves trans-granular cracking in alloy systems at low temperature, such as austenitic stainless steels and the other is inter-granular cracking that occurs at higher temperatures. In an aqueous environment, corrosion resistance in a system such as Iron-Nickel-Chromium (Fe-Ni-Cr) is strongly influenced by the presence of specific anions, usually oxygen and halogens, especially chloride. The environment-layer interaction results in the development of a surface defect, and the initiation and propagation of a trans-granular (crystallographic) crack. The susceptibility of a material to this process strongly depends on the base alloy composition, especially the nickel content in a fully austenitic system. Susceptibility reaches a maximum when nickel content is approximately 8 wt% in a nominal Iron-18 wt% chromium alloy. In additional,

a high degree of susceptibility requires the presence of a minimum oxygen concentration of approximately 0.15 ppm. Degradation processes involve an interaction between the anion, oxygen and the surface, in conjunction with mechanical stress, resulting in an initiated-propagating trans-granular crack. For both gaseous and aqueous environments, by comparison, the presence of oxygen is a key factor in the initiation and propagation of inter-granular cracks. When the critical nickel content is above the 8 wt% in the first model, inter-granular cracking now occurs with higher nickel (>50 wt %) contents. The presence of the grain boundary introduces an additional complicating factor (higher transport rates, variable chemistry, etc.), the key variable being the oxygen concentration, whether in a gaseous environment at high temperatures (T> 450°C) or in an aqueous environment at lower temperatures (~300°C). In both models, mechanical stress plays a key role in facilitating layer destabilization.

Successfully applying advanced modeling and simulation techniques to the problem of environmental cracking is a formidable challenge, even in the absence of radiation damage. Such an application is made difficult by the fundamental nature of chemo-mechanical phenomena that require that chemical reactivity and mechanical deformation be considered of equal importance.[28] Progress in applying such techniques to environmental cracking would very likely have a broad impact on the science and technology of materials performance.

4.4. Summary

Materials scientists face a tremendous challenge: to develop transuranic-bearing nuclear fuels, fuel cladding and structural components for advanced nuclear reactors that withstand ultra-high fuel burnups, neutron doses and temperature extremes. Meeting this challenge will require these scientists to push the limits of high performance computational materials modeling.

In the past, developing materials to meet such requirements has involved decades-long testing and examination. Such long lead times are a result of scientists' exclusive reliance on nuclear test reactor radiations to drive micro-structural and material property changes and their desire to create materials that can endure long service lifetimes. Certainly, economic considerations and fuel economies are part of the push for long material service lifetimes and the deep burn of fuels. These drivers will only exert greater pressure in the future.

The future holds the promise of high-fidelity predictive performance models not only to predict the lifetime and failure of fuels and components in a wide variety of advanced nuclear energy systems, but also to enable the design of new materials tailored for such aggressive environments. This report has documented a number of challenges that must be overcome before materials scientists can develop high fidelity nuclear materials performance models that are able to:

[28] R. Staehle, "Proactive Material Degradation Assessment," Department of Energy, Nuclear Regulatory Commission, Report NRC-PMDA-PIRT, Appendix A, 2005.

1. Bridge the multi-scale time and length (size) scales which characterize materials degradation in nuclear environments;
2. Deal with the complexity of multi-component materials systems, including those in which the chemical composition is continually evolving due to nuclear fission and transmutation;
3. Discover the controlling factors that are key to materials performance and include them in models in order to reduce the likelihood of technical surprises;
4. Transcend ideal materials systems to engineering materials and components; and
5. Incorporate error assessments within each modeling scale and propagate the error through the scales to determine the appropriate confidence bounds on performance predictions.

5. Final Whitepaper - Verification, Validation and Uncertainty Quantification Panel

5.1. Introduction

This whitepaper provides a framework for understanding the role that Verification and Validation (V&V), Uncertainty Quantification (UQ) and Risk Quantification -- collectively referred to as VU (Verification & Validation and Uncertainty Quantification) -- play in modeling nuclear energy systems. The first part of the paper explores the modeling of nuclear-energy systems. The next section discusses the critical elements of V&V as it applies to nuclear energy systems. This exploration covers a broad spectrum of scientific and engineering disciplines that include astrophysics, chemistry, physics, geology, hydrology, chemical engineering, mechanical engineering, civil engineering, electrical engineering, nuclear engineering and materials science. In the final section, we examine the critical issues and challenges that scientists need to address to develop a viable and sustainable VU program to support the modeling of nuclear energy systems.

5.2. Background on Modeling Nuclear Energy Systems

Nuclear energy systems and their associated fuel cycles involve complex, interacting subsystems. To model these systems requires expertise that spans many scientific and engineering disciplines. The modeling must include the main stages of the nuclear fuel cycle, such as mining and milling, conversion, enrichment, fuel fabrication, power production, temporary spent-fuel storage, separations, and nuclear waste disposal. The choices of fuel cycle (open or closed), fuel type and reactor type will determine which stages are important and the role each stage plays. Computational simulations of each fuel-cycle stage have played a major role in the advancement of nuclear energy, especially when we examine the history of power production, separations and nuclear waste disposal. An extensive array of experiments has validated these computational simulations, ranging from basic physics experiments on nuclear data, to single-effects experiments, to integral, system-level experiments. In total, these experiments have cost tens of billions of dollars over several decades, but there are still gaps in the experiments covering severe accidents and aging.

By employing an experimental base, scientists have been able to improve simulations. They have improved the models, numerical approximations, and input data. More recently, researchers have estimated uncertainties using best-estimate predictions by mathematically propagating the uncertainties in input data, initial conditions, and sub-models through simulators. The U.S. Nuclear Regulatory Commission has accepted this process in its Code Scaling, Applicability and Uncertainty (CSAU) methodology. Nevertheless, because current nuclear system simulations are not based upon micro-scale,

science-based models, but on macro-scale models, for example, a heat transfer sub-model, scientists can only evaluate uncertainties for a limited number of parameters.

As simulations become more science-based, they will rely more heavily on micro-scale sub-models. Because informed design decisions depend upon macro-scale responses, designers will make greater use of multi-scale modeling. In addition, because nuclear energy systems are like other complex systems and involve the interaction of a great many physical phenomena, tightly-coupled, multi-physics modeling will also play a larger role in the future. New VU capabilities will be necessary to support the development of multi-physics and multi-scale modeling. Advances in computing power will enable some of these required, new capabilities, but others will require improvements in the mathematical and algorithmic foundations of VU.

For nuclear energy systems, there are two motivations to perfect VU. The most obvious is to improve the confidence users have in simulations' predictive responses and our understanding of prediction uncertainties in simulations. Additionally, scientists must also perform VU for nuclear energy systems because the USNRC, the licensing body, requires it. This is based on the premise that an extensive experimental database can provide important insights about system attributes.

VU's objective is to predict with ***confidence***, using computer simulation models, ***best estimate*** values and the associated ***uncertainties*** of complex system attributes, while also accounting for all sources of error and uncertainty. This means:

- Modeling;
- Numerical treatment;
- Software errors;
- Epistemic uncertainties (i.e., data as well as correlations);
- Aleatoric, or contingent, uncertainties (i.e., random phenomena); and
- Initial and boundary conditions.

If VU satisfies this objective, it will support the following favorable outcomes:

- The ability to make confident, risk-informed decisions when considering alternative designs and operations.
- More specifically, the ability to:

  - Identify code development needs;
  - Identify and design the required validation experiments;
  - Make design decisions needed to manage margins; and
  - Present a risk-informed safety case to the regulatory body.

One challenge for VU when applied to nuclear systems is that it must predict any high-impact consequences of low-probability events with high confidence. This must be done factoring in aging effects, even if there is limited experimental data at the macro scale. This challenge is similar to the one associated with the stewardship of nuclear weapons.

Attributes of Nuclear Systems' Models

Given the diversity among the stages of the nuclear fuel cycle, there is considerable diversity in the associated simulation models. To illustrate the complexity of nuclear systems' simulation models, we can cite the nuclear fuel cycle's power production stage. To model a nuclear power plant, including the mechanical, electrical, and nuclear components and systems, structures, and the external environment, scientists must model a wide range of behaviors. These involve: 1) the thermal-hydraulic behavior of fluid circuits, including fluid-structure interactions; 2) thermal behaviors of components making up the system; 3) material behaviors factoring in radiation, temperature, pressure, and chemistry effects; 4) structural responses; 5) instrumentation responses; 6) control and protection systems logic; 7) reactor physics; and 8) radiation fields. In running simulations, most users recognize that weak to strong coupling exists between these effects due to natural or engineered feedback effects. Today, simulation packages such as TRACE, TRAC, RELAP and SASSYS, limit users not only in the detail they can achieve in modeling analysis, but also in the degree of coupling that models can represent. Introducing science-based, multi-physics, and multi-scale modeling will only exacerbate these modeling challenges, making them orders-of-magnitude more challenging when best-estimate calculations are considered.

5.3. An Overview of the Key Elements for Verification and Validation and Uncertainty Quantification

To restate the definitions of verification and validation:

> **Verification** is the process of determining as completely as possible: 1) if a computer code correctly implements the intended algorithms; and 2) how accurately the algorithms solve the intended equations.
>
> **Validation** is an assessment of the degree to which predictions of a code represent the intended physical phenomena. This quantifies how accurately the model equations represent physical reality for a specified regime of applicability.

Verification

Code verification is detecting mistakes in the implementation of the chosen numerical algorithms. Such coding errors can often be uncovered through a rigorous process of software quality assurance, utilizing such approaches as programming by contract, unit tests, and code coverage assessment tools. Once these standard techniques have been applied to make the code as bug-free and robust as possible, a variety of test problems can be used to search for remaining errors in coding. For example, by computing the

error at different grid resolutions and directly using benchmark analytic solutions, scientists can observe the order of accuracy of a solution. They can then compare the accuracy with the formal order of accuracy they expect for the discretized equations. Employing manufactured solutions can help with such studies by providing analytic solutions.

It helps to think about verification testing and test problems in three ways. First, what is the ***structure*** of the chosen test problems, the logical principles that support them? This explains why given test problems are chosen and how they are organized. Second, what is the specific ***construction*** of the test suite or the specific means chosen to populate the test problem suite? Finding or developing test problems that fully address the complexities of multi-physics codes is a tremendous challenge. Third, what is the ***assessment***, or the criteria applied to decide whether or not the code has passed or failed a given test problem? The verification of test problems is supposed to be a strong test of the code, so the assessment must be objective, rigorous, and well documented.

Solution verification quantifies the numerical error in a calculation. This answers the question, "What is the error in a given calculation?" Unfortunately, with complex calculations, it is all but impossible to estimate such errors rigorously while also covering the entirety of the calculation. Nevertheless, we can address error calculations partially and practically by employing explicit discretization robustness and convergence studies, formal error estimation procedures, inference from test problem suites, and – possibly at some peril – inference from previous experience (i.e., judgment). Past experience can count for a great deal if it is properly understood and presented.

Even if code verification could prove that the implementation of algorithms is perfect, calculations could still be inaccurate due to poor discretizations, i.e., a lack of converged calculations. In general, any verification of the correct functioning of algorithms cannot be partitioned as cleanly as we would like. Using available test problems, it may be impossible to determine that algorithms are failing; the failures may appear only on large-scale problems for which there is no reference solution. Some procedures that offer promise for addressing this are: 1) *a posteriori* error estimation; 2) convergence studies; 3) numerical error models; and 4) uncertainty quantification methods that treat the numerical error as an epistemic (lack-of-knowledge) uncertainty. Validation, discussed below, depends on verification. Validation must account for the numerical errors present in any calculation to be compared with experimental data. The fundamental question that must be recognized, if not completely answered, is "Does the numerical error corrupt the comparison with experimental data?" Without proper acknowledgment of this problem, a comparison with experimental data can be misleading.

Validation

Scientists determine the physical fidelity of nuclear energy system design equations for specific applications through comparisons with experimental data that test an application's physical accuracy. If there are limited resources, validation tasks should be given priority. As a result, the desire to achieve a complete validation of a complex code

used in a predictive, elaborate, multi-physics application must be balanced against these resources. The key elements of an experimental validation that are necessary, but may not be sufficient, are:

1. The precise specification of needed validation tests that optimize the alignment of validation calculations with executed experiments. This requires sophisticated, two-way communications between those executing validation experiments and those performing validation calculations. When experimental data is not of a high enough quality to support validation, the validation is weakened. Users expect that experiments are subject to verification and validation so they can provide the highest quality data. That is, **experimental verification** confirms that scientists executed an experiment correctly; **experimental validation** confirms that scientists executed the right experiment.

2. The performance of solution verification for all validation calculations.

3. The development of quantitative measurements and/or computational prediction comparisons that include quantified uncertainty. This requires: a) experimental error bars that include experimental uncertainty; and b) calculation error bars that estimate calculation uncertainty that is determined by a simulation to measure uncertainty quantification (UQ).

Validation calculations are used to check the physical accuracy of the associated calculations; they compare calculations with validation-quality experimental data. Validation calculations facilitate the assessment of the physical quality, physical accuracy, and/or predictive capability of the code for the application that the chosen validation data represent. When validation calculations are compared to ***experimental data,*** these data need to have certain characteristics to insure that the validation effort is effective. Among these are a quantified experimental uncertainty, reproducibility, and robustness of experimental data and data that is as directly comparable with calculations as is possible.

Experimental "***error bars***" indicate "quantified experimental uncertainty." This problem cannot be completely and rigorously solved when complex experiments are involved. Experimental bias and variability are the components of error bars and different factors can affect the size of these components. Scientists can present experimental error bars as based upon experimental data. To perform a validation, scientists approximate experimental "error bars" and use them as a starting point to make inferences about the experimental-computational comparisons. In general, factors that contribute to experimental uncertainty are diagnostic fidelity, experimental variability, and experimental bias. The more we expect to draw rigorous inferences from a validation comparison, the more we need to know about how experimental error bars quantify experimental uncertainty. For example, does an experimental error bar represent a central tendency of an underlying Gaussian distribution, a statistical confidence interval, a description of a uniform distribution, a possibility interval, or something else?

Uncertainty Quantification

Uncertainty quantification (UQ) in large-scale simulations plays an increasingly important role in code verification and validation. If scientists want to validate a simulation using the quantitative results of an experiment, they must understand the expected uncertainty inherent in the calculation's output metrics. They must also estimate the size of the error bars associated with an experiment's output metrics. In practice, it is not difficult to assess a simulation's accuracy when the experimental uncertainty is less than the simulation's predicted uncertainty. An experiment's error estimates of uncertainty usually require scientists to perform experiments with controlled parameters and understand the known systematic errors.

Dynamic Probabilistic Risk Assessment (PRA) and Rare Outcomes

A broad definition of UQ includes risk quantification. By risk quantification, we are not only interested in a system's response metrics' uncertainty, but also how response metrics impact risk. Risk can include economic risks, human health risks, and other types of enterprise risk. Completion of an UQ is a necessary, but not sufficient, requirement for quantifying risk. Risk quantification requires a model that takes the metrics for a system's response and their uncertainties as an input, and produces risk metrics and their uncertainties as the output. In all likelihood, the risk model itself may be uncertain, i.e., the impact of a dose of radiation on human health. This calls for the convolution of the probability distributions from the system response metrics with the probability distributions of the risk metrics.

Dynamic, probabilistic risk assessment (PRA) is a very different example of risk quantification. In PRA, the main concern is the chance that a given sequence of events will occur. PRA includes the uncertainty associated with a stated likelihood, such as the PRA of high-consequence, rare-outcome event sequences. As a rule, rare-outcome events are quite sensitive to assumptions about distributions. If limited experimental data do exist, it is possible that researchers can develop limited information about distributions. In the following discussion of UQ, we will assume that risk uncertainty is included in both of the instances mentioned above.

Extrapolation Beyond a Validation Regime

Quantifying uncertainty in large-scale simulations is especially important when a simulation becomes a predictive tool to describe phenomena in a regime outside of the bounds of previous experimental tests or known observations. Examples of this circumstance in nuclear energy systems include accident analysis of nuclear power plants, forecasts of the effects of aging on materials in hostile environments, and forecasts of long-term, high-level, waste repository performance. Without experiments to check the code predictions in such regimes, it is essential to quantify the code output's expected uncertainty. It also is essential to catalog in a careful way all of the differences

that experts can determine between the physical model equations and the reality of physical phenomena. Without measurements as a reality check, a thorough analysis by experts is the only way to identify model error that scientists can quantify through further work. This aspect of UQ is a complex undertaking for any simulation code that has non-linearly coupled multi-physics algorithms that represent underlying physical phenomena.

The Aggregation of Uncertainties from Multiple Sources

The determination of uncertainty quantification is complex. It is a current research topic. In a complex, multi-physics, simulation code, many aspects of the physics can have a parametric representation or a choice of physics models; i.e., each aspect can have its own degree of approximation. The range or bounds of parametric settings in physical models and the choice of physics models represent an area of uncertainty in the simulation. In practice, scientists employ simulation codes with a particular choice of input physics models and perhaps a typical choice of parametric settings. This can proceed without an effort to explore the full range of uncertainty in the simulation's outcome. Occasionally, some large-scale simulations will run different models to estimate the range or dispersion of output results. This provides a measure of the uncertainty that is often quite insufficient to determine the simulation's full uncertainty.

To begin uncertainty quantification, scientists identify the known sources of uncertainty in a simulation. This can encompass several types of uncertainties: 1) those associated with approximated models that describe the underlying physics; 2) those that are approximations in the numerical algorithms; 3) those associated with the settings of parameters used in physical models; 4) those that are settings that individual algorithms may require to operate in a stable fashion; 5) those associated with various levels of opacity tables and equation-of-state tables; and, of course, 6) those associated with performing a simulation at a given spatial resolution when the resolution is not converged.

Estimating Uncertainty Quantification is an exercise in how to reduce the computing requirements of the full uncertainty space by a substantial enough factor so that computing can provide a solution. If we recognize that a multi-physics code embodies many components of coupled physics, there are a great many possible sources of simulation uncertainty. Moreover, the uncertainties associated with these sources do not necessarily combine linearly. Uncertainties associated with various physics models may cancel each other or result in compensating effects. In a realistic multi-physics, multi-dimensional code, the number of parameters whose values can be bounded might be large. Consequently, the problem of examining uncertainty that results from all possible non-linear interactions among the uncertain components to its fullest extent is exponentially complex.

Addressing High Dimensionality

As noted in the previous sections, an initial step to Uncertainty Quantification is the identification of all of a simulation code's avenues of uncertainty. Once this is established, scientists must develop a sensitivity analysis to determine what components of uncertainty, i.e., algorithmic approximation, parameters, etc., are the main factors influencing the output's metrics. This analysis is likely to follow an iterative process that is not determined *a priori*. If scientists perform a sensitivity study to filter out those components of uncertainty that may not be determinants of the output's uncertainty, they must know the physically- or mathematically-reasonable bounds of any set of parameters that represent a physical model. But the determination of physically-reasonable bounds could require considerable research and the quantification of such bounds might be possible using knowledge gained from experiments, analytic analysis and scientific judgment. With a first estimate of the sensitive drivers of the code response to parametric and physical model variation, scientists can view the problem as how to navigate the uncertainty of dominant drivers in an N-dimensional space, where each dimension represents a parameter, physical model, degree of approximation, etc., for the underlying code physics.

To accomplish this, scientists must account for correlations within the N-dimensional space, a procedure that may reduce the dimensionality. Thus, it is essential to sample the full N-dimensional space using a set of simulations that represent all the dimensions of uncertainty within the bounds of those dimensions. As a consequence, the problem of uncertainty quantification becomes one in which all identifiable uncertainties, and their interactions with one another, are run through the simulation code. This provides a predictable total output uncertainty in the code response to variations over acceptable bounds of all the components. The uncertainty in code response to variations in all the key components of the code can be expressed as the total uncertainty in the code output's main metrics; these are one objective of the simulation.

5.4. Key Issues and Challenges in V&V and UQ

Scientists must resolve many grand challenges before there is more widespread use of VU methodology. These challenges include how to: 1) couple predictive simulations with dynamic, probability risk assessments (PRA) and rare-outcome events; 2) quantify uncertainties after extrapolation beyond the validation regime; 3) aggregate uncertainties arising from multiple sources; and 4) a high-dimensional space of model parameters that is often referred to as the "curse of high dimensionality." The previous section highlighted each of these issues. In the previous discussion, each issue became more complex because, in general, it involved nonlinear, coupled, multi-scale physical systems. We will discuss some of the challenges for these complicated systems later in this section.

Future exascale computing environments are likely to pose new challenges for V&V and UQ. They will also provide opportunities, such as the possible deployment of intelligent systems that could self-adapt to manage the VU process more efficiently. An especially

important hurdle is how to perform a quantitative assessment of the VU methodology. A wide range of assumptions, statistical models, and function expansions, etc., are incorporated into a given VU methodology. In addition, scientists can *execute* the methodology with different degrees of formality, rigor, or completeness.

A Quantitative Assessment of VU Methodology

Using computer simulation models, VU's try to predict with ***confidence*** the ***best-estimate*** values and associated ***uncertainties*** of complex system attributes. If optimal, they will account for all of a system's sources of error and uncertainty. An important goal is to facilitate ***confident***, risk-informed decisions for licensing, making it essential to quantify the confidence in any computed result. Thus, any confidence metrics must include: 1) a critical assessment of the assumptions that are part of the methodology; 2) an evaluation of how well the methods selected for the critical steps in the process (i.e., code and solution verification, sensitivity analysis, validation, and UQ) apply to the problem being analyzed; 3) the physics models' fidelity and robustness; 4) the computational model's geometrical fidelity; and 5) the documentation's completeness. Other important considerations related to the degree of confidence in a given VU methodology can include the quality and quantity of the experimental calibration and validation data and the type of quality engineering practices the software's developers employed.

In short, are the results of the VU methodology credible? In reality, developers always take shortcuts and use approximations because of budgetary constraints, their schedule, the technical feasibility, and political and legal obligations. How can we estimate how much the real world differs from the methodological assumptions? How can we know that the methodology is implemented correctly? In the end, we must rely upon expert judgment and it must help improve the level of confidence.

5.5. The Treatment of Nonlinear, Coupled, Multi-Scale Physics Systems

Verification

Testing is the main way that scientists verify computational science codes. It contributes substantially to the collection of verification evidence. The degree of confidence we have in the verification of software depends upon sufficient testing. Without adequate testing, the risk of a software malfunction increases.

First and foremost, testing must have well-defined ways to examine a code. Simple tests for individual code components can have strong assessment criteria. On the other hand, more difficult tests that include more physics and are numerically complex can be difficult to devise. For these complex tests, defining assessment criteria can be difficult. A critical problem for verification is the definition of such tests and the creation of robust assessment criteria to verify the test's results.

Scientists need benchmarks for code verification for a wide range of physics and engineering applications that emphasize coupled multi-physics. Some important areas where solutions are needed to semi-analytic, verification test problems include, but are not limited to:

- Component physics semi-analytic test problems and solutions in one, two, and three dimensions. Some examples of these are : hydraulics for a single-phase/single component, single-phase/multi-component, two-phase/single-component and two-phase/multi-component fluids; heat conduction through structures; a structural response to applied loads; isotopic composition with irradiation; neutron and gamma spatial interaction rates; and material thermal conductivity with applied irradiation and temperature.

- Coupled physics semi-analytic test problems and solutions in one, two, and three dimensions. Some examples of the main areas of interest are: thermal hydraulics, thermal neutronics; thermal materials; thermal structures; neutronic materials; hydraulic neutronics; hydraulics structures; hydraulics materials; structures and materials; neutronics/thermal-hydraulics; thermal-hydraulics materials; and thermal-hydraulics neutronics structures and materials.

- Semi-analytic test problems and solutions for neutron transport beyond flux-limited diffusion that have angle-dependent transport solutions. Radiation transport is one of the limited classes of physics problems where Monte Carlo simulations can provide meaningful test problem solutions.

A few of the research topics in solution verification are:

- Practical methods for estimating or bounding the numerical errors associated with spatial and/or temporal discretization;

- Methods to estimate the numerical errors that are associated with the parameters that control numerical algorithms' performance, such as artificial viscosity or hour glassing parameters, particularly when they occur along with other discretization errors.

- Practical methods to make validation or application decisions when dealing with under-resolved models.

- The use of parallel, asynchronous algorithms to create solution methodologies.

Validation

Well-characterized validation experiments are critically important for simulation and model development. Model accuracy is assessed through validation experiments and physicists usually divide such experiments into two categories: 1) component experiments for a single physics phenomenon; and 2) integrated experiments that cover

coupled physics phenomena. Component and integrated validation experiments can vary from application to application.

Component experiments

High quality experiments for component physics need to evaluate multi-scale, multi-physics, and multi-dimensional codes for nuclear energy systems. Due to the highly non-linear interactions that occur between physical processes, scientists need to insure that they can assess the accuracy of any isolated physical process they might consider. In integrated experiments, it can be difficult to distinguish an error in the coupling between component physics from an error in individual components, otherwise known as a compensating error.

Therefore, component physics experiments are a critical part of any validation process. Some component validation experiments that would be useful might include simulations such as: single effect thermal/hydraulic; zero power reactor critical; materials stress-strain; load deformation of structures; and chemical separations unit components.

Although there is a large amount of experimental data available to validate computational physics models of nuclear energy systems, there is a critical need for new experimental data. This data would address component performance under severe accident conditions, assess the aging of components, and evaluate fundamental parameters that might be used to predict fuel performance.

Integrated experiments

Most applications tend to be multi-physics in nature. As a result, the validation of coupled/integrated physics models is crucial. In most codes, since physics models are modular, operators must split or separate parts of the model. Due to this approach, high-quality, well-diagnosed, integrated physics experiments are needed for multi-scale, multi-physics, multi-dimensional codes and any multi-physics code must be able to simulate this class of experiments.

Some examples of this are integral thermal hydraulics for natural circulation systems; fuel performance in power reactors and integral, thermal hydraulics neutronic structural materials under degraded core conditions.

Validation Methodology

Beyond the validation of specific phenomena, scientists need to address methodological gaps. Scientists need to be able to support validation in a way that allows them to quantify the uncertainty in non-linear, coupled multi-physics, nuclear energy system applications. Some examples of the methodological gaps are:

- Advanced statistical methods to perform quantitative measurement and/or prediction comparisons, especially when non-negligible variabilities and uncertainties in diagnostics, initial conditions, boundary conditions, and other model inputs are present.
- Tools to automate the quantitative validation process.
- Validation inference methodologies that can apply to a hierarchy of validation experiments that range from simple material characterization tests to a series of increasingly complex experiments.
- Extrapolation inference that moves from a validation parameter space to an application parameter space that is significantly outside the validation database.
- Statistical methods for validation if there is only a single, well-instrumented test.

Uncertainty Quantification

Scientists must resort to intelligent statistical sampling techniques if they are to sample the full domain of an N-dimensional space of possible inputs, if other methods such as adjoint method and automatic differentiation are not appropriate. If the dimensionality is high (N>>10), then standard sampling techniques, such as Monte Carlo methods, will not be sufficient to cover the full domain of uncertainty with a computationally feasible number of calculations that are likely to be done in two or three dimensions. Scientists will have to develop adaptive sampling procedures that will efficiently sample regions in which the sensitivity is highest to variation in parameters, models, approximations, etc.

In addition, scientists can use intelligent sampling of the N-dimensional parameter space to examine how a code responds to the full mix of parameters in the physical models. This will provide an estimate of the output's total uncertainty due to uncertainty in model parameters. However, some combinations of parameters and their variations within this full mix may produce results that disagree with available data from experiments. As a result, it will be necessary to find the subset of models and associated parametric settings that at least agree with available data. To do this requires an intelligent filtering of the full ensemble of models that covers all of the uncertainty space of the simulation. Once scientists complete this filtering, they will need to develop techniques to propagate this filtered subset of models to regimes for which no experimental data exists. They will also need to use this set of models to predict the uncertainty of output quantities for those regimes.

The entire process of Uncertainty Quantification faces important challenges that scientists need to address. Research into these issues is fundamental to refining the UQ component of any plan for a V&V initiative. Scientists are exploring quite a few of these issues in V&V programs at DOE's national laboratories. They include:

1. What approaches might scientists develop to determine the dominant sensitivities in the code that drives the uncertainty in a large-scale simulation's output, especially when the outputs are highly non-linear functions of the inputs?

2. What approaches might scientists develop to propagate the uncertainty associated with a large number of uncertain parameters (N>>10) through a simulation to

predict the total uncertainty in a large-scale simulation's output metrics? Could this be done in a computationally efficient way, particularly when the dimensionality of a parameter space is high and the computing cost for a code run is very high?

3. What approaches might scientists develop to reduce or otherwise take advantage of the dimensionality of a high-dimensional UQ space, i.e., "The Curse of High Dimensionality"?

4. How sensitive is the final uncertainty of output code metrics to the input probability density functions of the physical models' code parameters' settings?

5. How many sample calculations might be required to measure a code simulation's output uncertainty for an arbitrary number of parameter dimensions, N? Can scientists measure the accuracy of the output uncertainty for a given number of sample simulations that include an arbitrary number of dimensions?

6. What techniques must scientists develop if they want to determine the completeness of a collection of models that fit known experimental data?

7. How do we perform V&V with a UQ methodology?

8. How might scientists compare quantitatively determined output uncertainties when they have used different UQ methodologies to estimate them?

9. How can scientists determine the level of confidence in a UQ methodology that analyzes the uncertainty in code output metrics if the experiments that might be able to test the methodology are not part of the desired regime of code simulations?

10. Are there benchmarking problems that scientists can resolve if they want to create a fair test of competitive methodologies for UQ and sensitivity analysis?

11. What methodologies exist for the aggregation and propagation of aleatoric or random and epistemic uncertainties?

12. How can scientists perform UQ when parameter and other sources of uncertainty are state-condition dependent for transient problems?

13. How can scientists efficiently propagate uncertainties through loosely coupled physics packages that may be typical of operator splitting or may extend across scales in multi-scale problems?

14. How can scientists complete UQ for PRA when they must include dynamic event sequences?

15. What special problems are likely to arise when scientists try to extend UQ analysis to exascale computing architectures where 10^6 simulations and UQ analysis may result in the creation of enormous data sets?

16. How can scientists develop future codes that intrusively propagate uncertainty as they run a simulation?

5.6. Summary of Recommended VU Research Priorities

Both single-component physics and the integrated physics of coupled or multi-scale systems can be critical to model outcomes and uncertainties. We have noted this in the preceding discussion of nuclear systems modeling and V&V/UQ.

Our top priority recommendation is that a V&V and UQ program for nuclear systems' simulation take a two-pronged approach. First, focus on research into the critical issues and challenges that we identified in V&V and UQ for nuclear systems. This could include the identification and/or acquisition of improved validation data for fundamental physical parameters that sensitivity analysis indicates are the most critical to model outcomes. Through such a program focused on basic science, modelers and experimentalists could work collaboratively to improve the quality and usefulness of validation data, as well as the fidelity of detailed, micro-scale, physics models. Second, a concurrent study using the V&V and UQ process to analyze a number of critical, integrated physics applications would provide a problem focus and address the issues of coupled multi-scale physics and UQ.

Several topics for current research in the V&V and UQ realm that we listed and discussed above deserve special emphasis in future nuclear systems modeling initiatives:

- For the quantitative assessment of VU methodology:
    - How can we verify that researchers have implemented a methodology correctly?
    - How do we determine the "confidence" level for a particular analytic approach?
    - How can we compare alternative methodologies?
    - How do we account for assumptions we make about a given methodology that might turn out to be inaccurate?

- When addressing high dimensionality, nonlinearity, coupling and multiple scales:
    - How can we design benchmarks for effective code verification testing, particularly if we need to deal with more challenging nonlinear or coupled physics problems?
    - Can we develop practical and effective methods for solution verification for nonlinear, coupled, multi-scale problems?
    - Can we design needed component and integrated validation experiments and acquire sufficient validation data?

- How can we deal with a range of possible model inputs that has the potential to become enormous and still insure adequate sampling?
- How do we treat the propagation and aggregation of uncertainties, when we deal with nonlinear models or multi-scale, multi-physics models?

- The aggregation of uncertainties from multiple sources:

  - How can we distinguish between and treat uncertainties due to numerical error, model inaccuracies, or input data that is imprecise or not well understood, even when such uncertainties may need to be addressed in a unique way?

- The extrapolation of results beyond the validation regime:

  - How do we quantify uncertainties when we extrapolate them to physical parameter regimes that are beyond the experimental database?
  - What role should "expert judgment" play?

- Coupling predictive simulations with dynamic, probabilistic risk assessment (PRA) and quantifying probabilities of rare outcomes:

  - Can we develop coupled tools that we can use to assess a given scenario and simulate a predicted outcome? Can we repeat this process to provide a dynamic system model?
  - How do we use UQ to help predict the likelihood of rare, but potentially catastrophic, events knowing that experimental data that describe such outcomes is difficult to find?

- New approaches for VU in the exascale computing environment:

  - Can we successfully manage and process the large quantity of numerical experiments that will probably be required to perform UQ studies and gather the necessary statistics, especially if the number of experiments might become very large?
  - Can we harness new levels of computing power to provide an "artificial intelligence" or self-adapting system that would be able to assess the source of different model uncertainties? Might such a system help scientists prioritize what future experiments and simulations they should perform?

6. Final Whitepaper - Systems Integration Panel

Building an "Open-Source," Flexible, and Extensible, Energy Enterprise Model

6.1. Introduction

Background

Human progress – viewed in terms of technology, economics, and social goals -- depends upon our ability to acquire and use energy. Energy use influences how we build shelter, what food we produce, what we manufacture, how we travel, and how we wage war. For the world's population, quality of life is linked to our access to affordable energy, chiefly electricity. Figure 1 shows how closely access to energy and human development are tied, based upon a comparison of the United Nations' Human Development Index[29] and per capita electricity consumption; the correlation is not so strong when we look at the highest levels of electricity consumption – at these levels, the correlation between increases in human development index and greater energy consumption is not strong, but at other levels it is very closely correlated.

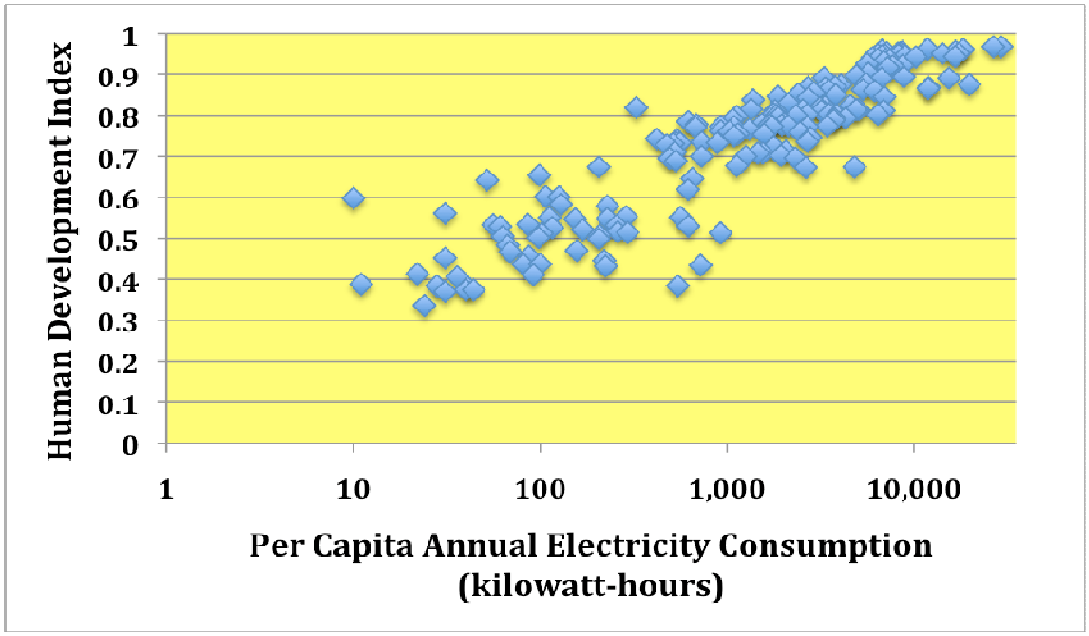

Fig. 1. The United Nations' Human Development Index compared to per-capita electricity consumption in 170 countries. Source: United Nations, United Nations

[29] United Nations, United Nations Development Program, *Human Development Report 2007/2008: Fighting climate change: Human solidarity in a crowded world*. Basingstoke, UK, and New York: Palgrave Macmillan, 2007.

Development Program, *Human Development Report 2007/2008: Fighting climate change: Human solidarity in a crowded world*. Basingstoke, UK, and New York: Palgrave Macmillan, 2007.

Over the past few years, a new consensus of public opinion has developed. It holds that our economic prosperity, environmental quality, and national security are closely related to our energy supply's security and affordability. By coupling these concerns, the public has presented policy makers with a test of whether they can develop better approaches to energy, environmental, economic, national security, and foreign policy issues. The National Commission on Energy Policy summarized the challenge:

> *"... The overall picture is vastly complicated by the inescapable linkages between energy production and use and the environment. In particular, the risk of global climate change from emissions released by fossil fuel combustion will exert a profound influence on the world's energy options and choices over the decades ahead. In this context, the old notion of energy security acquires new dimensions. Reliable access to the energy resources needed to support a healthy economy remains the core imperative, but in the 21st century energy security also means reducing the macroeconomic and terrorism-related vulnerabilities inherent in the current geopolitical distribution of oil supply and demand and coming to grips with the environmental impacts of the current energy system*." [30]

The challenge to policy architects and strategic planners is broad. In some cases, policy has faced barriers because different political philosophies have blocked effective policy formulation. In other cases, policy has stumbled because we don't have the data we need to characterize "ground reality." In general, our ability to reach a consensus on energy strategies is made more difficult by the many cause and effect relationships that are part of the behemoth system-of-systems that represent the U.S. and global energy enterprise.

Understanding the U.S. energy enterprise

The U.S. energy enterprise is a massive, "just-in-time" system to deliver and use energy. We can understand the magnitude of the U.S. energy enterprise by reviewing a few salient facts:

- The U.S. energy enterprise is a $1 trillion a year business that generates, delivers, and consumes approximately 100 quadrillion BTUs of primary energy a year, while emitting 5,800 MMT of CO_2. The electrical power sector consumes forty percent of this energy, transportation consumes twenty-nine percent, industry

[30] National Commission on Energy Policy, "Ending The Energy Stalemate: A Bipartisan Strategy to Meet America's Energy Challenges," Washington, D.C., December 2004. p. iv.

consumes twenty-one percent, and the residential and commercial sector consumes eleven percent.[31]

- In the United States, electricity generation draws upon several resources. Of the total, fifty-one percent is coal, twenty-one percent is nuclear, seventeen percent is natural gas, nine percent is renewables (chiefly hydro and biomass), and two percent is petroleum. The infrastructure to supply electricity includes over 600 coal-fired power plants, 104 nuclear reactors, and 180,000 miles of transmission lines operated by 500 companies.[32]
- The United States has 150 oil refineries and over two million miles of natural gas and petroleum transmission and distribution pipelines. We have over 117,000 service stations that sell fuel to over 140,000,000 passenger vehicles and trucks.

Besides these relevant facts, a number of factors complicate the way we use our energy system resources. These factors are likely to make future energy delivery choices more difficult and to constrain what we can do. This would limit how close we can come to creating an "optimal" energy strategy and narrow the path to a better energy future. For example:

- In geographic terms, primary sources of energy are not evenly distributed. Since access to coal, oil, hydro, wind, and solar energy varies considerably by location, extracting and refining them creates a wide range of environmental impacts and risks. As a consequence, since our regional economies depend on primary resource extraction (i.e., coal, oil, etc.), this can affect how we implement different energy policies.
- Solar and wind energy tax our system in other ways. Since their availability varies by time-of-day and by season, our nation needs to develop a viable and competitive, high-density, electrical-energy, storage technology. We must also enlarge the existing electricity grid if we want to expand our use of renewables and expand the market for plug-in electric vehicles and innovative transportation technologies.
- Our reliance on fossil fuels as a primary, energy-storage vehicle is an additional drag on our present system. Fossil fuels are also the way we accommodate monthly and seasonal shifts in demands in the electrical supply system.[33] As a result, load balancing depends on our worst green house gas (GHG) polluter.

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[31] U.S. Department of Energy, Energy Information Administration, Office of Integrated Analysis and Forecasting, "Emissions of Greenhouse Gases in the United States 2005," Report DOE/EIA-0573, November 2006, p. ix. http://www.r744.com/news/files/GHG_report_US_nov2006.pdf?PHPSESSID=070ffd8ba032d6387bd36dcee68a6310. The emissions figure of 5800 MMT of CO_2 is for 2000-2002.

[32] U.S. Department of Energy, Energy Information Administration, "The Impact of Increased Use of Hydrogen on Petroleum Consumption and Carbon Dioxide Emissions," Report SR-OIAF-CNEAF/2008-04, August 2008, http://www.eia.doe.gov/oiaf/servicerpt/hydro/hydrogen.html. U.S. Department of Energy, Energy Information Administration, "Electric Power Annual with data for 2007," Table 2.2, Existing Capacity by Energy Source, January 21, 2009. http://www.eia.doe.gov/cneaf/electricity/epa/epat2p2.html.

[33] Charles Forsberg and Stephen Goldberg, "Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale," White Paper for DOE/NE – DOE/SC Workshop on Science-Based Nuclear Energy Systems Enabled By Modeling and Simulation at the Extreme Scale, May 10-12, 2009.

- A patchwork quilt of existing regimes and policies regulates how different parts of the energy industry operate. These rules can spark conflicts between our goals for energy, the economy, and the environment.
- We lack a highly differentiated, national, energy-related, manufacturing infrastructure. In addition, large shifts in the cost of key commodities impacts our use of energy technologies in very different ways.
- Concerns about the relationship between energy production, land use, and water use are growing. This is especially true in the Southeast, where such concerns are a major political issue.
- Finally, our existing energy transmission and distribution networks (i.e., electric transmission lines and pipelines) are fragile and have capacity limits. These are likely to restrict the flexibility of new policies and limit our potential for growth.

The policy debate: asking (and answering) tough questions

As it is currently constituted, the U.S. energy system operates as a giant "machine" that puts watts on the electrical grid and moves people and goods. One unintended consequence is that this "machine" generates massive amounts of GHG and transfers a sizable portion of our national wealth to other countries.

This system is clearly unsustainable in both economic and environmental terms. Since it is, there are clear implications for national security and foreign policy. For one, the complexity of the energy-economic-environmental system is staggering; even if it is examined in its sub-national or regional dimensions, it is difficult to understand. Nevertheless, we must strive to achieve a better appreciation of the interlinked, "Gordian-knot"-like, network of cause-and-effect relationships of this system, if we are to formulate effective policies to address the most compelling challenges. The following questions are ones that our policy makers and strategic planners need to address:

- What are the economic and environmental impacts of different GHG mitigation strategies? Which ones should our nation pursue?
- What is the likely impact of developing new energy technologies, such as high-density, electrical, energy storage, carbon capture and storage, advanced-nuclear fuel cycles, and hydrogen-powered vehicles, etc.? How important is each technology to our energy future? What should our R&D priorities be?
- What tradeoffs are associated with centralized and distributed electric-power generation and storage?
- What physical and geographical limits are there for different energy production technologies?
- What role can nuclear power play in the transition to a low-carbon future?
- Is there a limit to the role that renewable energy sources can play in the U.S. energy system?
- What changes are needed in our energy infrastructure, particularly the electric transmission and distribution grid architecture, so it can respond to new technologies and increased demand?

- What should our priorities be as we develop new energy-system supply chains and manufacturing capacity?
- How much time should it take to achieve a sustainable energy policy, how much will it cost, and how will we pay for it?

We clearly need a new approach. We also need new tools to inform the forthcoming energy policy and planning debates. Similar challenges arose when the climate-change community debated a related range of issues. The climate-change community turned to large-scale, systems simulations to integrate a growing knowledge base, obtain greater insights, and develop more informed climate policies. We must adopt a similar approach to offer new solutions for the energy, economic, and environmental issues that will be part of the energy systems policy debate.
The rest of this paper will offer a critique of energy systems simulation initiatives and models, define attributes of recommended capabilities for energy-enterprise systems' simulation models, and identify how scientists should organize and implement the development of models.

6.2. A Critical Review of Available Models

We need to understand how our nation can deploy interoperable energy technologies. One approach would be to build upon models used to analyze energy use. In this overview, we consider two widely-used models: energy-environment models and grid simulation models. As the following discussion will underscore, these models tend to have limited applicability. In addition, it is not easy to overcome the limits because they were these models were not built to be architecturally extensible.

Energy-Environment Models

Since the 1970s, policymakers have employed models to understand our economy's use of energy and to evaluate energy policies. Over time, these models have gained the computing power needed to answer new science and policy questions. Today's models evaluate energy's environmental impacts by estimating emissions[34] or performing global climate simulations.

These energy-environmental models forecast future market adoption of different energy technologies and help us understand their potential benefits and limitations. One of the

[34] Brookhaven National Laboratory's Market Allocation (MARKAL) model is a leading energy-environmental model that is used to calculate emissions. It is widely used by the International Energy Agency as well as by other parts of the U.S. government. The paper by Johnson et al. is one example of how this model has been employed. The paper includes a concise description of MARKAL and discusses its limitations. See Timothy L. Johnson, Joseph F. DeCarolis, Carol L. Shay, Daniel H. Loughlin, Cynthia L. Gage and Samudra Vijay, "MARKAL Scenario Analyses of Technology Options for the Electric Sector: The Impact on Air Quality," U.S. Environmental Protection Agency, Office of Research and Development, Report EPA/600/R-06/114, September 2006. http://www.epa.gov/nrmrl/pubs/600r06114/600r06114.pdf

main outputs of an energy-environmental model is a forecast of energy consumption and production. Energy-environment models are based upon an assumption of competition among energy technologies subject to certain constraints. This allows models to determine the relative prices of energy produced using different technologies and then create forecasts for these technologies' deployment. Each model differs according to how prices in one part of the economy propagate through the balance of the economy.

The forecasts these models make for new technology deployments reflect the economic limits and growth potential of such technologies. While there are physical factors that constrain how technologies can be used, such as whether they can be accessed intermittently and if they are limited by water and land requirements, models do not always reflect these constraints. The model we propose in this White Paper makes these physical characteristics its main focus of attention.

Today's models differ according to the level of detail that they forecast and their intent. The National Energy Modeling System (NEMS) that the Department of Energy's Energy Information Agency uses is an intricate, detailed system of models that forecasts national energy use. In its different modules, NEMS captures a number of sub-parts of the energy system, such as the production and use of electricity and fossil fuels and the development of renewable energy.[35] To capture some of the variations in use, these modules provide annual forecasts that divide the nation into regions. NEMS describes how our energy system will deploy new technologies, but since it aggregates regional data, it cannot depict differences within specific regions. For instance, the electricity model has one region that includes Washington, most of Nevada, and much of Montana. As a consequence, it is impossible to know the size of Seattle's energy demand because its needs are averaged with those of the northern Rockies. Thus, the model cannot evaluate how offshore wind energy use in the Seattle area would differ from renewable energy use in mountainous areas.[36] Similarly, the model cannot compare the impacts of nuclear energy initiatives in Oregon with similar efforts that would be unquestionably difficult to build in arid parts of Nevada. As comprehensive as NEMS is, it is can only address some of the issues that will shape how our nation moves to its energy future.

Integrated assessment models are energy-environmental models that are gaining much attention. These models link physics-based, climate models with economic behavioral models to improve our understanding of how climate change and human behavior affect

[35] The U.S. Department of Energy's Energy Information Administration provides detailed documentation of the National Energy Modeling System (NEMS) and its related modules on its website http://tonto.eia.doe.gov/reports/reports_kindD.asp?type=model%20documentation. There is an overview of the basic design and operation of the model as well as its current parameter values in U.S. Department of Energy, Energy Information Agency, "Assumptions to the Annual Energy Outlook 2009," report number DOE/EIA-0554, March 2009. http://www.eia.doe.gov/oiaf/aeo/assumption/index.html

[36] For each region, the NEMS model attempts to account for many features of the electricity system. It includes a top-down approximation of time-of-day pricing variability and intermittent supply considerations. The U.S. Department of Energy's Energy Information Agency provides more details in U.S. Department of Energy, Energy Information Agency, "The Electricity Market Module of the National Energy Modeling System: Model Documentation Report," report number DOE/EIA-M068, May 2009. http://tonto.eia.doe.gov/FTPROOT/modeldoc/m068(2009).pdf

one another.[37] These models can predict how climate change might reduce economic growth. When examining energy production, these models quantify how much of each energy resource the economy is using, along with the related emissions and their impact on the environment.

Integrated assessment models are global in scope, but disaggregate the world into regions with different characteristics. Within each region, estimates of supply and demand for each technology's inputs and products determine energy prices. Once these are set, the models can select ways to allocate scarce resources efficiently. After these allocations are made, the resulting mix of energy resources follows economic logic. Policy makers model alternative policy choices by evaluating alternative cost scenarios for different technologies.[38]

The main focus of energy-environmental models is the long-term interaction between the economy and the environment, as well as the depiction of possible energy choices in the long run. Because of this long-run focus, such models do not lend themselves to a highly granular examination of U.S. energy alternatives. Since the models' time horizons are on the order of a century or two, they are not well-suited for an analysis of shorter term alternatives that may be of interest as part of long-term forecasts of climate trends. The fact that such models rely upon time horizons of five, ten, or even fifteen years means that they are appropriate for looking at long-term trends, but may not be suitable when policy makers try to understand the energy system's short-term variations.

[37] There are many integrated assessment models in use today, far too many to list them individually. A reasonably comprehensive and organized list can be found in Elizabeth A. Stanton, Elizabeth, Frank Ackerman, and Silvan Kartha, "Inside the Integrated Assessment Models: Four Issues in Climate Economics," Stockholm Environment Institute, Working Paper WP-UWUS-0801, 2008 and in Sergey Paltsev, "Economic Modeling of Energy and the Environment: Current Approaches and Challenges," presentation to the Center for Economic and Financial Research, Moscow, Russia, February 10, 2009. http://sust-rus.org/wp-content/uploads/2009/03/paltsev.pdf A discussion of many of the key models in use today and the strengths and shortcomings of different approaches appears in Derek Vollmer, *Assessing Economic Impacts of Greenhouse Gas Mitigation: Summary of a Workshop.* Washington, D.C.: The National Academies Press, 2009. The discussion here draws heavily upon the three models that the U.S. Climate Change Science Program uses for scenario analysis: MiniCAM (Pacific Northwest National Laboratory); IGSM-EPPA (Massachusetts Institute of Technology); and MERGE (Electric Power Research Institute). For a more thorough discussion, see Leon E. Clarke, James A. Edmonds, Henry D. Jacoby, Hugh M. Pitcher, John M. Reilly, and Richard G. Richels, "Scenarios of Greenhouse Gas Emissions and Atmospheric Concentrations," Report by the U.S. Climate Change Science Program and the Subcommittee on Global Change Research, Synthesis and Assessment Product 2.1a, July 2007. http://www.climatescience.gov/Library/sap/sap2-1/finalreport/sap2-1a-final-all.pdf

[38] A more comprehensive discussion of the economic approach and the assumptions it uses in integrated assessment models appears in Ackerman et al, Frank Ackerman, Frank, Stephen J. DeCanio, Richard B. Howrath, and Kristen Sheeran, "Limitations of Integrated Assessment Models of Climate Change," Working Paper, November 3, 2008. http://www.e3network.org/resources/DeCanio,%20Ackerman,%20Howarth,%20and%20Sheeran%20LimitsOfIAMsOfClimateChange.pdf

Electricity system models

Generation expansion and *system reliability models* are the backbone of the electric reliability (North American Electric Reliability Council, or NERC) community. These models forecast reserve margins and loss-of-load frequency as well as the probability of loss-of-loads for large electricity generation systems; this helps planners chart the future expansion of the electricity grid. By integrating and aggregating individual generating plant reliability and availability models with probability estimates of individual plant outages and hourly-system load models, these models forecast overall system reliability and behavior. A second class of models, power plant, transmission and distribution *siting models,* determine the location and size of generation and transmission capacity. Typically, these siting models include environmental, regulatory, and economic data that helps to optimize the placement and building of additional capacity.

A third type of "electricity systems model" is Argonne National Laboratory's Electricity Market Complex Adaptive Systems (EMCAS) system. For a single region, this model includes all of the electricity production, transmission and distribution systems.[39] In EMCAS, the physical electricity system works in concert with market actors' economic relationships that function under a regulatory framework. In the model, each actor, the electricity system and market actors, are agents that behave according to rules that govern their decisions; these decisions can change over time. When these agents interact, they result in market behaviors that cause producers to set energy prices that are transmitted to consumers. While prices are set on an hourly basis, planning horizons can extend for days, weeks and years. Since EMCAS examines the transmission and distribution aspects of the electricity system, it offers less insight into the tradeoffs associated with different production alternatives that may be of interest to policy makers.

A similar power grid simulation tool is the Pacific Northwest National Laboratory's Electricity Infrastructure Operations Center (EIOC). While focused on real-time monitoring and operations of the electricity grid, this simulation model includes near-term planning tools[40] and visually represents complex, electricity-transmission systems.

These grid simulation models could provide a foundation for the model that we propose here, but they would need to begin to account for the resource needs and waste by-products that energy production generates.

Summary of Current Modeling

[39] Information on EMCAS is available on the Argonne National Laboratory, Decision and Information Sciences web site, "Electricity Market Complex Adaptive System (EMCAS)." http://www.dis.anl.gov/projects/emcas.html. Koritarov and others provide an example of how this model was used in Poland. See V. Koritarov, G. Conzelmann, R. R. Cirilo and S. M. Goldberg, "Poland Becoming a Member of the Global Nuclear Energy Partnership: Volume 2 – Appendices," Argonne National Laboratory, Report L ANL-07/10 Vol 2, March 2007. http://www.dis.anl.gov/pubs/58914.pdf. Argonne National Laboratory's Generation and Transmission Maximization model, GTMax, has similar capabilities. See http://www.dis.anl.gov/projects/Gtmax.html .

[40] See Pacific Northwest Laboratory, "GridLAB-D: The next revolution in power systems simulation," Undated brochure. http://eioc.pnl.gov/brochures/gridlab_d.pdf

As should be evident from the preceding discussion, current modeling approaches don't respond well to the different groups that want valid, quantitative alternatives to make energy policy decisions. These constituencies range from non-technical individuals who are concerned with more general issues, such as whether it makes economic sense to replace gasoline with ethanol, to technical, subject-matter experts who focus on particularly detailed questions, such as what is the best design for a plug-in, hybrid, automobile, power train. Consequently, it is a challenge to explain the results of modeling tools to the broader public in ways that are credible and not couched in the language of experts. Few of the technical experts' models have much in common with each other. Many address different energy sectors and can focus on the same energy sector but at different levels of detail. Thus, it is difficult to marry the models' detailed modeling capabilities and to transfer the results of highly granular models to models operating at a higher-systems, but lower-granularity, level. Indeed, if we want to average results from different granular levels in a systems-level model, it can be difficult to know the best way to proceed; this problem is reminiscent of the issues posed by sub-grid modeling in computational fluid dynamics.

To amplify this point further, we know that the underlying equations in computational fluid dynamics are verifiable. This does not hold in energy models and scientists know that when they average results over different scales of time and size, it is computationally impossible to carry out simulations that encompass all the relevant physical scales. Nevertheless, it is not clear that one sub-grid model is preferable over another; this remains a subject for continuing research. In energy modeling, this problem is all the more pressing, since scientists don't know what "governing" equations to use. For this reason, energy system models must be sufficiently transparent. Maintaining this transparency is one of the only means by which users and consumers of such models can appreciate the models' inherent limitations. If we recognize these limitations, they are more likely to dampen the exuberance with which we employ such models and temper the enthusiasm with which we hail or disclaim their results.

The obvious question then is: where do the limitations of the today's models originate? We can offer some explanations, but this review is not meant to be exhaustive.

In basic terms, today's models take a hard-wired approach to details, i.e., granularity. Their code architecture reflects their origins, the tendency to have a narrower focus and a gradually expanded scope, but without re-engineering the code architecture – what might be called code growth by accretion. Of further note, today's models were designed when modern code architecture design had not yet gone beyond the constraints of computer science and become more sophisticated. Even in computationally sophisticate fields such as physics, modern code architecture design did not have a substantial impact until the early to mid-1990s, roughly a decade ago. As a consequence, many models are not modular, are not extensible, and do not take advantage of code reuse. Furthermore, experts must run the models and modify their interior structure, particularly their proprietary codes.

One result of this history is a lack of transparency. Sometimes this was intentional, as is usually the case for proprietary models whose reliability or believability rests solely on the reputation of the model's owner or owners. More often, the lack of transparency is an unintended consequence of a model design that is so narrowly specified that it is difficult for anyone other than the original model developers to modify it.

One goal that we should strive for is to allow different levels of sophistication among users who want to modify code internals. This could be done by segregating the more-sophisticated subcomponents of models in modules that only experts can access and providing "hooks" for such user-defined modules so that experts and intelligent users can modify or enhance their behavior.

Finally, few developers consider model extensibility and pay little attention to varying the scope or model granularity. Rarely do they provide a way to adjust a model's interface to a user's level of sophistication. Consequently, today's models evolve slowly and require the original model developers to rejoin any efforts to extend or modify a model. As a result, models are largely "fixed objects" that technically inexpert users run.

6.3. Recommendations: A Path Forward

The previous section outlined the weaknesses common to most, if not all, of today's energy system models and underscored the issues we believe are of greatest concern. In these recommendations, we discuss how to take a different approach to "doing business."

What Models Should Include

To define a new approach, we should specify what the most desirable elements for a model are. These are:

1. *Open-source architecture.* Whatever is built should be "open source," so that proprietary[41] aspects are minimized as much as possible. To deal with the inevitable issue of proprietary and/or sensitive data, details such as an electric grid's local characteristics or a commercial power plant's performance and security characteristics should be segregated in secure data input files. This should not alter the "open" nature of the modeling code. This approach would provide us with a tool that can be used around the world.

2. *Transparency*. Models must be transparent when users, whether they are experts or novices, run them and interpret their results. If our goal is to create a set of tools that meets the needs of the broadest possible audience, these users need to believe that they understand and can rely upon the models. Without transparency, this might not be true.

[41] By 'proprietary' data we mean data whose distribution may be restricted for either commercial reasons or for national/homeland security reasons.

3. *Modularity.* It is important to insist upon modularity in the underlying modeling code and consistency in code generation when constructing energy system analysis tools. This means the architectural design of new models has four distinct goals: 1) to make it easier to modify models in the future, including model extensions that are a central part of "open source" models. This should permit models to include more complex relationships or interactions between different types of energy systems, economic 'actors,' and environmental factors; 2) to decrease code complexity and make models more accessible to larger numbers of potential model builders and modifiers; this is a key characteristic of "open source" models; 3) to increase model efficiency via code reuse; this is more relevant as models become more complex; and 4) to provide for coding consistency and source code configuration control (possibly via a project-related host center), so that the subparts of models known as modules can always maintain their interoperability; this will insure code reliability. Modularity and consistency are also key architectural features of any model and make it easier to allow for different levels of specificity or granularity in a model's description and execution.

4. *Providing for differences in the sophistication of users and model builders*. Few people will be familiar with the sophisticated models we seek to build; for those who are, we will call them *developers*. A larger number of people will probably want to change different aspects of the "interiors" of models; we will call these people *modelers.* Finally, many users prefer to leave models' interior aspects alone, but want to modify the inputs or model, as long as no programming is required; we will call these the *users*. The code development techniques of modern computer science can satisfy all of these human-model interaction levels. We should rely upon these when we build these new models.

5. *An ease of data comprehension*. Since models are only valuable if their results can be readily understood, it is crucial that users understand how models operate and how they produce results. For this, the design of the Graphic Unit Interface (GUI) is essential. How the GUI displays or reveals the model to users, as well as how it presents the model's results, is critical.

6. *Efficiency*. One of the insights gained from large community modeling efforts, such as the Global Climate modeling program that the National Center for Atmospheric Research (NCAR) hosted, is that having a project-related resource center handling issues such as code debugging, regression testing, and porting, allows individual research groups to focus on science. Such a center spreads the costs of such work over the community and removes scientists from the role of acting as maintainers of codes. In addition, broadening the user community supports more effective code (and model) verification and validation. This would mirror the commercial software industry's beneficial practice of regularly releasing 'beta' versions of new software.

7. *Community building*. The global climate community has also shown how a community-based modeling program can produce a vibrant intellectual community that debates the core issues in the modeling effort. It demonstrates

how having such a community avoids time-consuming debates over competing models that have internal codes that can be shrouded in secrecy for proprietary reasons. As noted above, an "open source architecture" and transparency are crucial to building such a community model.

An Approach to Model Building

Building a set of systems level models similar to those we have described is a daunting task; we do not minimize the challenge.[42] Nevertheless, we know much about how to approach such an ambitious task. Ultimately, we hope this will result in energy system modeling tools that require computing resources comparable to those employed to run computational physics simulation codes.

First, we believe an *iterative approach* that starts from a very simple model[43] as the best way to develop to new systems models. Such an effort would build upon previous experience. We would argue that one cannot design the ultimate model architecture from a blank sheet. Experience tells us that the chances of doing this right are exceedingly limited. We already have models that are based on an iterative approach, but they probably are not designed in a way that lets their code evolve as users iterate the model.

Second, we believe the best approach is to select a *simple* systems-level model that already exists and use it as the base case. We can foresee using the model as a tool for examining dynamics and to consider the consequences of implementing different strategies over long periods of time. We can see how users could create "scenario explorations" from such efforts. Once developers refine these models, users would probably be interested in using them as tools to identify the best policy alternatives. Technically, this would be straightforward. The real challenge is to devise different cost functions or metrics to define what is optimal from a policy perspective.

As to specific steps, we suggest that after scientists identify the initial target model, they should choose a programming methodology that permits rapid prototyping. Our reason for suggesting this approach is the enormous speed-up that it will make possible during the implementation of a new systems model; the key is to expend as much effort as needed to define the code architecture and to save time for later efforts that involve building more sophisticated internals, such as sophisticated GUIs.

[42] Even in the case of relatively well-understood disciplines such as computational fluid dynamics (CFD), building new simulation codes is an effort that takes 5-10 years, at funding levels of $4-5 million a year, to produce a useful CFD research and analysis tool. The DOE/NNSA ASC/Alliance program that funded similar efforts at a number of universities is an instructive example of the challenges of building such modeling tools and the chances of success, if there is long-term funding and encouragement.

[43] For argument's sake, let us assume that this initial model operates at the uppermost system level, i.e., with minimum granularity; Conceptually speaking, one could equally well start at the maximum granularity level, but its key disadvantage is that the former approach has a much larger potential user base than the latter.

6.4. Immediate next steps

We will need a broad consensus to create such simulations and develop their associated modules. The consensus will also need to support how sensitive data is accessed and stored. Besides requiring due diligence, the development effort will need to identify and evaluate the capabilities of all of the simulation models that the government and private sector are using, as well as models that are used internationally.

To begin, the Department of Energy (DOE) should convene a workshop to address these topics that draws upon the success of the DOE's Office of Science's "Research Needs" workshops. This workshop, with participants from the federal and private sector as well as international partners, would identify simulation requirements, examine current simulation capabilities, and formulate a detailed strategy to begin a major development effort similar to the one we have recommended. The workshop would be an appropriate setting to discuss new systems models, especially a model's scope and the level of effort and funding needed to create it. Due to the urgent nature of this modeling effort, we recommend that DOE establish a workshop steering committee as soon as possible. This committee should organize the workshop and complete its deliberations no later than December 2009.

7. Conclusions and Recommendations

7.1. Introduction

The Joint Office of Science and Office of Nuclear Energy Workshop on
Advanced Modeling and Simulation for Nuclear Fission Energy Systems provided a thorough examination of the potential role of this technology to advance a scientific understanding of nuclear energy technology. The workshop identified many of the technical hurdles that must be addressed by future research and development activities. It also provided an excellent perspective of the potential role of extreme scale computing in addressing these issues.

The following is a brief summary of the results and recommendations provided by each whitepaper.

7.2. Integrated Performance and Safety Codes Panel:

Conclusions

The use of extreme computing is likely to improve the modeling and design of nuclear energy systems significantly. Nuclear energy science and engineering simulations will drive the need for exaflop-scale, computing power to create robust, predictive simulations that have quantifiable uncertainties. The creation of IPSCs faces considerable technical challenges that range from improvements in software engineering and numerical methods, to the development of more accurate and fully-integrated physics models.

Recommendations

Given the increase in computing power and the scientific issues that should be addressed in this area, the following research and development subjects require attention and additional analysis:

- Multi-scale methods that allow direct up-scaling of micro-scale science simulations to meso-scale simulations (in both length and time, perhaps even in the same source code, in some cases);
    - Atomic-scale physics in IPSC for nuclear fuels;
    - First-principles informed mechanistic models; and
    - Algorithms that support scaling from *ab initio*, to molecular dynamics, to continuum.

- Advances in computer science to support new techniques, algorithms, and integrated codes on emerging architectures. This should include:
    - Solvers and physics-based preconditoners;
    - Acceleration methods for Monte Carlo transport algorithms at the extreme scale;
    - Hybrid, deterministic and Monte Carlo transport methods, particularly in support of IPSC multi-physics coupling;
    - Advanced Boltzmann solvers that can replace the homogenization techniques that are in common use today;
    - Spatial p-refinement, multilevel preconditioners and weighted partitioning for load balancing in deterministic transport solvers;
    - Adaptive deterministic methods that solve all seven dimensions of the Boltzmann transport equation;
    - Asynchronous transport schemes;
    - An integration of RANS, LES, and DNS methods;
    - The development of advanced, adjoint radiation transport, thermal hydraulics, and coupled-physics solutions;
    - Software platforms that facilitate the development of new methodologies and the integration of multi-physics;
    - 3-D models that accurately incorporate nonlinearities, such as steel yielding, concrete cracking, and strength degradation specific to a nuclear power plant;
    - Material damage and failure models scaled up to a plant level

- Development of new models of physical behaviors that are usable on advanced extreme scale computing platforms. This should include:
    - New models for understanding fission gas production, gas transportation and formation, void migration, and bubble detachment;
    - Methods that achieve a tighter integration of reactor depletion and kinetics;
    - Improved boiling, two-phase flow and critical heat flux methods;
    - The structure and chemistry of waste forms' radionuclide-bearing phases and their corrosion products;
    - The measurement and prediction of thermo-chemical parameters for nuclear materials and an extended thermodynamic and kinetic database;
    - Theory, models, and data to predict the migration of radionuclides under various geochemical and geologic conditions;
    - New dissolution models for spent fuels;
    - Improved models of unit operations, distillation columns, mixing, and off-gas recovery in fuel reprocessing operations;

7.3. Materials Behavior Panel

Conclusions

Scientists and Engineers face a tremendous challenge: to develop transuranic-bearing nuclear fuels, fuel cladding and structural components for advanced nuclear reactors that withstand ultra-high fuel burnups, neutron doses and temperature extremes. Meeting this challenge will require these scientists to push the limits of high performance computational materials modeling.

In the past, developing materials to meet such requirements has involved decades-long testing and examination. Such long lead times are a result of scientists' predominant reliance on nuclear test reactor radiations to drive micro-structural and material property changes and their desire to create materials that can endure long service lifetimes. Certainly, economic considerations and fuel economies are part of the push for long material service lifetimes and high burnup of fuels. These drivers will only exert greater pressure in the future.

The future holds the promise of high-fidelity predictive performance models not only to predict the lifetime and failure of fuels and components in a wide variety of advanced nuclear energy systems, but also to enable the design of new materials tailored for such aggressive environments.

Recommendations

This report has documented a number of challenges that must be overcome before scientists and engineers can develop high fidelity nuclear materials performance models. Therefore, we recommend that the following research and development subjects require attention and additional analysis in areas that:

- Deal with the complexity of multi-component materials systems, including those in which the chemical composition is continually evolving due to nuclear fission and transmutation;
- Discover the controlling factors that are key to materials performance and include them in models in order to reduce the likelihood of technical surprises;
- Transcend ideal materials systems to engineering materials and components; and
- Incorporate error assessments within each modeling scale and propagate the error through the scales to determine the appropriate confidence bounds on performance predictions.

7.4. Verification, Validation and Uncertainty Quantification Panel

Conclusions

For nuclear energy systems, there are two motivations to perfect Verification, Validation and Uncertainty Quantification (VU). The most obvious is to improve the confidence users have in simulations' predictive responses and our understanding of prediction uncertainties in simulations. Additionally, scientists must also perform VU for nuclear energy systems because the USNRC, the licensing body, requires it. This is based on the premise that an extensive experimental database can provide important insights about system attributes.

VU's objective is to predict with ***confidence***, using computer simulation models, ***best estimate*** values and the associated ***uncertainties*** of complex system attributes, while also accounting for all sources of error and uncertainty. This means:

- Modeling;
- Numerical treatment;
- Software errors;
- Epistemic uncertainties (i.e., data as well as correlations);
- Aleatoric, or contingent, uncertainties (i.e., random phenomena); and
- Initial and boundary conditions.

If VU satisfies this objective, it will support the following favorable outcomes:

- The ability to make confident, risk-informed decisions when considering alternative designs and operations.
- More specifically, the ability to:
  - Identify code development needs;
  - Identify and design the required validation experiments;
  - Make design decisions needed to manage margins; and
  - Present a risk-informed safety case to the regulatory body.

One challenge for VU when applied to nuclear systems is that it must predict any high-impact consequences of low-probability events with high confidence. This must be done factoring in aging effects, even if there is limited experimental data at the macro scale. This challenge is similar to the one associated with the stewardship of nuclear weapons.

Recommendations

Our top priority recommendation is that a V&V and UQ program for nuclear systems' simulation take a two-pronged approach. First, focus on research into the critical issues and challenges that we identified in V&V and UQ for nuclear systems. This could include the identification and/or acquisition of improved validation data for fundamental

physical parameters that sensitivity analysis indicates are the most critical to model outcomes. Through such a program focused on basic science, modelers and experimentalists could work collaboratively to improve the quality and usefulness of validation data, as well as the fidelity of detailed, micro-scale, physics models. Second, a concurrent study using the V&V and UQ process to analyze a number of critical, integrated physics applications would provide a problem focus and address the issues of coupled multi-scale physics and UQ.

Several topics for current research in the V&V and UQ realm that we listed and discussed above deserve special emphasis in future nuclear systems modeling initiatives:

- For the quantitative assessment of VU methodology:
    - How can we verify that researchers have implemented a methodology correctly?
    - How do we determine the "confidence" level for a particular analytic approach?
    - How can we compare alternative methodologies?
    - How do we account for assumptions we make about a given methodology that might turn out to be inaccurate?

- When addressing high dimensionality, nonlinearity, coupling and multiple scales:
    - How can we design benchmarks for effective code verification testing, particularly if we need to deal with more challenging nonlinear or coupled physics problems?
    - Can we develop practical and effective methods for solution verification for nonlinear, coupled, multi-scale problems?
    - Can we design needed component and integrated validation experiments and acquire sufficient validation data?
    - How can we deal with a range of possible model inputs that has the potential to become enormous and still insure adequate sampling?
    - How do we treat the propagation and aggregation of uncertainties, when we deal with nonlinear models or multi-scale, multi-physics models?

- The aggregation of uncertainties from multiple sources:
    - How can we distinguish between and treat uncertainties due to numerical error, model inaccuracies, or input data that is imprecise or not well understood, even when such uncertainties may need to be addressed in a unique way?

- The extrapolation of results beyond the validation regime:
    - How do we quantify uncertainties when we extrapolate them to physical parameter regimes that are beyond the experimental database?
    - What role should "expert judgment" play?

- Coupling predictive simulations with dynamic, probabilistic risk assessment (PRA) and quantifying probabilities of rare outcomes:

- Can we develop coupled tools that we can use to assess a given scenario and simulate a predicted outcome? Can we repeat this process to provide a dynamic system model?
- How do we use UQ to help predict the likelihood of rare, but potentially catastrophic, events knowing that experimental data that describe such outcomes is difficult to find?

- New approaches for VU in the exascale computing environment:
  - Can we successfully manage and process the large quantity of numerical experiments that will probably be required to perform UQ studies and gather the necessary statistics, especially if the number of experiments might become very large?
  - Can we harness new levels of computing power to provide an "artificial intelligence" or self-adapting system that would be able to assess the source of different model uncertainties? Might such a system help scientists prioritize what future experiments and simulations they should perform?

7.5. System Integration Panel:

Conclusions

The Systems Integration Whitepaper outlined the weaknesses common to most, if not all, of today's energy system models and underscored the issues we believe are of greatest concern. And yet, having a robust energy system analysis capability is critical to providing sound analysis of important policy decisions.

The challenge to policy architects and strategic planners is broad. In some cases, policy has faced barriers because different political philosophies have blocked effective policy formulation. In other cases, policy has stumbled because we don't have the data we need to characterize "ground reality." In general, our ability to reach a consensus on energy strategies is made more difficult by the many cause and effect relationships that are part of the behemoth system-of-systems that represent the U.S. and global energy enterprise.

In these recommendations, we discuss how to take a different approach to "doing business." To define a new approach, we should specify what the most desirable elements for a model are. These are:

- *Open-source architecture.* Whatever is built should be "open source," so that proprietary[44] aspects are minimized as much as possible.

[44] By 'proprietary' data we mean data whose distribution may be restricted for either commercial reasons or for national/homeland security reasons.

- *Transparency*. Models must be transparent when users, whether they are experts or novices, run them and interpret their results.

- *Modularity.* It is important to insist upon modularity in the underlying modeling code and consistency in code generation when constructing energy system analysis tools.

- *Providing for differences in the sophistication of users and model builders*. The code development techniques of modern computer science can satisfy all of these human-model interaction levels. We should rely upon these when we build these new models.

- *An ease of data comprehension*. Since models are only valuable if their results can be readily understood, it is crucial that users understand how models operate and how they produce results.

- *Efficiency*. One of the insights gained from large community modeling efforts, such as the Global Climate modeling program that the National Center for Atmospheric Research (NCAR) hosted, is that having a project-related resource center handling issues such as code debugging, regression testing, and porting, allows individual research groups to focus on science.

- *Community building*. The global climate community has also shown how a community-based modeling program can produce a vibrant intellectual community that debates the core issues in the modeling effort.

Recommendations

The Department of Energy (DOE) should convene a workshop to address these topics that draws upon the success of the DOE's Office of Science's "Research Needs" workshops. This workshop, with participants from the federal and private sector as well as international partners, would identify simulation requirements, examine current simulation capabilities, and formulate a detailed strategy to begin a major development effort similar to the one we have recommended. The workshop would be an appropriate setting to discuss new systems models, especially a model's scope and the level of effort and funding needed to create it. Due to the urgent nature of this modeling effort, we recommend that DOE establish a workshop steering committee as soon as possible. This committee should organize the workshop and complete its deliberations no later than December 2009.

7.6. Overall Workshop Conclusions:

This workshop builds on a series of workshops the Office of Science sponsored in the summer of 2006 to explore the role of modeling and simulation in advancing the research

needs of advanced nuclear energy systems. The output from these workshops, published in the following documents: Basic Research Needs for Advanced Nuclear Energy Systems, July 31 – August 3; Report on the Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop, August 10-12, and Workshop on Simulation and Modeling for Advance Nuclear Energy Systems, August 15-17, represents a roadmap for a strong modeling and simulation effort for advanced nuclear energy systems. This workshop will builds and extends the results of these previous workshops. Given that the previous workshops were held almost three years ago, it would be useful to have an assessment of the technical status of the various elements of the existing program.

We believe this workshop report is a concise, but thorough study of the issues associated with building modeling and simulation at the extreme scale of fission nuclear reactor systems. We also believe the recommendations provided in the whitepapers will serve as an excellent foundation for the subsequent research and development supported by the Office of Science and Nuclear Energy and we urge that they be implemented as soon as practical.

Appendix A: Charge for the Workshop

Department of Energy
Washington, DC 20585

SEP 30 2008

Dr. Robert Rosner
Director
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

Dr. Ernest Moniz
Department of Physics
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, MA 02139

Dear Drs. Rosner and Moniz:

Thank you for agreeing to organize and conduct an international workshop to examine the role of computing at the exa-scale in meeting the foremost challenges for the future of nuclear energy. A key goal for the workshop is to present the nuclear energy community with the opportunity to shape the appropriate role for exa-scale scientific computing in the quest to advance these scientific frontiers.

As you know, the United States and the world are likely in the early stages of a nuclear renaissance in which nuclear fission energy, along with many other forms of energy, is being developed and deployed to provide abundant "carbon-free" power. If this leads to multi-terawatt deployment of nuclear power in this century, new nuclear reactor, fuel, and fuel cycle technologies will be needed. Furthermore, these technologies will call for new levels of system integration. Development of the new technologies and associated analytical tools is an expensive multi-decadal proposition, and we must embark on program development expeditiously if we are to meet the needs in a timely way. The question for this workshop is: What is the role of exa-scale modeling and simulations in accelerating the development and deployment of these new reactor, fuel and fuel cycle technologies? What are the DOE program requirements for developing and implementing the essential tools? We believe this workshop can play a seminal role in understanding the issues and possible solutions.

This workshop will build on a series of workshops the Office of Science sponsored in the summer of 2006 to explore the role of modeling and simulation in advancing the research needs of advanced nuclear energy systems. The output from these workshops, published in the following documents: Basic Research Needs for Advanced Nuclear Energy Systems, July 31 – August 3; Report on the Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop, August 10-12, and Workshop on

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Simulation and Modeling for Advanced Nuclear Energy Systems, August 15-17, represents a roadmap for a strong modeling and simulation effort for advanced nuclear energy systems. We expect your workshop will develop a report that builds on the results of these previous workshops.

The report from your workshop is expected to be a document that should not exceed 100 pages and should be completed by the end of April 2009, if at all possible. I would like to stress that this is to be a collaborative effort between NE, NP, NNSA and ASCR. I would also welcome any other recommendations on program content, emphasis, or balance. This effort, I realize, is a large undertaking. However, nuclear energy systems are likely to play an important role in our nation's energy future well into the later half of this century and it is the responsibility of DOE and the scientific community to develop the key technology options.

A desired outcome of these meetings, and as a step in preparing for the final workshop and subsequent report, is to develop a short list of "global challenge" computational problems. Solving these problems should have the potential to transform our understanding of science and its impacts and to improve our ability to apply knowledge in applications important to science, engineering, industry, and society. This list should include:

Physics Issues Surrounding Nuclear Energy: These issues include but are not restricted to reactor core and safety simulations, nuclear fuel performance simulations, separations and safeguard simulations, waste forms and repository simulations, and materials simulations.

Systems Integration: The use of modeling and simulation to understand the interactions between complex nuclear systems from the energy source itself up to and including the entire fuel cycle.

Verification, Validation, and Uncertainty and Risk Quantification: This topic should discuss the challenges of verification, validation and uncertainty quantification for large exa-scale level simulations of fission nuclear energy systems. It should explore possible methods for understanding the contribution to overall risk quantification of nuclear energy systems.

Computational Technologies: The topic should address the computation resources and software development necessary to support exa-scale modeling and simulation for nuclear systems.

An effort should be made to identify the scope of the funding required to achieve success.

SEP 3 0 2008

Mr. Alex Larzelere of the Office of Nuclear Engineering Research and Dr. Walt Polansky of the Office of Advanced Scientific Computing Research are the program managers responsible for this workshop. Alex and Walt will be contacting you shortly to discuss the schedule, deliverables, logistics and administrative needs.

If, at any time, you have questions about current plans, priorities and strategies, please feel free to contact us. Many thanks for your willingness to lead what we hope will be a landmark workshop in the field.

Sincerely,

Dr. Michael Strayer
Associate Director of Science
Office of Advanced Scientific Computing Research

Dr. Paul Lisowski
Deputy Assistant Secretary
Office of Nuclear Energy, Fuel Cycle Management

Appendix B: Workshop Agenda

Monday, May 11th		
	Session	**Lead**
8:00am	Opening Remarks – Workshop Charter	Ernie Moniz Bob Rosner
8:15	Program Perspective	Michael Strayer Alex Larzelere
8:30	Future Computing Environments	Thomas Zacharia
9:00	Charge to Breakout Groups	Ernie Moniz Bob Rosner
9:30	**Coffee Break**	
10:00	Parallel Breakout Sessions with Presentations of Whitepapers at Each Session	Session Chairs
12:00	**Working Lunch**	
1:00	Continue Parallel Breakout Sessions	Session Chairs
2:30	**Coffee Break**	
3:00	Initial Session Report - Integrated Performance and Safety Simulations of Nuclear Energy System	Stephen Lee Moran Parviz
3:30	Initial Session Report - Advanced Material Behavior Modeling	Brian Wirth Tomas de la Rubia
4:00	Initial Session Report - Verification, Validation and Uncertainty Quantification for Nuclear Energy Simulations	Marv Adams Richard Klien
4:30	Initial Report - Nuclear Energy System Integration	Vic Reis Yves Kaluzny
5:00	Day One Observations and Wrap Up	Ernie Moniz Bob Rosner
5:30	Adjourn	

Tuesday, May 11th		
	Session	**Lead**
8:00am	Day Two Welcome and Opening Remarks	Ernie Moniz Bob Rosner
8:15	Continuation of Breakout Sessions	Session Chairs
9:30	**Coffee Break**	
11:00	Budget Planning and Priorities: A Perspective from OMB and Congress	
12:00	**Working Lunch**	
1:00	Final Session Report - Integrated Performance and Safety Simulations of Nuclear Energy System	Stephen Lee Moran Parviz
1:45	Final Session Report - Advanced Material Behavior Modeling	Brian Wirth Tomas de la Rubia
2:30	**Coffee Break**	
3:00	Final Session Report - Verification, Validation and Uncertainty Quantification for Nuclear Energy Simulations	Marv Adams Richard Klien
3:45	Final Report - Nuclear Energy System Integration	Vic Reis Yves Kaluzny
4:30	Steps Forward for ASCR and AFCI	Bob Rosner& Ernie Moniz
5:00	**Adjourn**	

Appendix C: Workshop Attendees

Workshop Role	First Name	Last Name	Organization
Integrated Performance and Safety Code (IPSC) Panel			
Panel Chair	Stephen	Lee	Los Alamos National Laboratory
Panel Chair	Parviz	Moin	Stanford University
Pre-workshop Whitepaper Author	Tom	Downar	Purdue University
Pre-workshop Whitepaper Author	Andrew	Siegel	Argonne National Laboratory
Panel Member	James	Blanchard	University of Wisconsin
Panel Member	Christen	Chauilac	CEA
Panel Member	Bob	Hill	Argonne National Laboratory
Panel Member	Art	Kerman	MIT
Panel Member	David	McCallen	Lawrence Berkeley National Laboratory
Panel Member	John	Mitchiner	Sandia National Laboratories
Panel Member	Patrick	O'Leary	Idaho National Laboratory
Panel Member	Rick	Stevens	Argonne National Laboratory
Panel Member	John	Turner	Oak Ridge National Laboratory
Workshop Organizer and Panel Member	David	Nowak	Argonne National Laboratory
Material Behaviors Panel			
Panel Chair	Tomas Diaz	de la Rubia	Livermore National Laboratory
Panel Chair	Brian	Wirth	UC Berkeley
Pre-workshop Whitepaper Author	Marius	Stan	Los Alamos National Laboratory
Pre-workshop Whitepaper Author	Sid	Yip	MIT
Panel Member	Tom	Arsenlis	Livermore National Laboratory
Panel Member	Chaitayna	Deo	Georgia Tech
Panel Member	David	Dixon	University of Alabama
Panel Member	Moe	Khaleel	Pacific Northwest National Laboratory
Panel Member	Doug	Kothe	Oak Ridge National Laboratory
Panel Member	Yves	Limoge	CEA
Panel Member	Paul	Lisowski	Office of Nuclear Energy
Panel Member	Mark	Lusk	University of Colorado
Panel Member	Michael	Pernice	Idaho National Laboratory
Workshop Organizer and Panel Member	Alex	Larzelere	Office of Nuclear Energy
Verification, Validation and Uncertainty Quantification Panel			
Chair	Marv	Adams	Texas A&M
Pre-workshop Whitepaper Author	Richard	Klein	UC Berkeley
Pre-workshop Whitepaper Author	Paul	Turinsky	North Carolina State
Panel Member	Hany	Abdel-Khalik	North Carolina State University
Panel Member	John	Kelly	Sandia National Laboratories
Panel Member	Jim	Stewart	Sandia National Laboratories
Panel Member	Rizwan	Uddin	University of Illinois

Workshop Role	First Name	Last Name	Organization
Panel Member	Cetin	Unal	Los Alamos National Laboratory
Workshop Organizer and Panel Member	Paul	Messina	Argonne National Laboratory
Systems Integration Panel			
Panel Chair	Vic	Reis	Department of Energy
Panel Chair	Yves	Kaluzny	CEA
Pre-workshop Whitepaper Author	Steven	Goldberg	Argonne National Laboratory
Pre-workshop Whitepaper Author	Charles	Forsberg	MIT
Panel Member	Leonid	Bolshov	IBRAE
Panel Member	Dana	Christensen	Oak Ridge National Laboratory
Panel Member	Matt	Crozat	Office of Nuclear Energy
Panel Member	Sherrell	Greene	Oak Ridge National Laboratory
Panel Member	Mark	Peters	Argonne National Laboratory
Panel Member	Glen	Sjoden	University of Florida
Panel Member	Gil	Weigand	Oak Ridge National Laboratory
Co-Chair and Panel Member	Bob	Rosner	Argonne National Laboratory
Others			
Observer	Pete	Beckman	Argonne National Laboratory
Observer	Jay	Billings	Oak Ridge National Laboratory
Observer	David	Brown	Livermore National Laboratory
Observer	Lali	Chatterjee	Office of Science
Observer	Phil	Colella	UC Berkeley
Observer	Julian	Cummings	CalTech
Observer	Lori	Diachin	Livermore National Laboratory
Observer	Anath	Grama	Purdue University
Observer	Mark	Guiton	Cray Inc.
Observer	Barbara	Helland	Office of Science
Observer	Thuc	Hoang	National Nuclear Security Agency
Observer	Leland	Jameson	National Science Foundation
Observer	Ken	Koch	Los Alamos National Laboratory
Observer	Bob	Little	Los Alamos National Laboratory
Observer	Rusty	Lusk	Argonne National Laboratory
Observer	Barney	MacCabe	University of New Mexico
Observer	William	Martin	University of Michigan
Observer	Jeffery	Nichols	Oak Ridge National Laboratory
Observer	Valerio	Pascucci	University of Utah
Observer	Ahmed	Sameh	Purdue University
Observer	Thomas	Sterling	Louisiana State University
Observer	Tim	Tautges	Argonne National Laboratory
Speaker	Miachael	Holland	Office of Management and Budget
Speaker	Buzz	Savage	Office of Nuclear Energy
Speaker	Thomas	Zacharia	Oak Ridge National Laboratory