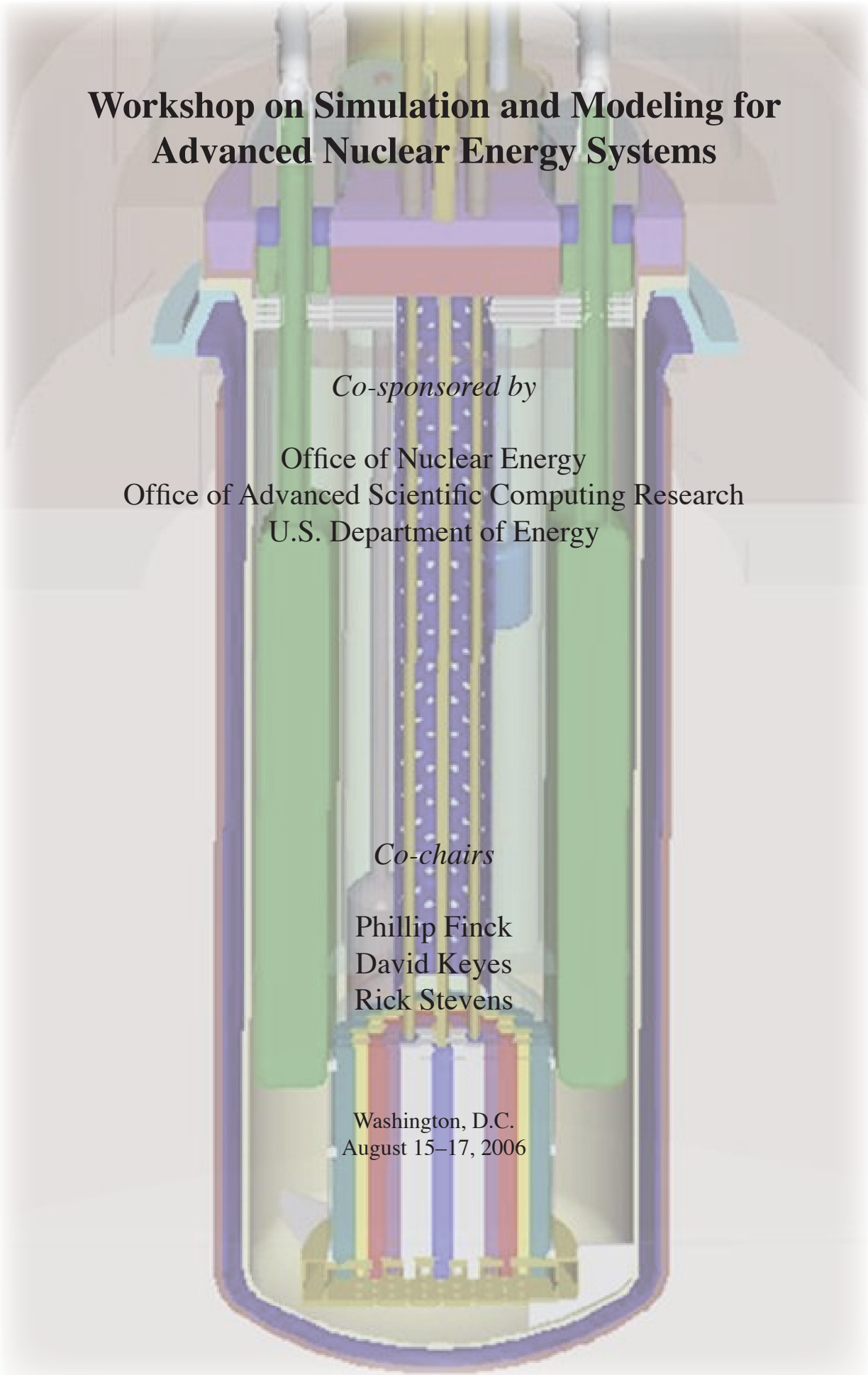
Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems



Co-sponsored by

Office of Nuclear Energy
Office of Advanced Scientific Computing Research
U.S. Department of Energy

Co-chairs

Phillip Finck
David Keyes
Rick Stevens

Washington, D.C.
August 15–17, 2006

Contents

Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems

August 15–17, 2006

Executive Summary

A joint workshop of the Department of Energy Office of Nuclear Energy and Office of Science was held August 15–17, 2006, in Washington, DC, to explore the simulation and modeling needs for developing advanced nuclear energy systems. The purpose of the workshop was to obtain community input on the role of computational science and high-performance computing in the DOE Advanced Fuel Cycle Initiative (AFCI) and the emerging Global Nuclear Energy Partnership (GNEP).

The open workshop was attended by over 170 participants, representing 20 American universities, 10 DOE national laboratories, the nuclear and computer industries, and international collaborators (France and Japan). Approximately two-thirds of the representatives at the workshop were drawn from the nuclear engineering and nuclear energy community.

Effort was made to ensure that participants explored the entire spectrum of research and development opportunities, in both the short term (1–5 years) and the long term (5 years and beyond), since the GNEP program unfolds over several decades. Special attention was paid to tie workshop findings and recommendations both to the Office of Nuclear Energy needs and to current and expected future capabilities of the Office of Science, and in particular, the Office of Advanced Scientific Computing Research. This objective was facilitated by a series of plenary talks providing overviews of current and planned activities of these Offices.

Technical discussions began with breakout sessions organized by experts in the nuclear energy and focusing on six areas where simulation and modeling are clearly relevant to the GNEP program: reactor core simulation, seismic/structural mechanics/balance-of-plant, validation, repository, separations chemistry, and materials and fuel design. The goal was to define opportunities for collaboration between the nuclear energy research community and the applied mathematics and computer science communities. These sessions were followed by breakout sessions led by computer scientists and focusing on six areas where advanced simulation techniques could benefit the nuclear energy community: mathematical and geometrical modeling; validation, verification, and uncertainty quantification; scalable and multiscale algorithms; software tools and software engineering; computing facilities, data, and networking; and data analysis and visualization.

Several crosscutting issues in the enabling technologies emerged as themes during the workshop and are likely fertile ground for investment and collaboration.

- Uncertainty quantification and error estimation in simulations
- Methods for systems that couple multiple models
- Movement away from empirical models toward physics-based, first-principles models
- Methods for systems with multiple scales
- Algorithms and software that scale well on high-capability computational platforms
- Simulation workflow management, including data archiving and automated discovery

The following are the high-level findings of the workshop:

1. The code base currently used for advanced nuclear systems is insufficiently predictive to guarantee attainment of the ambitious technology stretch goals of the Global Nuclear Energy Partnership.
2. A significant opportunity exists to apply advanced modeling and simulation and high-performance computing to improve designs of future reactors, reduce uncertainty in facilities development and construction costs, improve safety, and reduce development times of new fuel types needed to close the nuclear fuel cycle.
3. Significant research challenges remain in developing and scaling multiscale and multiphysics codes to the performance levels on advanced high-performance computers needed for fundamental studies, as well as for design and engineering use. These research challenges are similar (but not identical) to those faced in other science and engineering domains; thus many methods can be leveraged from other disciplines.
4. Accomplishing the development priorities of GNEP will require investment in existing nuclear energy codes and software tools to address short-term design and planning use, simultaneously with investments to start longer-term projects aimed at future needs that have long development times.
5. The United States has some of the required expertise but also needs to continue to develop younger scientists and engineers. The nation is capable of deploying computational infrastructure to begin building a new generation of nuclear energy simulation codes that could shift paradigms in the development of new nuclear energy systems. To reap the benefits of an approach that uses computation to reduce the scope, cost, and time latency of required experimentation will, in turn, require a sustained software development activity and a corresponding buildup of human resources and large-scale faculties.
6. The creation of new physics-based high-fidelity simulation codes offers the possibility of accelerating the licensing process, if the regulatory process can be modified to incorporate first-principles simulations as a basis for risk analysis and design approvals.

High-level recommendations include the following:

1. Establish a significant number of multidisciplinary teams comprising experts in applied mathematics, computer science, nuclear engineering, materials science, physics, chemistry, and advanced software engineering to begin the development of next-generation simulation codes based on models closer to first principles aimed at deployment in the five- to ten-year time frame. These teams should have the explicit goal to develop open source community codes that will be used for next-generation design of nuclear fuels, power plants, separation plants, and repositories. Experiences with the DOE Scientific Discovery through Advanced Computing and Advanced Strategic Computing programs offer confidence that this goal can be achieved, as well as offering much software for leveraging.
2. Establish a requirements-driven process that will enable the community to define accuracy and validation goals for each computation tool and for an integrated simulation system.
3. Establish and support teams of software engineering and parallel computing experts to work with the established nuclear engineering community on existing codes, to port these codes to modern platforms in the near term, to integrate them into modern engineering workflows, and to support near-term design and engineering.
4. Establish a scientifically demonstrated validation process that will provide sufficient assurance of the predictive capabilities of simulations—first of components and ultimately of integrated systems—that stakeholders beyond the technical realm will be able to rely on simulation to support capital investment and both national and international policy making.
5. Create a long-term research program including a mix of university and laboratory research aimed at advancing the cross-cutting issues (e.g., new approaches to uncertainty quantification and error estimation, multiscale and scalable algorithms, and development and validation of coupled multiphysics codes). This work should be motivated by the actual research and development needs of the GNEP program and should be supported at a level that permits rapid acceleration.
6. Dedicate significant resources on DOE's large-scale facilities for proof-of-principle runs, development of new methods, and the production use of existing and new tools by the U.S. nuclear energy community and its international GNEP partners.
7. Develop a foundation (university programs and laboratory internships) for training the next generation of computationally oriented nuclear engineers and scientists in related disciplines needed to support the long-term redevelopment of nuclear energy in the United States and the world.

1. Background and Objectives

In the past year, the federal government announced the Global Nuclear Energy Partnership (GNEP), which seeks to develop consensus on enabling expanded use of economical, carbon-free nuclear energy to meet growing electricity demand. A principal objective of the 2006 Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems was to identify the research opportunities and priorities for advancing the use of simulation and modeling in the research and development of advanced nuclear energy systems.

Another objective of the workshop was to encourage increased communication between nuclear energy researchers and computer scientists and applied mathematicians. Often, software developers have developed useful tools that have not been transferred to the nuclear energy community; and often, this same community needs special tools that the computer scientists are unaware of. By bringing these two groups together, the workshop sought to identify what enabling simulation software is available and what tools are needed for making the GNEP program successful.

This was one of four workshops sponsored by the federal government this summer. Two DOE agencies were involved:

- Office of Nuclear Energy
- Office of Advanced Scientific Computing Research

In the remainder of this report, we summarize the activities of the 2006 meeting on Simulation and Modeling for Advanced Nuclear Energy Systems. These activities included keynote addresses, breakout discussions, working group sessions, and presentations. We conclude with an evaluation of the three-day meeting and suggestions for bringing the GNEP vision to fruition.

2. Modeling and Simulation Needs for Advanced Nuclear Energy Systems

GNEP envisions the implementation of a novel set of nuclear technologies to enable long-term sustainability of the nuclear fission power option. GNEP will, in particular, extend long-term energy resources, dramatically reduce the need for geologic repositories and the proliferation risk associated with the inevitable global expansion of nuclear energy.

To achieve these objectives, GNEP proposes replacing the current once-through nuclear fuel cycle with a nearly closed fuel cycle, relying on a combination of technologies:

- Commercial reactors, mostly light water reactors (LWRs), will continue to operate in their current mode and, as a result, will produce significant quantities of spent nuclear fuel (SNF).
- The SNF, instead of being sent to temporary storage or to geologic disposal, will be treated to separate its constitutive elements. Certain elements will be encased in novel waste forms to be disposed of, whereas the transuranic elements (TRUs) will be transmuted (mostly via the fission process) in specialized fast reactors.
- Specifically, the TRUs will be sent to a fuel fabrication plant, where they will be incorporated in novel forms of fuel.
- The novel fuels will be irradiated in a fast neutron reactor, where a fraction of the TRUs will be destroyed. The irradiated fuel will be treated to separate its constitutive elements. The extracted TRUs will be sent back to the fuel fabrication plant, whereas other elements will be incorporated in specialized waste forms for ultimate disposal.

New nuclear technologies are generally extrapolated from existing technologies over a long gestation period, following which there is strong confidence that their implementation will be technically successful. Nevertheless, a number of issues remain, including technical feasibility issues (can the GNEP requirements be met?); cost issues (will GNEP be affordable?), and regulatory issues (can the GNEP technologies be licensed?).

For example, in the area of separations technology, key technical feasibility issues include the needs to reduce separations losses to a very low level, create waste forms that will last for extremely long periods, and track materials throughout the plant with high precision. Losses, and the concomitant need to clean up and recycle waste streams, contribute to increased costs. Finally, a licensing approach for separations plants needs to be established; this will likely impose additional requirements on the design approach.

For another example, in the area of transmutation fuel fabrication and irradiation, advanced fuels with significant quantities of minor actinides have not yet been demonstrated; this is the key feasibility issue for all of GNEP. The current approach to fuel development is empirical, relying on sequential experimentation, with significant

implications for schedule and cost. The scientific understanding of fuel irradiation behavior is limited and creates additional constraints on the licensing process.

During the first part of the workshop, the nuclear energy community discussed these issues, beginning with an overview of the state of the art in six areas of advanced nuclear energy systems: reactor core; materials and fuels; separation chemistry; repository modeling; seismic, structural mechanics, and balance of plant; and validation. In each of these areas, an effort then was made to identify ways in which the injection of improved simulation techniques and modeling tools could help address the issues. (Because the discussion of validation interfaced so closely with the verification/validation and uncertainty analysis discussions by the computing science community, those topics were combined and are presented together in Section 3.1.)

2.1 Reactor Core Simulation

The objective of reactor core simulations is to predict a series of plant parameters (fluxes, temperatures, stresses, damages, etc.) during normal and off-normal events, during static and transient events, for short-term operational times up to the plant lifetime. These quantities are important for the plant efficiency and safety and for single-component and system reliability and lifetime.

Current Status

Reactor core simulation and modeling involves neutronics, fluid and heat transfer (called thermal hydraulics by some engineering disciplines), thermomechanics, fuel behavior, chemistry, and balance of plant—all with feedback effects. The current methodology for reactor core modeling is to rely on experiments, then prototype operation, and ultimately full-scale demonstrations to provide a degree of confidence in simulation tools. Costly testing is essential because of the lack of confidence in the simulation tools and associated parameters. Most of these tools were produced many years ago and lack advances in physics, numerical algorithms, software engineering, and high-performance computing. Design margins could be significantly improved by better reactor core modeling. For example, a challenging problem is the design of passive safety features for a sodium fast reactor where a complex sequence and combination of neutronic reactivity, thermal-hydraulic, and thermomechanics effects must be considered.

Needs

The major reactor core challenges are related to safety and economic competitiveness and, for GNEP in particular, to the simulation of fast reactor transient and accident response. For more traditional reactors challenging problems are nucleate boiling, critical heat flux (with mixing grids effect), pressurized thermal shock, reflooding, and fluid structure interaction. These call for better physical modeling, better applied mathematics

algorithms, multiresolution and adaptivity for multiresolution of multiphysics multiscale problems, and an innovative approach for integration level of solvers (e.g., writing the integrated governing equations for the coupled problem). As a consequence one will be confronted with problems related to the parallelization of the solvers, the software architecture for an efficient integration, and some intractable (even with petascale generation of computers) number of unknowns (e.g., deterministic neutronics 10^{15}, DNS fluid and heat transfer 10^{16}, for static problems). Verification and validation of simulation software will prove a major challenge because of the difficulties associated with uncertainty propagation through multiphysics multiscale simulators and lack of integral experiments. Section 3.4.2 considers in detail the problem of parallelization of codes in the nuclear industry, and Section 3.4.3 discusses advanced frameworks for GNEP.

Enabling a New Simulation System. Adopting a first-principles approach utilizing advances in both hardware and software tools will make possible a new simulation system with extraordinary capabilities. An integrated high-fidelity system of software tools would describe the overall nuclear plant behavior taking into account coupling among the different systems and physical phenomena during reactor operations or safety-related transients. This coupling would link neutronics, fuel behavior, fluids and heat transfer, and structural mechanics. The system must also be coupled with the balance-of-plant software model. The new system should perform sensitivity and uncertainty analyses to assess margins, qualify, validate, and optimize designs.

2.1.1 Neutronics

Simulation and modeling of nuclear reactor physics are an important aspect of the GNEP program. Most industry modeling is specific to current reactor designs. Departures from these designs, such as using reprocessed fuel, will require higher-fidelity simulation tools based more on first principles than on normalization to current designs.

Current Status

Two methods exist for simulating and modeling nuclear radiation, particularly neutron interactions. Although deterministic methods are fast for one-dimensional models, both methods are slow for realistic three-dimensional problems.

- ***Deterministic Methods***. Deterministic neutronics plays a fundamental role in reactor modeling and simulation. A first-principles treatment requires solution of the linearized Boltzmann transport equation. This task demands enormous computational resources because the problem has seven dimensions: three in space, two in direction, and one each in energy and time. Indeed, experience in the ASC program indicates that the resource requirements of transport dominate those of all other physics components in multiphysics simulations. Parallel algorithms are difficult to develop for transport because the basic source iteration technique used to solve the equations requires the solution of a block lower-

triangular system. Good efficiencies have been achieved for terascale computers using thousands of processors, but the existing algorithms will fail at the petascale level.

- ***Monte Carlo Methods***. Monte Carlo methods model the nuclear system (almost) exactly and then solve the exact model statistically (approximately) anywhere in the modeled system. Monte Carlo methods promise greater accuracy and efficient parallel algorithms at the petascale level but also face many challenges. Orders-of-magnitude faster convergence is required in full-core reactor simulations to achieve acceptably accurate solutions throughout a reactor. In addition, memory requirements can be large because, in contrast to deterministic methods where domain decomposition can be used and only the descriptive data for a single subdomain saved on a single processor, Monte Carlo methods are not naturally amendable to decomposition.

Needs

With regard to ***deterministic methods***, fundamentally new solution algorithms will be required to achieve acceptable parallel performance at the petascale level (see Section 3.3 for discussion of scalable algorithms). Furthermore, the need for predictability will require adaptation in all seven dimensions. Current adaptive methods generally relate only to spatial adaptivity. Extension of such capability to angle is required. Improved energy discretization techniques are critical to achieving predictability and estimating uncertainty. Tens of thousands of energy grid points are required to fully resolve the energy dependence of neutron interaction cross sections. Even at the petascale, a brute-force resolution of this dependence is not practical. Current energy discretization methods are based on gross homogenization and are not compatible with a posteriori error estimation. Thus, novel subgrid models for treating the energy dependence must be developed.

With regard to ***Monte Carlo methods***, more sophisticated tally analysis is needed to ensure numerical stability and true convergence when coupling to fluids and heat transfer algorithms, CAD geometries, and deterministic codes on nonorthogonal grids. Another challenge is that there is currently no continuous-energy adjoint capability for algorithm acceleration. The adjoint capability is also needed for the calculation of sensitivities and uncertainties for reactivity parameters and for cross-section sensitivity analysis. Other challenges include the possibility of generating cross sections for deterministic calculations with Monte Carlo methods, “real-time” Monte Carlo analysis, and direct modeling of fission product transport and material damage. As for Monte Carlo needs, the first priority is the efficient accumulation of high-precision fluxes (everywhere) throughout a reactor geometry on a nonorthogonal grid of cells to support multiphysics coupling, to more accurately calculate parameters such as reactivity coefficients, and perhaps to generate multigroup cross sections. New methods are needed to accelerate global convergence, to estimate the propagation of cross section and statistical

uncertainties throughout the reactor depletion process, and to enhance burn-up depletion capabilities.

For reactor core modeling and simulation, deterministic methods will be used principally in the short term (3–5 years) with Monte Carlo as a benchmarking tool. In the intermediate term (5–10 years) Monte Carlo methods could be used as a hybrid tool with multiphysics coupling to deterministic neutronics and thermal hydraulics codes. In the long term (>10 years) multiphysics codes using nonorthogonal grids will provide complete, high-accuracy design tools, fully integrated into reactor core design and operation.

2.1.2 Fluids and Heat Transfer

Modeling fluid flow and heat transfer is necessary, not only for core modeling, but also for the whole plant, including steam generators, pipes, pumps, and condensers. Because of the complexity of the phenomena and geometries involved, current codes often rely on empirical correlations. It is often not clear whether these correlations can be readily extrapolated to new situations. The scientific challenges are in physical modeling, numerical methods, and computer science. Physical modeling must rely on more first-principles methods for single-phase and multiphase-multifluid flows, for steady and unsteady flows, and with or without heat transfer. Numerical methods must be more robust and provide the optimal mix between accuracy and stability. Codes must deal with billions of mesh elements and enable easy multiscale and multiphysics coupling.

Current Status

The main problems to solve in the short term (2–5 years) for light water reactors (LWRs) are pressurized thermal shock, gravity-driven flows, and fluid-structure interactions. For sodium-cooled fast reactors (SFRs) detailed core flow modeling is needed. In the intermediate term (5–10 years) reflooding and thermal fatigue of LWRs and transients and severe accidents for SFRs must be addressed. In the long term (>10 years) critical heat flux for LWRs and the fluids and heat transfer portion of the numerical reactor simulation for both LWRs and SFRs must be developed. Development is needed in four areas: (1) direct numerical simulation (DNS), the closest scale to first-principles approach: front-tracking, diffuse interface models, particle methods, and lattice Boltzmann techniques; (2) computational fluid dynamics (CFD) in open media (detailed calculation within one subchannel or within plena), with a focus on large-eddy simulation and high Reynolds numbers; (3) CFD in porous media (for multichannel analysis); and (4) system scale (overall plant calculation).

Needs

The focus should be on multiscale and multiphysics coupling and on complex geometries (see Section 3.2 for recent techniques that may address these needs). For the physical

modeling of multiphase, multifluid flows, the main development is needed in multifield models, interfacial area transport, and transition between flow regimes. For numerical methods, the main development is needed in unstructured grids with adaptive mesh refinement, porous media modeling with provision for nonisometric permeability, all for a range of boundary conditions. Moreover, development is needed in uncertainties (input data plus propagation) and validation and verification. In particular, for better validation, new generic experiments are needed with detailed instrumentation.

2.1.3 Multiphysics Coupling

In order to correctly include feedback effects and other reactor core simulation requirements, multiphysics coupling is needed to link neutronics (both Monte Carlo and deterministic) to fluids and heat transfer algorithms, structural mechanics, and fuel behavior, on nonorthogonal grids. Such coupling, for instance, is critical for correctly calculating reactivity-initiated accidents. In the case of SFR, of particular importance is to take into account structural mechanics deformations induced either by heat or stress. These algorithms could be linked to reactor transient analysis codes for accident modeling. Coupling statistical algorithms to deterministic algorithms is also a challenge. Very large numbers of grids cells with differing material characteristics may require domain decomposition on parallel computers (i.e., for a problem too large to be loaded on each processor).

Current Status

The current approach to multiphysics coupling is static coupling of separate codes. The accuracy and efficiency of static coupling are not well understood: "code coupling" is first-order accurate in time (at best), and this loose coupling presents convergence challenges. The fact that a coupled solution displays numerical stability does not guarantee accuracy. Multiphysics coupling faces many challenges. First is devising parallel coupling algorithms that overcome low-order time accuracy and provide rapid steady-state convergence. Next is including mesh, time-step, and physics model (multiscale) mesh adaptivity. Finally, a means is needed to assess the predictive capability of multiphysics simulations. (For further discussion of the coupling of codes, see Section 3.4.1.)

Needs

Two areas for multiphysics coupling algorithms research clearly are critical: ***development of second-order (at the least) in time coupling methods,*** and ***development of coupling approaches*** that support sensitivity analysis, data assimilation, and PDE-constrained optimization. Possible starting points include Strang splitting, predictor-corrector methods, implicit-explicit methods, and Jacobian-free Newton-Krylov methods.

There also exists a need to develop ***software architecture*** for efficiently treating the coupled problems. An example is the ability to define and plug in new and different combinations of physics-module implementations to study different phenomena, define and combine different numerical techniques, configure the code easily to run on new platforms, and develop new physics components without expert knowledge of the entire system. For further discussion of coupling multiple codes and examples of successful code coupling in large-scale simulations, including the Common Component Architecture work of the DOE SciDAC program, see Section 3.4.1.

2.1.4 Sensitivity Analysis

The predictive capability of reactor core simulation can generally be assessed with sensitivity and uncertainty analysis (SU). Uncertainty originates from errors in physical data, manufacturing uncertainties, and modeling and computational algorithms. SU is required to address cost, safety, and licensing needs and should be applied to all aspects of reactor core simulation. SU can guide experimental, modeling, and algorithm development R&D.

Current Status

Current SU relies on derivative-based methods such as stochastic sampling methods and on generalized perturbation theory to obtain sensitivity coefficients. Neither approach addresses all needs.

SU capabilities must be developed for comprehensive multiphysics simulation (e.g., radiation transport, fluids, thermal sciences, mechanics, chemistry, materials science, isotopic balance) with nonlinear feedback mechanisms. For licensing applications, the capability must accurately evaluate low-probability "wings" of uncertainty distributions (e.g., power peaking factor not being exceeded at 95% probability/95% confidence level) and discrete events (e.g., impact on core trip time during accident progression), in addition to sensitivity coefficients and covariances. SU must address both loosely coupled (e.g., sequence of coupled codes via I/O) and tightly coupled simulations. Clearly needed is knowledge of uncertainties in input parameters and data (e.g., cross sections, correlations, dimensions, and compositions), as well as knowledge and understanding of sources and uncertainties and biases in analytic and numerical modeling approximations. When using stochastic sampling of input parameter distributions or perturbations to obtain sensitivity coefficients, computer execution time limits the utility of these approaches to small input datasets. On the other hand, when adjoint-based methods are used, the utility of the approach is limited by the programming burden, treatment of nonlinearity, and computer execution times when considering loosely coupled codes or large numbers of responses.

Needs

Sensitivity and uncertainty analysis methods need to be considered an integral part in the development of multiphysics methods. SU adjoint-based methods are required, as well as SU algorithms that are noninvasive (e.g., forward perturbation, random sampling, subspace). Of particular importance are innovative methods that address nonlinearity, can predict responses' probability distributions, treat discrete events, and handle simultaneously large input data and response fields in a computationally efficient manner.

2.2 Materials and Fuels

Advanced nuclear energy systems such as those proposed for GNEP involve the production and exposure of a broad range of actinide-bearing fuel and structural materials to extremely challenging irradiation environments. Of highest priority are those materials constituting a single transuranic (TRU) fuel pin—the fuel and structural cladding. The TRU fuel pin not only is exposed to (in fact, is the source of) the highest irradiation damage rates but also involves novel chemistries, physics, materials structures, and compatibility issues not previously examined. Hence, the TRU fuel itself poses a unique set of problems that must be resolved to allow production, facilitate licensing without excessive regulatory margins, and enable commensurate reduced performance limits and higher costs. The materials performance issues for the driver fuels, the fuel cladding, and other core structural materials are generally similar but somewhat less severe and can be addressed within the envelop of research described below.

2.2.1 Current Status

The primary variables influencing material behavior include complex actinide components, temperature, neutron flux (damage rate), neutron fluence, and mechanical loading conditions. Chemical interactions between the coolant and the structural materials and at the fuel-cladding interface lead to complex corrosion behavior that is also influenced by irradiation (e.g., irradiation-assisted stress corrosion cracking). Taken together with the fact that multiple structural materials are involved, it becomes impossible to probe the complete required space experimentally. In addition, the costs and time associated with irradiation experiments and postirradiation examination provide further incentive to reduce the number of required experiments. Thus, the first-order impact of computational modeling and simulation can be to provide interpolation and modest extrapolation of the available or obtainable experimental database in support of GNEP design in the near term.

On a more fundamental level, advanced computational methods and hardware are expected to enable new capabilities in computational materials science. This development provides the potential for a greater understanding of material behavior to enable the development of new materials that offer improved performance options for future plants.

2.2.2 Areas of Opportunity

The following six technical areas will benefit significantly by application of advanced computational methods.

1. ***Radiation-induced microstructural evolution*****.** The nature of radiation-induced microstructural evolution and the associated property changes require a multiscale approach to their understanding and mitigation. Primary damage formation occurs on a time scale of femtoseconds to picoseconds in a volume of a few cubic nanometers. This involves very high local energy transfer events (both electronic and elastic), creating both point defect and fission product formation. These defects and newly created impurities diffuse and aggregate over much longer time scales (ks to Gs) and length scales (μm to mm), leading to phenomena such as fuel restructuring, fuel cracking, fission gas release, fuel-cladding mechanical interactions, and fuel and cladding creep and swelling. Over this same time solid fission product formation drives a complex evolution of fuel chemistry. Currently, there exist models or methods that can be applied at each of the relevant scales, although the quality or fidelity of these models varies. Fundamental material and defect properties for most materials (with the exception of actinides, as described below) can be provided by electronic structure methods, which support atomistic simulations employing molecular dynamics or Monte Carlo methods. The mesoscale microstructural evolution can be simulated by using models based on reaction rate theory, phase field, Monte Carlo, and discrete dislocation dynamics. At the largest scale, continuum elasticity and finite element models can be used. The primary deficiencies in this multiscale modeling scheme are well-defined methods for directly linking the models that operate at different scales and a strategy for determining when tight linking is appropriate (as opposed to simple information passing).

2. ***Electronic structure methods for actinides*****.** A major scientific challenge is the need to develop robust electronic structure methods for actinides in which the behavior of 5f-electrons is strongly correlated and requires the consideration of relativistic effects. The now standard density functional theory employing the local density approximation or generalized gradient approximation, which has been successfully applied to many other materials, fails to describe the behavior of the actinides. A new underlying theory is needed in order to compute fundamental properties such as defect formation and migration energies in both the pure metals and compounds (oxides, nitrides, carbides) involving these metals.

3. ***Thermodynamic quantities in UO_2, PuO_2, and mixed-oxide fuels*****.** A fundamental understanding of thermodynamic quantities in UO_2, PuO_2, and mixed-oxide fuels is needed. This problem is strongly related to the electronic structure issue described above in (2). The presence of the actinides makes the chemistry of nuclear reactor fuel initially complex, and continuous loss of U and Pu and formation of a broad range of new species due to fission introduce a challenging time-dependence to this chemistry. The fuel ultimately contains multiple f-electron elements: U, Pu, Am, Np, and Cm as well as many lighter elements. This situation leads to the potential formation of many phases that can influence critical physical properties such as thermal conductivity. The integration of new *ab initio* results with available thermodynamic databases is necessary to enable the

prediction of phase equilibria and oxidation states in fuel that contains fission products that may have been generated in situ or mixed into fresh fuel. An additional complicating factor is the influence of irradiation on phase equilibria due to the presence of persistent defect/solute fluxes and radiation-enhanced diffusion. Scientists need to better understand the behavior of the fuel in service, in order to support the fabrication of new fuel forms that incorporate long-lived actinide waste and to predict the behavior of the waste forms ultimately sent to a repository for long-term storage.

4. ***Mesoscale modeling***. Model development is required at the mesoscale for simulation of microstructural evolution of fuel and the effects on thermomechanical response of fuel. The challenges are both computational and conceptual. Defect generation information obtained from atomistic simulations indicates the need for simulating the interaction of irradiation-induced point defects with the microstructure (grain boundaries, dislocations, second phase precipitates, gas bubbles, and voids) and its evolution. Such simulations must incorporate all relevant grain-boundary and dislocation processes, gross deformation processes such as crack nucleation and propagation, and transport phenomena to account for fission product migration and precipitation. There are obvious links to the development of thermodynamic properties discussed in (3) above. The primary tools currently employed were mentioned in (1): reaction rate theory, Monte Carlo, and phase field models, along with discrete dislocation dynamics. Approaches for combining methods such as front tracking and phase field models into an integrated mesoscale model may offer the opportunity to advance the state of the art.

5. ***Modeling of fuel cladding and core structure***. The modeling and simulation needs for fuel cladding and core structural materials are generally similar to those of the fuel, without the complication of dealing with the actinides and fission products. Current *ab initio* theory is generally adequate, with the primary need being the ability to scale up from pure metals to complex, multicomponent alloys and to properly account for magnetism in ferritic alloys. The primary phenomena of interest are radiation-induced hardening and embrittlement, thermal and irradiation creep, and void swelling. Mechanical contact between the fuel and cladding increases heat transport from the fuel but can also lead to cladding failure, and chemical interactions with fission products can lead to thinning of the cladding by corrosion. Greater understanding of the thermodynamic behavior and complex chemistry at the fuel-clad interface is therefore important.

6. ***Integral fuel performance code***. The development of a next-generation integral fuel performance code that is based on state-of-the-art physics models is a major engineering need for GNEP. This development and use of this code have direct safety and licensing implications; for example, the chemical form and location of fission products and fuel cladding integrity largely dictate the source term in many accident scenarios. Current codes largely employ empirical and phenomenological models in a 1D or 2D geometry and have been heavily influenced by LWR fuel performance. Fast reactors involve much higher linear power ratings, temperatures, and fuel burnups. The desired code must be able to predict the 3D thermal and mechanical performance of a fuel pin while accounting for the full range of relevant phenomena, including heat transfer (conductive, convective, radiative), radiation damage and thermally fuel restructuring and microstructural evolution (creep, swelling, cracking), chemical species diffusion and

aggregation/precipitation (solid and gaseous fission products), fuel-cladding mechanical interaction, and chemical reactions leading to corrosion of the cladding on the outside by the reactor coolant and on the inside fission products. As mentioned above in (1), a strategy must be developed to determine which phenomena should be integrated into a single code as opposed to providing boundary conditions for the fuel pin simulation. For example, the fuel pin code may be tightly coupled to a CFD model to obtain cladding surface temperatures, or the relevant information may be simply passed from a separate CFD model.

2.2.3 Computational Issues

A number of common computational approaches can be brought to bear in resolving the technical issues:

- Potential development of a suite of community codes for each of the scales that must be simulated (e.g., a standard molecular dynamics kernel, visualization tool sets)
- Development of order-*N* methods for *ab initio* data
- Access to substantial capacity computing resources as well as high-capability resources
- Automatic extraction of data from high-fidelity simulations for coarse graining (e.g., *ab initio* data for interatomic potential development)
- Good algorithms for fitting interatomic potentials to large experimental and computational datasets
- Fast solvers for elastostatics, electrostatics, and similar problems involving long-range forces
- Discretization techniques that can handle dynamics and account for microstructural heterogeneity
- Coupled heat transport and species diffusion heterogeneous materials
- Methods for finding global ground states of multicomponent system
- Combining "front tracking" and continuum field approaches into a single computational framework
- Mathematical and statistical approaches to error and sensitivity estimation and propagation
- New algorithms and methods to simulate long-time behavior, an area that has proven to be less amenable to parallelization than large system size

2.2.3 Needs

Accelerated progress must be made on the scientific challenge of actinide chemistry to define thermodynamic stability of complex TRU fuels and ensure their fabricability and stability, as well as underpin the required research in all the other areas. This is a clear near-term priority. Algorithm development toward the goal of order-*N* methods and large-scale computing will have a substantial role to play as understanding of the underlying physics is obtained. The multiscale linking problem is also one in which work

should be initiated in the near term, with a need for both conceptual development and computational resources; such work may be expected to last for several years (see Section 3.3.2 for further discussion of the challenges in communicating multiscale information). The research required to support the development of an advanced fuel pin performance code has both near-term and long-term aspects. The near term shares much with the multiscale linking problem, involving the development of strategies and efficient algorithms for incorporating the necessary physical models. However, details of the physical models for fuel performance cannot be developed until progress is made on the actinide chemistry issue.

Validation of the fuel performance code for licensing purposes will take place over a longer term, involving technical validation by comparison of the code predictions with complex integral irradiation experiments, as well verification of the computational methods and performance; this issue is analyzed in depth in Section 3.1.

2.3 Separation Chemistry

As shown in Figure 2.3.1, separations of elements for further use either as a fuel or as waste is a critical part of the overall nuclear power system but is not independent of the system. Separation processes are intermediate in the overall system, since they are affected by other steps (e.g., the fuel that is input for the separation), and the extent of separation processes affects other steps (e.g., the form of the waste form or of the reprocessed fuel). A separations facility has a substantial number of constraints, including energy demand, nonproliferation, environment, economics, and public policy and regulatory issues. The separations facility comprises three critical stages, all of which can significantly benefit from modeling and simulation: preparation of the fuel feed by chopping and dissolution; a variety of coupled separations processes, currently including UREX for U and Tc separation, CDC-PEG for Cs/Sr separation, and TRUEX and TALSPEAK for dealing with the transuranics; and the form of the product fuel or of the waste form.

2.3.1 Current Status

Critical environmental issues involve extensive heat and energy integration and waste optimization, including water recovery, solvent lifetime (including reconstitution and elimination as waste), acid recovery and management, solids management through calcinations, and off-gas treatment to capture radionuclides, notably Kr, Xe, T, ^{129}I, and ^{14}C as well as CO_2 and NO_x for current technologies. The management of liquid, solid, and gaseous waste can be one of the important cost items in a separations plant. Appropriate models are expected to contribute substantially to NRC licensing requirements and certification. A critical aspect to meet regulatory and national security issues is inventory control, and tools are needed in terms of data management and process simulation that work well with advanced sensors and other measurement approaches.

Processor simulation tools for plant modeling include commercial packages such as ASPEN, HYSYS, and PRO-II and laboratory-developed codes such as Argonne's AMUSE code for solvent extraction. For most of the processes of interest to GNEP, however, no thermodynamic data packages are available for the solvents and actinide compounds. Computational chemistry codes for electronic structure and molecular mechanics are available for use in ligand design for separation systems, especially in the gas phase, as well as for predicting the thermodynamics for the synthesis of new solvent systems such as ionic liquids. Codes also exist for predicting the structures that can connect optimal binding sites. Molecular dynamics calculations are being used for predicting the behavior of liquid-liquid interfaces and the transfer of ions across them, as well as for ionic liquid behavior.

2.3.2 Challenges

At a high level, the six areas outlined below will have a large impact on GNEP.

1. Plant-scale simulation. The overall goal is to construct and operate a separations facility that is chemically, operationally, and economically efficient. Achieving this goal requires development of an integrated toolset to enable the full-scale simulation of the plant in terms of the chemistry, mass transport, energy input, and physical layout of the plant. Today a variety of tools can be used for plant design, but they are not well integrated for dynamic plant models. For example, if a new solvent is proposed, there is no modeling tool to speed plant design. Plant deployment usually has a timeline of 15–20 years.

2. Computational fluid dynamics. Many of the separations take place in centrifugal contactors (Figure 2.3.2), and it is vital to be able to model the mixing and flow in these systems. Such CFD simulations must be able to treat multiple liquid phases plus the gas and solid particles phases over length scales from the submicron to the meter. Current approaches tend to employ single-phase models. The flows are complicated by the need to deal with aggregation of solids and gases to form bubbles and droplets (<1 μm to 1 mm) that can become entrained in the flow. The flows themselves are on the order of tens of liters per minute with fully developed turbulence, non-Newtonian flows, gases at modest pressures, and reactions that include physical processes such as aggregation and separations at the interfaces, as well as radical chemical processes due to the presence of ionizing radiation. Current commercial CFD codes, which are the workhorse of the chemical industry, cannot treat the complicated flows needed for the separation and processing of nuclear fuels and waste.

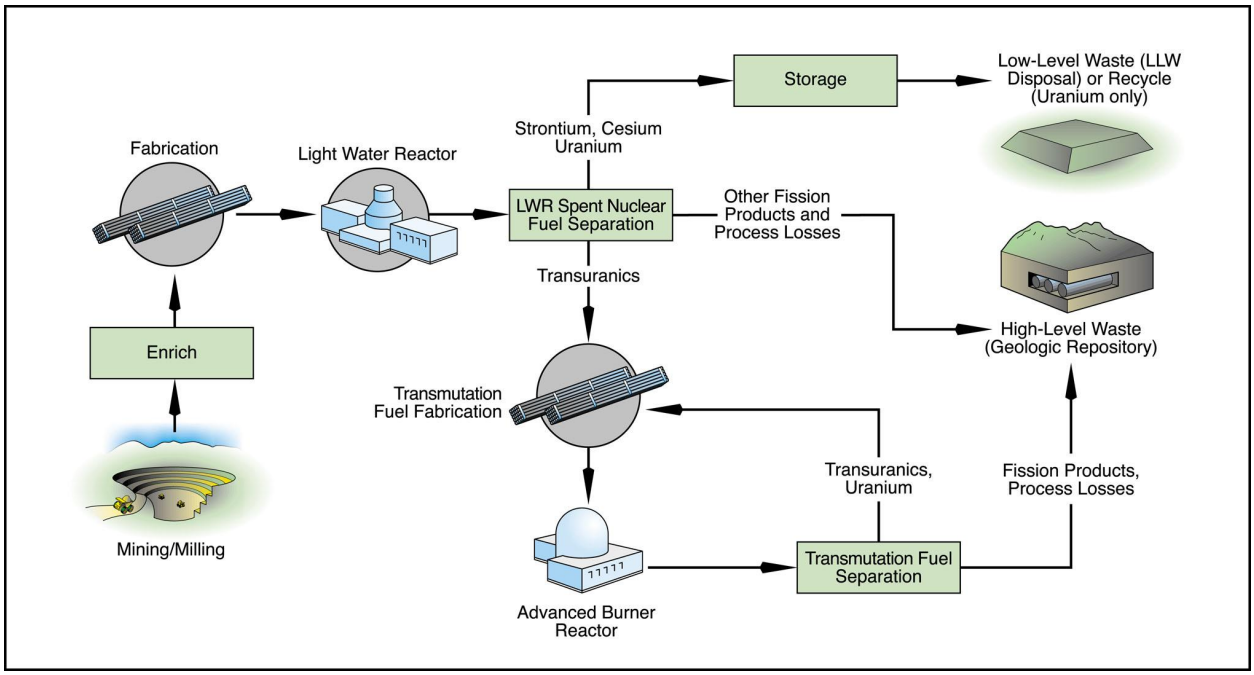


Figure 2.3.1. GNEP material flow diagram

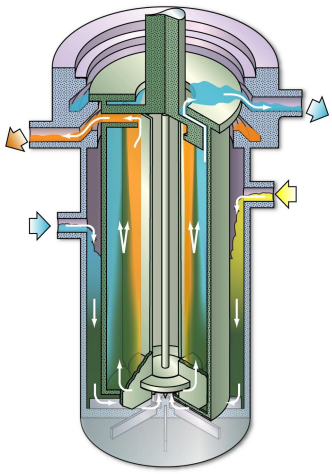


Figure 3.2.2. Centrifugal contactor

3. Predictive methods for thermodynamics and kinetics data as input to process simulators. The nuclear process separation industry cannot use most of the available databases for the chemical and petrochemical industries, because of the use of novel solvents and the presence of radioactive materials and heavy elements such as the actinides and lanthanides. In order to extend the currently limited thermodynamics data reliably into broader ranges of parameter spaces, thermodynamic predictors must incorporate limited experimental data and use computational chemistry approaches

including statistical mechanics and statistical modeling. Tools also must be able to capture the properties of neoteric solvents (including ionic liquids and molten salts) and the minor actinides in very dilute solutions and must be flexible enough to handle different fuels from different feeds and processes. Another important consideration is the ability to predict nucleation processes reliably. Current theories of nucleation and aggregation are inadequate, for example, for defining when a particle is formed. Similar issues must be addressed for polymerization processes as well as for colloid formation and suspensions as precursors to aggregation.

4. Rational design of the separations system from first-principles physics and chemistry. A major scientific challenge is the inverse design problem for chemicals and materials: Given a set of properties, predict what groupings of atoms as molecules will have the desired properties and can be synthesized. These molecules will have to exist in solvents; therefore, to predict the separations properties, scientists will have to be able to reliably predict the properties of liquids, solvation, and kinetics in solution. The issues dealing with predicting solution phase processes involve being able to predict entropy in complex systems involving coupling of strong and weak interactions. Many weak interactions need to be treated as collective phenomena. However, the large number of potential structures demonstrates the need to develop new phase space sampling methods that can deal with this currently computationally intractable problem for realistic systems.

5. Connecting/crossing time and length scales with uncertainty quantification. Many of the advances described above require the ability to make quantifiable predictions of processes that occur across many temporal and spatial scales and to make such predictions with a quantified uncertainty at all of the scales in an integrated fashion. This is critical to acceptance of designs by the regulatory agencies and for provision of optimal safety margins to dramatically minimize construction and operations costs. Equally important is the ability to go to long times in simulations. The sequential time problem in a simulation is linear in processor speed, and current and proposed computer architecture plans will not be able to provide access to longer times without dramatic changes in theoretical and algorithmic approaches. A critical spatial regime is the mesoscale, lying between 1 nm and 1 μm. Below 1 nm, currently available computational chemistry approaches can be used; and above 1 μm, continuum approaches work well. In the mesoscale, however, much less is known about the behavior of materials and about ways to predict behavior in this regime. Advances in this regime will require benchmarking and insights from experiment, for example, new measurements from the DOE nanoscience facilities.

6. Data management and visualization. Substantial issues arise in the underlying computer science technologies dealing with data. Data must be captured, managed, integrated, and mined from a wide range of sources to enable the optimal design and operation of separation processes for GNEP. Visualization will be a key tool in data analysis and presentation and will be important in enabling optimization based on simulations across scales.

A number of issues concern computer resources and access. Full-plant simulations will initially have to be performed on centralized systems because of the scarcity of resources at the petascale. These calculations will also provide benchmarks so that simpler versions can be run at each plant (say at the 10 TFlop/s to 100 TFlop/s level). There also are substantial export control issues in terms of models (e.g., flow sheets), data, and software, especially for separations systems because of nonproliferation issues.

2.3.2 Needs

Critical needs have been identified in each of the six areas outlined above.

1. Plant-scale simulation. There is a substantial need to improve individual and unit operations, such as distillation column, centrifugal contactors with entrainment and mixing, evaporators (including flow modeling and nucleation phenomena), recycle units for acid recovery (nitric plus nontraditional such as organics), water, organic solvents, and separations agents, unconventional acids, and off-gas recovery, both radioactive and nonradioactive. Similarly, there is a substantial need to develop models that involve full linking and integration of unit operations in a dynamic mode. Models also are needed that include all of the mass transfer in the plant—particularly for scheduling of operations and for accounting for differences in the input fuel streams. Critical issues include (1) the need to provide uncertainty information across the entire model of the plant to reduce the cost in construction due to lack of knowledge of the uncertainty; (2) the ability to capture, manage, and mine the broad array of fuel stream input and sensor data, in order to achieve order-of-magnitude advances in monitoring TRU for safety and nonproliferation issues; and (3) the need to develop effective and computationally efficient optimization strategies beyond linear programming for complex systems varying in time, with a broad range of constraints as discussed above. Moreover, the optimization and data management and archival strategies must be coupled, so that in the optimization effort one can investigate which changes can affect the optimal running of a process and can track the history of the design of the process. In addition, such information can be used to develop effective operator training and accident scenarios. The codes that can be used to predict accidents or criticality are complex, and both probabilistic and deterministic elements are needed to predict accidents and determine how to deal with them. (see also Section 2.1.1 on the role of deterministic methods in reactor modeling and simulation).

2. CFD. There is a critical need to include CFD in the simulation portfolio for process optimization. Questions that need to be addressed include the following: How do we treat these types of flows from the atomic level up to the continuum (and vice versa)? Is it appropriate to use a mix of stochastic and deterministic mathematical approaches to treat the CFD in separation systems?

3. Predictive methods. Thermodynamic modeling tools are needed that accurately predict partition or distribution coefficients for vapor-liquid, liquid-liquid, and solid-liquid equilibria. Such prediction requires, for example, the ability to predict phase diagrams for a variety of solvents and solutes over wide concentration ranges including third phase

formation. The prediction of reliable kinetics for separation processes must also include the dimension of time in order to predict the rate of change of a given species. Significant theoretical issues also must be addressed and new theories incorporated in efficient algorithms. In addition, design tools must be developed to predict particle morphology based on chemical composition for optimal fuel structure and composition. All of these predictions will need to include quantifiable error limits.

4. Rational design of separations system. Accurate and computationally efficient methods are needed for relativistic quantum chemistry in order to make reliable predictions of the thermodynamic and kinetic properties of molecules and solutions containing actinides including dealing with the f-electron problem (multiplets, spin-orbit, other relativistic effects), the lack of accurate density functional approaches for heavy elements based on a firm theoretical foundation, and the lack of reliable experimental data for benchmarking and model building. In addition, advances are needed in the development of force fields to enable classical molecular dynamics (MD) simulations of solutions and new methods to enable MD to reach long times (improved phase space sampling). New techniques also are needed for predicting the effects of radiolysis, which introduces trace species with cascading chemical effects leading to damage to surfaces and materials. Currently it is difficult to predict reaction rates of radicals in solution, especially for fast reactions, much less the reactions of highly excited states formed from the interaction of radiation and molecules. Finally, new techniques for optimization and sampling large realms of parameter space need to be developed if we are to develop new solvent systems (e.g., ionic liquids) that could help to minimize environmental concerns.

5. Time and length scales. New methods need to be developed to deal with uncertainty beyond current Monte Carlo approaches, which are computationally very time consuming and cannot adequately sample large domains of phase space. Uncertainty in the input data, the parameters, and the solvers is also of concern; especially needed are clearly defined goals of what the uncertainty is. (The issue of uncertainty analysis is discussed in depth in Section 3.1.)

6. Data management and visualization. A critical need is the ability to extract key features from the data for different data users. Feature extraction must provide quantified measures of key characteristics and the ability to view the data from different technical perspectives. In addition, visualization must enable people to view data from different perspectives, including those from scientists and engineers, plant management, plant technicians and operators, regulators, and the public. (Advances in data management and visualization, as well as the need for integrated efforts in these areas, are discussed in Section 3.6.)

All of these needs and the complexity of the science and technology will necessitate an integrated, multidisciplinary team approach to address these issues, as no one scientist or engineer has all of the capabilities needed to solve these large problems. In order to address these issues, teams involving scientists and engineers from academia, national laboratories, and industry with input from regulators will need to be formed in order to attain the final goal for GNEP of the optimized construction and operation of a

separations plant based on a firm scientific foundation with the necessary safety and non-proliferation issues under tight control. The complexity of the computational issues will require close interactions between application and domain specialists, applied mathematicians, and computer scientists to develop the approaches, theories, models, algorithms, and data management and analysis tools needed to make substantial advances. Efforts are needed immediately to advance plant design; at the same time, sustained work in this area is needed in order to continually improve plant design and operation over the lifetime of GNEP.

2.4. Repository Modeling

One of the motivations for the GNEP program is to reduce the impact of the nuclear fuel cycle on a geologic repository. Hence, modeling of the performance of waste forms in the environment of a geologic repository is essential to the success of GNEP. The implementation of a closed fuel cycle will mean that waste streams will be sent to a geologic repository that are very different from the waste stream (mostly commercial LWR spent fuel) currently planned for the Yucca Mountain repository. This new waste stream, consisting mainly of fission-product wastes from recycling, will ultimately require that a repository be analyzed for compliance with Nuclear Regulatory Commission regulations and have a design that takes advantage of the significantly reduced loadings (heat loading, mass loading, and much shorter overall half-lives) and radiotoxicity that the new waste stream will represent.

2.4.1 Current Status

The motivating challenge for repository modeling is to provide a realistic assessment of the long-term performance of an arbitrary waste form in the presence of a complex geochemical environment. This assessment must include a quantification of uncertainties in the overall performance due to individual uncertainties inherent in the long-time scales of the problem. A number of major issues and challenges are involved in accomplishing this goal. In addition to the wide range of spatial (10^{-2}–10^{3} m) and temporal (10^{1}–10^{8} s) scales involved in the physical processes, the upper boundary of those ranges lead to specific and often unique challenges: substantial reliance on modeling and simulation with little opportunity for direct experimental validation and the dominant role of consequent uncertainties in the model parameters. A wide array of chemical and physical processes interacting in complex ways requires a systems analysis approach to assess the performance of the waste form and repository system.

The state of the art of repository modeling is a total system performance assessment (TSPA) model designed specifically for the analysis of the proposed Yucca Mountain repository. The TSPA model integrates results of several physical and chemical processes to calculate projections of long-term repository performance. While this model is specific to the YMP, the fundamental physical and chemical processes that are simulated are common to any geologic repository:

- Multiphase flow and multicomponent transport through variably saturated porous media
- Heat and mass transfer within the waste emplacement drifts
- Thermal geohydrology in the host geologic medium surrounding the waste emplacement drifts
- Evolution of the chemical environment in the engineered system and geosphere
- Degradation of engineered systems including the waste forms and the packaging for those waste forms
- Transport of radionuclides in the biosphere
- Impact of disruptive geologic events

In the current system these processes are represented by loosely coupled simplified models that are either abstracted from physics-based process models or are based on empirical correlations derived from experimental data. Monte Carlo simulation with Latin hypercube sampling of up to 400 input parameters is used to estimate the uncertainty in projected long-term repository performance. Typically, several hundred independent Monte Carlo simulations, each with a Latin hypercube sampled set of model parameters, are required to produce stable estimates of repository performance metrics. Statistical analysis of the set of probabilistic results provides a quantitative measure of the uncertainty in the performance of the waste form or repository system and permits comparison between repository performance metrics and quantitative regulatory requirements. Monte Carlo simulations of repository performance thus provide a means for the defensible analysis of system behavior, incorporating processes and parameters based on scientific observations.

2.4.2 Needs

The vision for a future repository modeling system is a tightly integrated suite of physics-based models of the fundamental processes with a rigorous treatment of uncertainty propagation. A total-system performance model will require massively parallel computing hardware and a software framework that supports a large, diverse set of improved complex, multiphysics application codes. While all physical processes will benefit from a migration toward physics-based models, three specific areas for improved capability have been identified.

1. Waste Form and Material Degradation *(>10 yrs).* Whereas current models for waste form degradation are based on conservative empirical correlations of well-known waste forms, advanced modeling and simulation capabilities are required to predict thermodynamic, chemical, and radiation stability of advanced materials such as tailored ceramics, composite materials, and superalloys. This advanced modeling, combined with focused experiments, will allow for development of optimal waste forms and disposal canisters and minimization of environmental impacts. The improvement of individual process models will be facilitated by tools for high-performance computing capabilities,

including dynamic domain decomposition, efficient parallel solution algorithms, and load balancing.

2. High-Fidelity Assessment of the Chemical Environment *(3–5 yrs).* Modeling the local chemical environment that determines waste form behavior requires a tightly coupled multiscale simulation of the heat and mass transfer and chemical reactions in the waste package, emplacement drift (tunnel), and nearby host rock. High-fidelity modeling is necessary to incorporate the effects of local variations in the environment due to heterogeneities in the thermal and chemical system and localized failure mechanisms of the engineered systems. Such modeling includes turbulent multiphase, multicomponent natural convection fluid dynamics with radiative, convective, and conductive heat transfer within the drift coupled to two-phase chemically reactive flow and heat transfer in the porous media of the host rock. These processes control the local environment that drives the degradation of all engineered components. This chemical environment also determines the mobility of radionuclides released from the waste form. Tight coupling of high-fidelity solutions to disparate physical models requires the transfer of those solutions among dissimilar meshes and multiple spatial and temporal scales. Advanced tools will help manage this process in a high-performance computing paradigm.

3. Software Infrastructure for Coupled System Performance Assessment *(5–10 yrs).* An innovative software infrastructure is necessary to facilitate improvements in individual physical and chemical process models, to enable tight and mathematically rigorous coupling between different physical process models, and to manage the integration of simulation results into a transparent, defensible set of performance metrics. Such a software infrastructure is required for design and analysis of the entire waste form and repository system performance. Key capabilities include tools for uncertainty propagation, statistical analysis of results, waste form performance specifications, and repository design optimization. Moreover, in order to satisfy regulatory requirements, the infrastructure must ensure transparency, reproducibility, and traceability by rigorous management of data and workflow. Advanced frameworks intended to meet these requirements are discussed in Section 3.4.4.

Research and improvements are needed in several other areas as well:

- In ***uncertainty propagation***, there exists a clear need to be able to dynamically judge the convergence of the performance metric distributions derived from the Monte Carlo process. In addition, it is necessary to assess the relative contributions of model error (due to physical, mathematical, and numerical approximations) and statistical error (due to total system uncertainties and their approximation). This assessment can be used to optimize the use of computation resources for predictive simulations and for obtaining reliable and defensible estimates of their accuracy and of the level of confidence that can be placed in such estimates. Possibilities may also exist for deterministic propagation of some input uncertainties based on sensitivity analysis, adjoint methods, and polynomial chaos expansions.

- ***Visualization*** of Monte Carlo results and their statistical measures would be greatly facilitated by automated integration of large four-dimensional ensemble datasets that are distributed across multiple data storage sites and are too large to consolidate at a single site. The challenges and possibilities of visualization are discussed further in Section 3.6.

- ***High-fidelity assessment*** of chemical environments could be achieved in the near term (3–5 yrs) by first modernizing and parallelizing existing legacy codes that model the relevant physical and chemical processes. Incorporating feedback between models requires coupling different physical processes with a given domain as well as coupling multiphysics solutions across domain boundaries. This task will require collaborations among existing efforts in parallel meshes and efficient PDE solvers and should consider the modular structure consistent with an advanced software infrastructure. One approach is to embed computational scientists into a team of physicists and engineers to provide a continuing interface between the scientific models and the enabling technologies. The computational tools are best managed by national laboratories with a consistent user-base. The university environment offers an efficient mechanism for testing the applicability of those tools to a specific problem. If successful, the final integration will take place at the national laboratories with the input of the university participants. The modeling of the environment in and near a *single* drift (tunnel) may not push the boundaries of petascale computing. However, once integrated in a software infrastructure that incorporates the modeling of multiple drifts (tunnels) in a repository using a Monte Carlo uncertainty propagation methodology, the required computing resources will be substantial. Iterations for design optimization would further expand the required computing resources.

2.5 Seismic Analysis and Design, Structural Mechanics and Balance of Plant

A common theme in discussions of seismic analysis and structural mechanics is the fact that the nuclear energy industry is still relying on tools more than two decades old. In the short term, then, adoption of already existing computational tools will greatly benefit the nuclear energy community. In the longer term, new tools will be needed to address challenging 3D problems associated with structural dynamics and mechanics.

2.5.1 Seismic Analysis and Design

The potential for a major earthquake occurrence has been a critical design criterion for nuclear power plants. Historically, many of the most confounding and controversial siting challenges for nuclear plants were associated with earthquake considerations. In the 1960s and 1970s, the nuclear power industry drove the major advancements in the field of earthquake engineering with critical developments in the areas of probabilistic seismic hazard assessment (PHSA), soil-structure interaction (SSI), structural dynamics, and

structural mechanics. Some of the early computational tools, most notably in the area of structural mechanics, have continued to advance in the intervening years because of interest in other industries (e.g., aerospace, automobile). However, many of the critical tools developed specifically for nuclear power plants (e.g., SSI) have advanced very little, and the industry is reliant on tools that are fundamentally similar to those developed 20 to 30 years ago.

Current Status

A strong motivation exists to update and modernize many of the seismic simulation tools. Enabled by modern solution algorithms and high-performance computing, more rigorous and realistic seismic simulation tools are now possible. These tools can significantly increase our understanding of seismic events, enable performance-based design for significant cost savings, and increase design efficiency through the implementation of modern computer graphics and data analysis.

The phenomenology of earthquake events, which spans from energy release at the causative fault, to energy transport through seismic wave propagation in a highly heterogeneous media, to ultimate shaking and response of the structure, is very complex (Figure 2.5.1). The phenomenon is inherently three dimensional, and the response occurs in two distinctly different but closely coupled domains: the earth and a structural system.

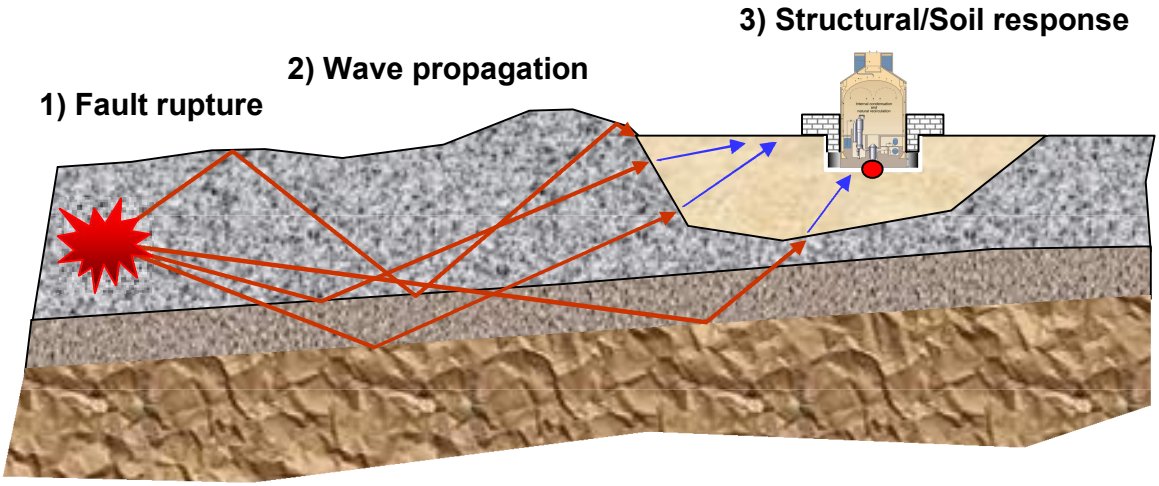


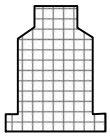
Figure 2.5.1 The end-to-end seismic response problem

Needs

Because of the complexity of the problem, and the limitations of 1970s vintage simulation tools, significant simplifying idealizations were invoked. These included estimation of the bedrock ground motion at the site by probability-based inspection of historical earthquakes of equivalent magnitude, one-dimensional site response simulation

assuming a wavefield of pure vertically propagating shear waves to estimate the local site response, and linear elastic analysis of the structural system. All of these methods can be augmented or replaced with more rigorous methodologies as described below.

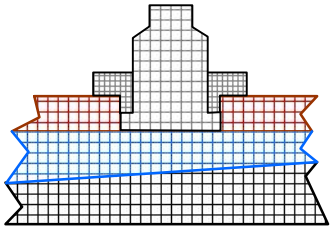
1. Nonlinear Structural Mechanics (near-to-intermediate term goal)



Modern performance-based engineering design methodologies can provide a much clearer understanding of expected structural system designs by defining clear structural performance goals (as opposed to traditional prescriptive design requirements) and provide for more cost-effective designs by allowing acceptable damage for very rare, extreme seismic events. However, full realization of performance-base design can be achieved only when simulation tools are developed that permit accurate predictions of nonlinear structural response.

Both explicit and implicit time integration structural mechanics codes have advanced tremendously in recent years, and the solution of many highly nonlinear structural system response problems are achievable. For nuclear fuel cycle structures, these simulation tools can be brought to bear for fully nonlinear analysis if adequate nonlinear material and structural element models are developed and implemented. Working closely with seismic design experts in the U.S. and international nuclear communities, structural components (e.g., reinforced concrete shear walls prevalent in nuclear power plant structures) that could be allowed to undergo significant nonlinear behavior under extreme events should be identified, and appropriate nonlinear mathematical models should be developed, validated, and implemented in modern nonlinear mechanics software. For more complex nonlinear elements (e.g., the cyclic degradation and softening behavior of cracking concrete components), there will be computational challenges to the solution of the global system of nonlinear equations, particularly when simulations up to structural collapse are desired. The computer science and mathematics communities can provide significant assistance through the development of robust, advanced solution algorithms for highly nonlinear structural systems (see Section 3.3). Such tools would have immediate and important impact in enabling cost-effective performance-based seismic design.

2. Fully Three-Dimensional, Time-Domain, Soil-Structure Interaction (near-to-intermediate term goal)

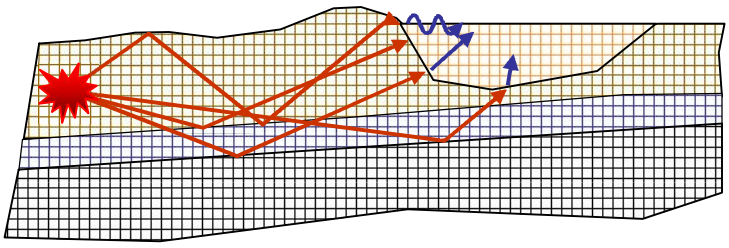


The computational limitations of existing soil-structure interaction (SSI) simulation tools necessitate a coarse discretization of the superstructure (e.g., reactor and foundation) system, and the soil domain surrounding the structure can be discretized over only a relatively small volume. In addition, existing codes for soil-structure interaction are frequency domain programs and lack the capability for visualization of transient response results, a significant problem when attempting to debug detailed models or to understand the details of the computed seismic response of the coupled structure/soil system.

Application of high-performance, massively parallel computations to the SSI problem would significantly improve the ability to simulate the 3D coupled system response. Parallel computations would allow more realistic 3D models that include very detailed nonlinear structural models, fully coupled to a 3D "soil island." The development of such a detailed, time-domain model would permit better representation of the dynamics of the superstructure, the load paths in the superstructure, and the coupled response of the structure/soil system. Implementation of effective visualization tools would also aid in the understanding of the complex response of the coupled system. To date, no one has "observed" the transient response of a detailed coupled power plant/soil model via computer visualization.

Nuclear power plants contain secondary equipment systems that are sensitive to dynamic motions in the frequency range of 25–30 Hz. Resolution of such frequencies in an SSI model will require extremely fine discretization of the superstructure and soil system. Ideally, one would like to perform implicit time integration of the steel and concrete superstructure (where elastic wave speeds are very high and thus time-step prohibitive in a Courant sense), and explicit time integration in the soil (where elastic wave speeds are slow). The applied mathematics and computer science communities could greatly assist in developing optimal hybrid solution schemes for nonlinear SSI system models.

3. Three-Dimensional Regional Seismic Wave Propagation (longer-term goal)

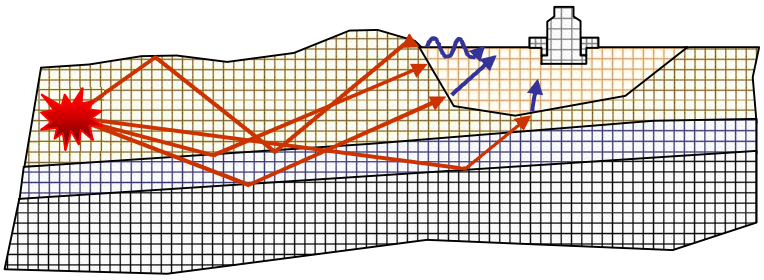


Recent research in the seismological community has demonstrated the utility of massively parallel simulations of regional seismic wave propagation. Such simulations are providing the first insight into the mechanisms driving the complex spatial variability of earthquake ground motions. Accurate simulation models of seismic wave propagation would significantly improve abilities to predict earthquake motions at a specific site, and these models could be integrated directly into existing PSHA frameworks.

A number of computationally related challenges must be resolved before the benefits of such models can be fully realized. Because of the high-frequency characteristics of nuclear power plant systems, it would be necessary to resolve high-frequency components of earthquake ground motions; however, there is insufficient understanding of the subsurface geologic heterogeneities at short wavelengths to compute such motions deterministically. The only current solution path is through a stochastic characterization of the geologic structure. There are no defined methods for creating stochastic geologic properties models. Such models must be constrained and consistent with sparse existing geologic data. In addition, the ensemble statistics of the realizations must be understood so that an appropriate suite of geologic realizations are included to capture statistically appropriate ground motions.

The extreme computational requirements for regional-scale models also present a significant challenge. Recent research efforts at modeling a region of large extent (the Las Angeles Basin) has indicated that resolving ground motion frequencies up to 3 Hz for a region of large extent would require a petaflop-scale machine. Resolution of higher frequencies would obviously limit the region of consideration to a region of substantially smaller extent. The successful realization of regional-scale simulations will require taking advantage of all possible simulation economies, such as adaptive gridding.

4. Causative Fault–to–Structure Simulations (longer-term goal)



The ultimate aim for computational seismic analysis is full 3D simulation of the fault rupture-to-structural (nonlinear) response process. This computationally intensive problem will require efficient coupling of the SSI model indicated in (2) above, with the regional wave propagation model in (3) above, necessitating advanced computational techniques and computer systems.

2.5.2 Structural Mechanics and Balance of Plant

Over the past 30 years, structural mechanics software development has been driven by such applications as aerospace, automobile industry, national defense, civil infrastructure, and, in the 1970s and 1980s, nuclear reactor technology. These developments have led to a number of finite element-based computer programs that have mature element technologies and solution algorithms.

Current Status

Existing software relevant to the structural mechanics of nuclear energy can be divided into three categories: linear finite element programs, implicit time integration nonlinear finite element programs, and explicit time integration nonlinear programs.

While the software used to calculate thermomechanical events has made significant progress and has enabled certain industries to move to a design by analysis approach, it is not clear whether the data and material constitutive laws have made the same progress. For example, it is not unusual in fast reactor analysis to see the results of very detailed transient thermomechanical analyses used along with very coarse damage models to predict plant lifetime.

Needs

In terms of major issues, there is a compelling need for development and implementation of advanced material constitutive models that can accurately represent the time-dependent behavior of materials in extreme environments. These models should address the effects of high irradiation levels, extreme temperatures, and chemical interactions on material behavior. Advanced materials models should account for fully 3D, multiaxial states of stress both at low strain rates (normal operations) and at high strain rates (accident scenarios).

- A ***multiscale approach*** is needed that couples processes for the entire structure, from materials to structures (Figure 2.5.2). Homogenization and localization processes may help to precisely describe the behavior of structures, including aging and temperature effects in time and space.

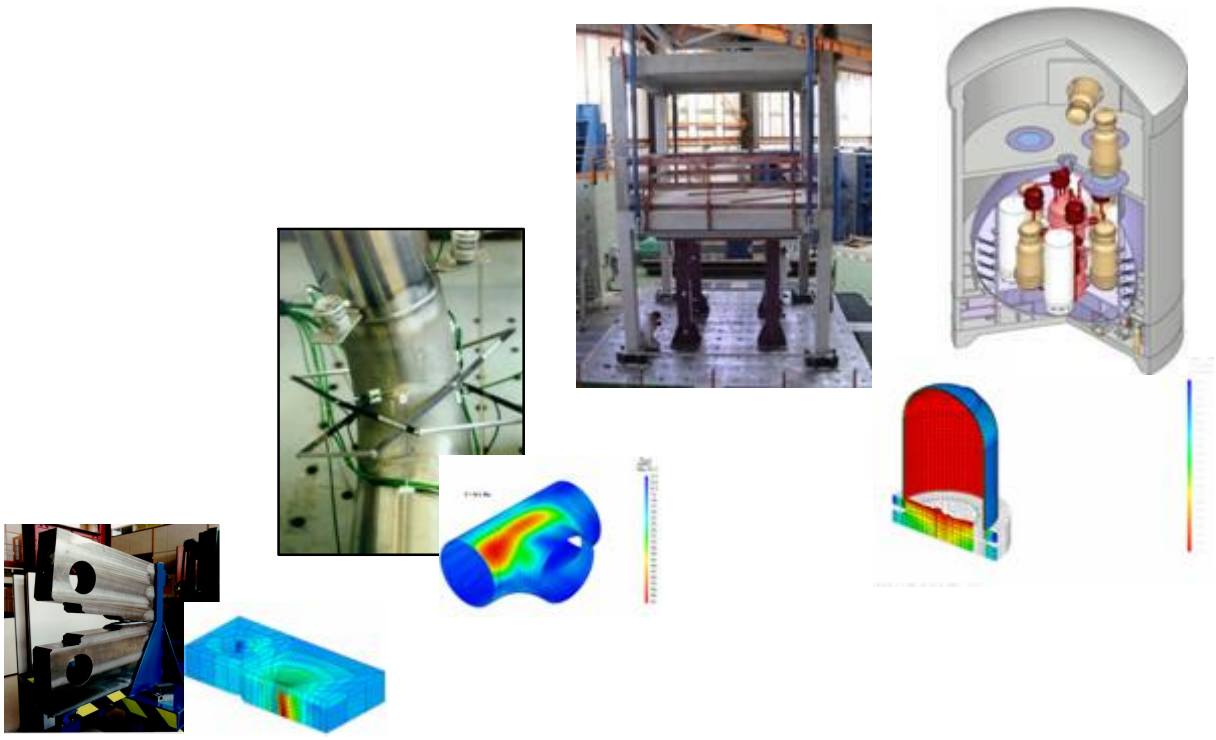


Figure 2.5.2: Multiscale approach for structural mechanics simulation

Multiphysics simulations also raise new requirements—for example, to model soil-structure interactions, fluid structure interactions, and corrosion in reinforced concrete or thermal fatigue of structures.

- ***Code coupling*** will be needed in order to determine vibrational response in heat exchangers or soil-structure interaction for earthquakes. Inverse analyses also will be needed for identification of material data or initial state of the structure.
- Advanced technologies will be needed to ***optimize the design*** of the structures under multiple constraints such as cost or safety.

Currently, for large structural mechanics simulations such as those needed by the nuclear industry, linear finite element and implicit time integration nonlinear finite-element programs use direct solvers that are today parallelized on shared-memory computers.

- For large-scale simulation on distributed-memory computers, however, ***new algorithms or new paradigms*** are needed. Dynamic problems that use explicit solvers are already running on these machines. Adaptive load balancing for structural mechanics applications may consider new models (enriched FE, multiscale models), requiring development of new algorithms or new elements.
- Localized damage in structure implies the need for ***load balancing*** to achieve efficient algorithmic scaling on parallel computers.

Another goal for numerical modeling in structural mechanics concerns the simulation of brittle materials.

- Numerical algorithms will be needed to ***treat smoothened materials*** (concrete, ceramics, fuels, etc.).
- Additionally, ***adaptive mesh refinement*** or enriched elements using XFEM will be necessary in order to achieve robust and efficient simulations of crack propagation.

3. Research Opportunities and Challenges in Applied Mathematics, Computer Science, and Facilities

The Office of Science holds simulation assets—scientific software tools, hardware platforms, and interdisciplinary research staff—without equal in the world. As the nation architects an internationally competitive next-generation nuclear industry, these strengths in large-scale simulation confer advantages that offset lack of recent experience in designing plants. At the same time, the GNEP research program challenges the limits of our simulation capabilities in multiple directions, making GNEP a worthy focus of simulation leaders. Opportunities for a mutually beneficial collaboration abound.

Favorable trends in capability and cost of large-scale simulation are transforming science and engineering into substantially simulation-based activities. As measured by the Gordon Bell peak performance prize, sustained processing rates on science and engineering tasks formulated similarly to GNEP applications—as systems of particles, partial differential equations, and so forth—have improved by five orders of magnitude over the 17 years of prize history and is expected to remain on this trajectory. Another metric, the Gordon Bell special prize, tracks steady progress for unstructured adaptive applications of billions of degrees of freedom on many thousands of processors. As measured by the Gordon Bell price-performance prize on the same set of applications, acquisition cost per sustained processing capability has dropped by four orders of magnitude over the same period. Although simulations cannot replace experiments altogether, their vastly greater affordability creates an incentive to employ simulation to bypass experimentation wherever possible.

Simulation has the potential both to focus experimental effort on the most important parametric regimes and to reduce the long lead times of experimentation in yielding understanding.

For simulation to achieve its potential in the nuclear energy arena, close collaboration will be required between tool developers in the Office of Science and users in the Office of Nuclear Energy. The promised return for this investment of the time of valuable personnel in learning new techniques and applications is a computational lever that will raise human productivity for scientific advancement and engineering design. DOE's SciDAC programs have amply demonstrated that large-scale simulation can enhance research and design programs in both expected and unexpected ways, the latter including re-examination of trusted models on the applications side and breakthroughs driven by new challenges on the computational techniques side.

During the second part of the workshop, the participants focused on the state of the art in six areas of computing science: verification, validation, and uncertainty analysis; mathematical and geometrical modeling; scalable and multiscale algorithms; software tools and environments; computing facilities, data, and networks; and data analysis and visualization. Cognizant of the needs and challenges raised in the first breakout sessions, the participants focused on how researchers can harness the growing capabilities of

computation to improve the fidelity of the modeling of multiscale, multirate, multiphenomena physics, on the one hand, and lower the threshold of expertise required to employ "best practices" and scalable software, on the other.

3.1 Verification, Validation, and Uncertainty Analysis

One of the key needs of the GNEP program is to have available predictive simulation tools that include a sound and credible prediction of uncertainties and biases (predictive validation). These tools are particularly important as we launch into the design of new technologies and facilities based on novel processes and want to avoid, as much as possible, the costly and lengthy procedures of having to build representative mockup experiments that confirm—but do not explain—our predictions. Verification and predictive validation must be based on a well-established set of scientific approaches that will allow us to announce a priori, and with strong confidence, the calculational uncertainties, both for cases that are well known (e.g., where strong experimental evidence exists in the form of confirmatory mockups) and for cases that are less well known (e.g., for novel design where only elementary experimental evidence is available). The framework for this predictive verification and validation should enable a graded, science-based approach, with application ranging from scoping-type design activities to generating information for the regulatory arena (e.g., the U.S. Nuclear Regulatory Commission, where the ability to accurately and convincingly predict behavior is particularly important). Additionally, both selected legacy codes and new codes will require verification and validation (V&V).

The current approaches to V&V in the nuclear energy field are diverse and depend not only on the discipline but also on the origin of the code being validated. In general, industrial codes have relied on comparisons of predictions with representative mockup measurements to establish calculation to uncertainty biases and uncertainties (often estimated by expert judgment); these biases and uncertainties are then applied to project calculations. R&D codes often rely on a more formal V&V process, where the individual sources of V&V are identified and quantified and then propagated to the final solution by using statistical techniques.

The following comments apply to the various disciplines:

- Neutronics has probably the most well-established formal V&V process, where the uncertainties on the basic nuclear data can be formally propagated through the constitutive equations and treated statistically along with information available from integral experiments.
- Fluid flow and heat transfer V&V is less formally established, where the V&V effort relies on code-to-code experiments to assess models, singular experiments, and large-scale experiments to indicate overall biases.
- In mechanical analyses both the constitutive equations and the data are well known, but boundary conditions (e.g., seismic loads) are usually poorly known. These analyses rely on experimental validation at several levels, from simple fundamental tests to complex mockup experiments (e.g., large shaking table).

- Fuels and materials performance, in particular fuel irradiation behavior, is dominated by the coupled effects of several phenomena and relies uniquely on very expensive and time-consuming confirmatory mockup experiments (e.g., multiyear irradiations), with little or no predictive capability. This is possibly the most challenging problem we face, but it also has the highest potential payoff.
- Systems-level analysis tools are primarily predictive because they are evaluating systems that typically do not exist; the tools currently in use have undergone little if any V&V.

We note that when coupled phenomena occur, in particular for safety analyses, validation has been restricted to either mockup or component-level experimental comparison, with little predictive capability

3.1.1 Current Status

A conceptual framework for V&V and uncertainty quantification (UQ) has developed during the past 10 years, primarily as a result of work conducted for the Waste Isolation Pilot Plant program, Yucca Mountain project, the ASC program, and nuclear safety analyses in bounding methods and probabilistic risk assessments. This evolving framework comprises the following elements: code verification, solution verification, model validation, and predictive estimation of system responses with uncertainty quantification. Procedures for the first two are relatively well developed, but concepts and procedures for validation and predictive estimation are still in the developmental stage.

Code verification involves activities that are related to software quality assurance (SQA) practices and to activities directed toward finding and removing deficiencies in numerical algorithms used to solve partial differential equations (PDEs). SQA procedures are needed during software development and modification, as well as during production computing. SQA procedures are well developed in general, but improvement is needed with regard to software operating on massively parallel computer systems. Numerical algorithm verification addresses the software reliability of the implementation of all the numerical algorithms that affect the numerical accuracy of solutions produced by the code. Numerical algorithm verification is conducted by comparing computational solutions with benchmark solutions: analytical solutions, manufactured solutions, and highly accurate numerical solutions. Although procedures are available, there remains a lack of applicable benchmark solutions needed for all of the elements of GNEP.

Solution verification, also referred to as numerical error estimation, deals with the quantitative estimation of the numerical accuracy obtained when PDEs are solved by using discretization methods. The primary goal in solution verification is the estimation of the numerical accuracy of all of the solution quantities of interest in a given simulation. Solution verification is related to the topic of adaptive mesh refinement; however, the goals of AMR are more restrictive than those of solution verification. The discretization errors must be quantified so that they can be separated, in principle, from other error and uncertainty sources, such as physics modeling errors and variabilities in

physical properties. The primary shortcomings in present methods are (a) the computational expense of estimating discretization errors by using solutions on multiple mesh resolutions and (b) the lack of robustness of existing methods in complex physics simulations.

Model validation, used here in a restrictive sense, emphasizes the quantitative assessment of computational model accuracy by comparison with high-quality validation experiments—that is, experiments that are well characterized in terms of measurement and documentation of all the input quantities needed for the computational model, as well as carefully estimated and documented experimental measurement uncertainty. These validation experiments can be conducted on hardware that represents any level of simplification or disassembly of the actual, or complete, system of interest, for example, even experiments conducted on simple geometries with only one element of physics occurring. Although the statistics community has expended significant effort in comparing computations and experiments, the emphasis has been on calibration, or tuning, of input parameters of the model being compared with data. Model validation, in contrast, emphasizes assessing the accuracy of physics-based models in blind comparisons with experimental data. This emphasis is directly aligned with the goal of predictive capability in modeling and simulation. The state of the art in model validation addresses issues of (a) assessing model accuracy when several system response quantities have been measured and compared and (b) comparing system response quantities from multiple realizations of the experiment with computational results that are characterized by probability distributions.

Predictive estimation (PE) starts with the identification and characterization of errors or uncertainties from all steps in the sequence of modeling and simulation process that leads to a computational model prediction. This includes (a) data error or uncertainty (input data such as cross sections, model parameters such as reaction-rate coefficients, initial conditions, boundary conditions, and forcing functions such as external loading), (b) numerical discretization error, and (c) uncertainty (e.g., lack of knowledge) in physics processes being modeled. The result of the PE analysis is a probabilistic description of possible future outcomes based on all recognized errors and uncertainties.

Predictive estimation for computer experiments has three key elements. First, calibration addresses the integration of experimental data for the purpose of updating the data of the computer model. Important components include the estimation of discrepancies in the data, and more important, estimation of the biases between model predictions and experimental data. The state of the art of calibration of models is fairly well developed; however, significant computational effort is required. Second, extrapolation addresses prediction uncertainty in new environments or conditions of interest, including both untested parts of the parameter space and higher levels of system complexity in the validation hierarchy. Extrapolation of models and the resulting increase of uncertainty are poorly understood, particularly the estimation of uncertainty that results from nonlinear coupling of two or more physical phenomena that were not coupled in the existing validation database. The third element is estimation of the validation domain of the physics models of interest, that is, estimation of contours of constant uncertainty in the

high-dimensional space that characterizes the application of interest. Practically, this involves the identification of areas where the predictive estimation of uncertainty meets specified requirements for the performance, reliability, or safety of the system of interest. The state of the art in estimation of the validation domain is very early in both conceptual and mathematical development.

Sensitivity analysis is the apportioning of prediction uncertainty to various contributing sources of uncertainty and error. Sensitivity analysis is especially important for resource allocation, as it can help prioritize, for example, whether predictive estimation would be reduced more by reducing uncertainty in input data, or improving numerical accuracy, or by improving physics model fidelity. Sensitivity analyses are fairly well developed, although the linkage between statistical and applied mathematics techniques is poor.

3.1.2 Needs

Improvements in numerical algorithm verification methods and tools are needed in the following areas:

- Development and formal compilation of ***accurate benchmarks*** are needed in each of the elements of GNEP: reactor core simulation (including fluid flow and heat transfer and neutronics), materials and fuels, separation chemistry, seismic and structural response, systems- and safety analysis tools, and repository modeling. These benchmarks will, by necessity, be a variety of analytical solutions, manufactured solutions, and highly accurate numerical solutions. New benchmarks are particularly needed in multiphysics modeling and in atomistic and molecular modeling to assess the code correctness and numerical algorithm reliability for these types of models.
- Existing and future computer codes, both government laboratory-developed and commercial software, need to be able to accommodate the addition of source terms in the PDEs; that is, the capability must exist to add analytical terms to the right-hand side of the ***physics-model PDEs*** programmed in the code.

Improved solution verification methods are needed in the following areas:

- Improvement and extension of existing recovery methods and ***residual-based, or adjoint, methods*** to unsteady (parabolic) and hyperbolic problems. Existing methods have been developed for very restricted physics applications for elliptic PDEs. A critical need exists for extending these methods to engineering quantities of interest, multiphysics simulations, and atomistic simulations.
- Development of numerical methods capable of addressing the elements of ***numerical approximations*** occurring in many simulations: mesh discretization, temporal discretization, iterative solution of nonlinear equations, and statistical sampling error when multiple simulations are computed for probabilistic simulations. These methods are needed so that the proper balance can be

achieved for each error contributor in a complex simulation, without wasting excessive computational effort on one contributor.

Model validation requires advancements in two areas:

- Improved quantitative methods are needed for ***statistical comparison*** of simulation results and experimental results for situations where very few experimental realizations are available but a large number of spatially or temporally distributed measurements are available at locations, or times, over the system of interest.
- Improved methods are needed for quantifying and properly interpreting, for informed decision-making, ***differences in probability distributions*** from computations and experiments for various system response quantities. Two examples are (a) How should differences in mean response quantities be weighted relative to tails in each distribution? and (b) How should multiple modes in structural responses be compared in assessing model accuracy in structural dynamics?

Predictive estimation in its application to GNEP faces three primary research challenges:

- ***Development of new sampling methods***. Predictive estimation and sensitivity analysis require ensembles of multiple related runs of the code. In multiphysics and multiscale physics models with nonlinear coupling and large numbers of input parameters, each code run is computationally expensive. New and efficient sampling techniques are needed that employ a combination of statistical features and applied mathematics features of the PDEs (e.g., the elliptic nature of the PDEs).
- ***Uncertainty propagation for systems of systems***. Simulations of the full closed-fuel cycle will have codes with different physical understanding and different levels of validation. This situation will require extension of current capabilities in calibration of models, particularly physics-model form uncertainty, to estimate credible prediction uncertainty.
- ***Extrapolation to higher levels in the validation hierarchy***. Within GNEP, there will be more data for component and subsystem testing and less for mockups and full system testing. An open question is how to integrate this data to make credible predictions with defensible uncertainty estimations at the full system level.

3.2 Mathematical and Geometrical Modeling

Advanced mathematical and geometrical modeling for numerical simulations is a ubiquitous need for the GNEP program. In particular, the numerical solution of PDEs appears in almost all of the simulation and modeling areas: separations (process or plant design), reactor core (neutron transport, fluid dynamics and heat transfer in multiphase

flows, fluid-structure analysis), seismic response (structural and seismic analysis), repository modeling (fluids and heat transfer in the drift, subsurface flows), and materials (phase field models).

3.2.1 Current Status

The specific capabilities required to perform physics-based simulation in these areas range from simulation of a single physical process in a geometrically complex environment to simulations that require the coupling of models for multiple diverse physical processes. For the most part, the existing simulation codes in these areas are based on algorithmic and software approaches that are 30 years old. Since that time, new technologies have been developed that have the potential for making the substantial improvements in simulation capabilities required to make the transition to physics-based modeling. For example, these include higher-order or high-resolution discretization methods for problems in complex geometries, adaptive mesh refinement, techniques for automating the grid generation process, and front tracking methods. All of these techniques have been implemented in software frameworks that enable high-performance parallel implementations, and have been used to perform a variety of high-fidelity multiphysics calculations.

While much can be accomplished by leveraging existing technologies, there are also a number of simulation and modeling problems in GNEP that require new mathematical and algorithmic ideas. Examples include upscaling microscale simulation data to obtain meso- and macroscale models; molecular dynamics algorithms for ionic fluids to obtain thermodynamic and transport properties; automated methods to extract macroscopic features such as defects and grain boundaries from molecular dynamics simulation data; and multiresolution grid generation techniques to automatically remove unwanted details from CAD data in the grid generation process. The design of multiphysics simulation codes requires a careful analysis of the coupling between submodels to understand the numerical stability of the combined methods, and to optimize the accuracy and performance of such simulations. Moreover, GNEP simulations will require the use of the largest computational facilities available, and scaling simulations of physically and geometrically complex systems to the petascale remains a fundamental open problem. Scalable algorithms and multiscale methods are discussed further in Section 3.3.

3.2.2 Needs

Our findings indicate that the GNEP program requires advanced models and numerical techniques that can do the following:

- Handle complex geometrical domains such as those defined by CAD models for plant and reactor design or in the modeling of extremely heterogeneous material such as the earth's subsurface for seismic modeling.
- Significantly improve accuracy and reduce computational cost through advanced numerical methods such as spatial/temporal/model refinement, the use of high-

order methods, and implementations that can leverage leadership class computing infrastructures.
- Address the coupling needs of multiscale, multiphysics applications; both algorithmically to ensure numerical accuracy and stability and with the appropriate software infrastructure.

CAD tools. The solution of numerical PDEs often requires that the computational domain be divided into a union simple cells (the computational mesh), and the PDEs are approximated, or discretized, on those mesh elements. The approximated system is then solved by using the appropriate numerical methods and software. Generating the computational mesh from a CAD description can be a time-consuming, multistep process requiring significant human interaction. To reduce this cost, recent work to develop advanced tools for CAD repair and cleanup and for selectively eliminating small, unnecessary features have been used in related engineering and scientific domain areas. Many of these tools are directly applicable to GNEP needs and can be used with modest customization. However, to address the advanced needs of coupled, multiphysics simulations, the incorporation of uncertainty quantification techniques directly into the simulation pipeline, or the use of design optimization techniques will require the development of new tools to support geometry access, simplification and modification. For example, capabilities to automatically support different levels of detail in the geometric model for different aspects of the solution process do not exist, and general geometry modification and derivative computation tools for design optimization needs are only now being explored.

Mesh technologies. Generating the computational mesh on complex geometries has been the subject of active research for many years, and two primary classes of technologies have resulted. The first class, *structured meshes,* uses a logically regular arrangement of mesh cells to represent the computational domain. Methods developed by using structured grids are typically very efficient, in terms of both memory usage and computational speed. Recently, variations of these methods that use "cut-cell" techniques, or overlapping grids, have been developed to handle complex geometries while preserving most of the efficiency advantages. The second class of technologies, *unstructured meshes*, uses simple cell types (tetrahedron, hexahedron, prisms, etc), connected in an arbitrary way, to cover the computational domain. Because of their flexibility, these meshes have long been used to represent complex geometries and a large number of methods and technologies are well understood and widely available for these mesh types. Both technologies have been and will continue to be used in GNEP simulations. Recent work to help automate the mesh generation process is available for both mesh types and can be leveraged by the GNEP program. As the solution proceeds, adaptive spatial and temporal techniques have been developed and used to reduce computational cost and improve accuracy in a number of related scientific and engineering areas including combustion, particle accelerators, fusion, and climate modeling. Such techniques include spatial refinement to concentrate grid points in regions needing high accuracy, interface tracking methods to follow moving fronts, temporal refinement techniques to reduce computational cost, and, more recently, adaptive model methods. Many of these tools have been used in the context of a single

simulation or physical process; to move to complex multi-physics simulations will require significant new development. For example, if a single mesh is being used to represent multiple physical processes, the refinement criteria in adaptive methods become more complicated. If different meshes are being used, a general hierarchical infrastructure that supports coupling multiple meshes to each other and to a single geometrical representation of the computation domain is required.

Multiple scales. Advanced mathematical models along with the solution algorithms and software that can leverage different mesh types have been developed for coupled multiple time- and length-scale multiphysics systems in complex geometries. Examples include stable and accurate operator split methods, semi-implicit, predictor-corrector methods, and fully implicit Newton-Krylov techniques. Stable and high-order spatial and temporal discretization methods have been used successfully in, for example, computational fluid dynamics problems, and wave propagation modeling. Although these developments have been made in related scientific areas, each new system to which they are applied requires careful analysis to determine which techniques are appropriate and how they must be modified to address the current need.

Teamwork for customization. Many of the technologies discussed above are similar to those needed in other engineering and scientific domains, but every application has specific details that require problem-dependent customization of the technology. These customizations of existing software, along with the development of a new generation of GNEP-specific software tools, will require multidisciplinary teams of mathematicians, computer scientists, and domain scientists. Such teams have been used successfully in the DOE SciDAC and ASCI programs, and the GNEP program can leverage many of the new mathematical models, numerical methods, and software tools that have resulted from these investments. These programs have demonstrated that multiple technologies can be shared across application areas to some extent, but have also shown that each new application domain yields new challenges and opportunities that must be addressed. In addition, these programs also highlight the need to invest significant time (5–10 years or longer) and resources to carefully formulate requirements, implement advanced software tools, and verify and validate the simulation results before they are trusted in critical design and analysis scenarios.

In summary, the GNEP program would benefit from the following.

- A collaborative effort between the applied mathematics and NE communities to develop the **next generation of simulation codes for PDE-based modeling**, based on the new algorithmic and software technologies described above. Such an effort would leverage the expertise and software infrastructure developed under the DOE SC and NNSA research programs in computational science and high-performance computing over the past 15 years and has a very high probability of success in the short to medium term. However, the development of a new simulation capability for an application domain is an expensive undertaking, and multiple GNEP application areas need new simulation capabilities.
- Investments in long-term **research in support of the fundamental open questions** in mathematical and geometrical modeling as highlighted above. For

many of these problems, new mathematical ideas and algorithms are required. For these areas, the principal forms of support required will fund people, specifically collaborations between domain scientists and applied mathematicians; and the funding of some specialized software to support rapid prototyping of new ideas in these domains. Petascale computing presents a unique problem that will probably require experimentation across the entire range of issues from models to algorithms to programming models.

3.3 Scalable and Multiscale Algorithms

A recurrent theme in discussions of GNEP requirements for simulation and modeling is scalability. To exploit the ever-increasing computational power and to address the increasingly complex engineering problems posed by the nuclear energy community, new algorithms will be needed that are scalable both in reducing the simulation time and in being able to treat multiscale phenomena to the required accuracy.

3.3.1 Scalable Algorithms

High-fidelity analyses based on first-principles simulation will require significant increases in spatial and temporal resolution. Current practice in seismic analysis, for example, is limited to a frequency response of 3 Hz. Elevation to the target frequency of 25 Hz will require a thousandfold increase in resolution. Similar examples are found in other GNEP areas, such as neutronics, thermal hydraulics, and thermal-mechanics of the core, fuel separation, and materials analysis. Access to these high-fidelity regimes will not be enabled by petascale computing alone. The underlying numerical algorithms and software must scale linearly (or at most as a small power) with the number of unknowns, and, in many cases, multiscale analysis must be employed to span several orders of magnitude in space scales and time scales.

Current Status

Several aspects of scalability need to be addressed to reach petascale performance. The first is the algorithmic scalability, which refers to the computational cost (operation count and memory demands) as a function of problem size, n. An algorithm is said to be scalable if the cost grows linearly with n or, at most, $n \log n$. The second is the degree of dependency. For example, long time integrations of small systems of ordinary differential equations (ODEs) have a cost that is linear in n (here, the number of steps) but are intrinsically serial and do not parallelize well. Similar dependencies arise when solving neutron transport methods by using discrete ordinate methods. A third concern is sufficient scalability of the problem, which typically implies $n/P \sim 10^4$, in order to amortize communication overhead. Many PDE-based computations require global vector reductions (e.g., inner products in conjugate gradient methods). Architectures that provide fast support for such operations will be important in moving beyond $P=10^4$

processors. Accuracy issues are also a concern at the petascale, where relatively long-time integration of small scale phenomena is susceptible to accumulated numerical truncation error. Moreover, scalable software is essential for petascale deployment. With $P > 10^5$, the adverse consequences of Amdahl's law will be palpable in any serial portion of the simulation process (e.g., boundary conditions, I/O, visualization, data transfer).

Fortunately, many of the GNEP technology areas are in a position to leverage advances in parallel numerical algorithms and software that have been developed within DOE over the past several years. First, the majority of the simulation problem areas are expressed as partial differential equations, which often require the solution of linear or nonlinear systems of equations. State-of-the-art parallel software for solving such systems has been developed by DOE and could form the kernel for next-generation NE codes. Examples include Hypre, PETSc, Sundance, SuperLU, and Trilinos. These codes have different strengths but in many cases are accessible through a single interface, which ultimately leads to more flexibility as the software evolves with changing needs. Second, the problem sizes are large enough to ensure that first-principles-based simulations will scale. Scalability has already been demonstrated, for example, in thermal-hydraulics analysis of wire-wrapped fuel pins (P=2048 on IBM's Blue Gene) and in mechanical analysis of fuel behavior (P=2048 on the Earth Simulator). Recent electronic structure configuration interaction eigenproblems in computational chemistry have been solved with up to $n=10^{11}$ unknowns. The core algorithms in all three of these cases will scale to $P \sim 10^5$–10^6 provided that $n/P \sim 10^4$ or greater.

In other areas, algorithmic breakthroughs and further core software development are still required. For example, two of the key simulation approaches to neutron transport have known limitations. For $P > 10^4$, the usual approach to distributing independent Monte Carlo simulations to different processors suffers from having more processors than processes. Lack of memory per processor is also a possible constraint. Deterministic approaches suffer from long dependency graphs that are intrinsically serial. The number of parallel threads is anticipated to scale as $P \sim n^{2/3}$. In structural and seismic analysis of the plant, direct methods are currently the most effective approach to solution of the linear equations. The cost of these scale as $n^{7/3}$ and memory as $n^{5/3}$, far in excess of the optimal O(n) that has been achievable in many fields through the use of multilevel iterative methods.

Needs

The advancement of GNEP goals would benefit from the following:

- Establishment of ***high-fidelity ("gold standard") computational benchmarks***. Ideally, these benchmarks should be validated against companion experiments so that they may serve as surrogates for detailed experiments at the component level. They will thus provide validated baselines for upscaled multilevel models (e.g., as first-principles fluid dynamics simulations do for subgrid-model-based simulations). Because much of the single-component (e.g., materials, fluids,

seismic) software exists today, high-fidelity gold-standard simulations in the NE arena could be carried out as hero computations on near-term petascale architectures.

- Development of ***coupled codes*** based on high-fidelity algorithms. In moving forth with the development of new scalable software for NE applications, one should exploit the opportunity to have this software interact with other codes; a common interface for such interactions can take place will be essential. There may also be a need for multiple-program multiple-data (MPMD) programming models, for example, to support petascale multiphysics/multicode applications.
- Next-generation codes that leverage multipurpose high-performance ***scalable solvers.*** When considering scalability, one must distinguish between scalable algorithms and scalable software. Software design for petascale and beyond will require addressing every element of the code for parallelism. Because the core (scalable) algorithms typically constitute only 10% of a production-level engineering code, considerable effort will be required to ensure that all aspects of the software will scale to hundreds of thousands of processors in the near term and millions of processors in the >10-year timeframe.

3.3.2 Multiscale Methods and Algorithms

Large variations in time and spatial scales in reactor physics pose mathematical and computational challenges. A model of the full fuel cycle comprises reactor physics, fuel design, processing and reprocessing, waste repository, and so forth. The physical processes and theories range in scale from angstroms to kilometers in space and femto-seconds to years in time—from electronic structures computation for separation chemistry to the material models of dislocation, brittleness, corrosion and cracks propagation for the fuel, concrete, and metal, to the thermal hydraulics of the full reactor and seismic effects on the reactors.

Current Status

The models are principally described by coupled PDEs, ODEs, and integrodifferential equations encapsulating the different physics valid at the different scales of interest. The multiphysics models pervasive in development of an integrated simulation tool for nuclear reactors warrant new or improved scalable multiscale algorithms in addition to the need for scalable, adaptive, multiresolution higher-order and higher-resolution time-space discretization methods described in Section 3.2 and Section 3.3.1.

Needs

Several areas have been identified that warrant attention.

1. Monte Carlo methods. Monte Carlo methods are often applied to solve many problems in neutronics (e.g., Boltzmann's equation), in high-dimensional sampling and phase space methods, in stochastic models, and in sensitivity analysis and validation. Although Monte Carlo methods scale well with the number of processors, as a class of algorithms these methods converge slowly.

New fast, $O(N)$, scalable and accurate mathematical techniques and algorithms for representing high-dimensional functions and associated calculus, high-dimensional quadratures, and multiscale sampling methods can be applied to obtain faster and more accurate solutions. The application of these methods will also permit accurate five- and higher-dimensional phase space calculations that are desired for neutronics computations and the solution of Boltzmann's equation, as well as the ability to reduce high-dimensional problems to low-dimensional manifolds.

For example, mathematical and software developments in high-order and adaptive multiresolution methods (e.g., calculus for low-rank separability) currently permit high-fidelity analysis of six- and higher-dimensional problems. This approach is demonstrably scalable—to 4096 CPUs on the Leadership-class Computing Facility at ORNL.

2. Multiscale physics. Rigorous methods for communicating information between multiscale physics models is required. Some of the needs are software based (Section 3.3.2), but the main difficulty lies in ensuring that relevant information is exchanged at the right spatial and temporal scales to provide a robust and accurate overall simulation capability.

3. Coupling physics models of disparate time scales. In many cases the time step is dominated by the physics at the finest scale. Application and leveraging of current adaptive time stepping and integration methods to accelerate the solution methodology are attractive. In some cases (e.g., molecular dynamics), however, new solution methods will be required to accelerate the computation of trajectories based on the properties of the particle interactions. Transient analysis for reactor safety analysis is another area that requires methods for simulating disparate time scales.

4. Improved solution time for coupled physics models of disparate time scales and time stepping schemes. Improved homogenization, statistical, and probabilistic methods for sampling will improve current stochastic and Monte Carlo methods, sensitivity analysis, and upscale lumping of parameters required for coupling physics codes and validation and verification. New mathematical techniques for time splitting of operators and treatment of multiscale and multilevel boundary conditions will be required for accurate solutions of PDEs. For transient reactor safety analysis the performance of stiff time evolution equation solvers will need to be improved.

5. Mathematical techniques for treating complicated multiscale and multilevel boundary conditions. Such techniques will be required for accurate solutions of PDEs. In many GNEP applications different PDE- and continuum-based models are applied in the interior domain with a particle based method (e.g., lattice Boltzmann, molecular

dynamics, lattice gas) simulating the regions near the interface or near the boundaries. New scalable methods will be required to couple these methods accurately and rigorously.

6. Adaptive methods for coupling multiphysics models from the core neutron transport models to the thermal hydraulic scale and onto the whole plant. One important aspect of this simulation will be the thermal hydraulics. New developments of multiscale methods are required for treating Newtonian and non-Newtonian flows in complicated geometries with phase change, particle interactions, bubble interfaces and interactions, turbulence, chemical reactions, and free surface phenomena. Achieving this objective will require improved and rigorous methods for linking subgrid models in continuum models as well as subscale physics models. Effective computational methods will also be needed for fluid/structure interaction and front tracking of chemical reactions. Accurate numerical models of turbulent porous media flow with complex geometry are also needed in several reactor core applications (e.g., pebble bed).

7. Multiscaled methods for constrained optimization. For plant design optimization as well as economics, multiscale methods for constrained optimization with multiphysics models will be required with a feedback loop for convergence through self-consistent loops. Effective inverse methods will be required for faster and more robust estimations for reliability and safety analysis in reactor design, operations, and seismic analysis.

3.4 Software Tools and Environments

Major findings associated with software tools and software engineering are related to code coupling, parallelization, and parameter studies. Unresolved coupling issues that will need to be addressed include appropriate architecture to facilitate coupling; reuse of legacy codes or parts of such codes; validation, verification, and uncertainty quantification of coupled codes; and issues associated with interfacing codes that have disparate spatial, temporal, and data structure characteristics. Parallelization issues also exist, in addition to the need to obtain high-fidelity computations that are associated with the need or lack thereof to parallelize serial legacy codes.

The need for GNEP component and enterprise systems-level design studies introduces a requirement for multiobjective optimization software that should be robust and exhibit good parallel scaling. Other requirements include sensitivity and uncertainty analysis (addressed in Section 3.1), workflow management (addressed in Section 3.6), and techniques for identifying and minimizing errors that occur in large codes.

A crosscutting finding is that early work on software tools and software engineering will require a comprehensive survey and assessment of existing software, along with a plan that gives guidance to their integration into the GNEP program.

3.4.1 Coupling of Codes

Important system behavior issues involve interactions of phenomena captured by various codes that currently have difficulty sharing data. They typically use different data structures and mesh representations, inconsistent equations of state and other properties for a given material, and incompatible I/O variables and formats. For example, the coupling of codes representing the reactor core and vessel with those simulating the balance of plant piping, pumps, structures, and other important components generally cannot be done without enormous investment of time and effort. Similarly, detailed fuel rod performance codes providing high-fidelity response cannot be easily used to provide information to full-core simulations. Furthermore, codes representing physics that must be tightly coupled (such as fluid flow and heat transfer, thermomechanical response, and neutron transport in the core) cannot be easily run together at all. Finally, most current codes use independent and incompatible graphics tools that significantly complicate the ability of an analyst to understand the larger picture. This lack of interoperability stems from the lack of standards for key areas where independent codes could interface.

Current Status

Coupling multiple codes (here, "code" means anything from a library routine to a full application program) is a complex problem that requires both computer-science solutions, in terms of software architecture and data structure choices, and a carefully chosen mathematical representation of the data to be exchanged between the codes. The kind of coupling required ranges from one-way coupling (e.g., using the climate to provide conditions for repository modeling) to very tight two-way coupling (e.g., in a fluid-structure interaction). A well-developed and architected system for coupling codes also provides an effective way to manage the complexity of developing, testing, and parallelizing collections of codes. In addition, experience in software engineering has shown that modularity can improve the robustness and correctness of codes. For codes that must be certified as part of the regulatory process, a modular approach may allow faster and more confident certification, which in turn will reduce barriers to innovation. Such a system also provides an evolutionary approach for making use of current (so-called legacy) applications without requiring complete rewrites or re-engineering of those codes. This is an important consideration for achieving near-term computational goals, since full program development often takes years. In addition, such a system enables collaboration, particularly between institutions, by establishing clearly designed interfaces and requirements.

Code coupling has been successfully carried out in several large-scale simulations. The Community Climate Model has faced many of these issues and has addressed both the problems of the mathematical representations (needed to ensure accuracy and stability) and data structures and data exchange for parallel computation, in this case using the Model Coupling Toolkit. Similar problems have been addressed in the fusion community. Other tools, such as MpCCI, have been used for fluid-structure interactions. The SciDAC

Center for Component Technology for Terascale Simulation Software has focused on the issues of building a common component architecture.

Needs

Despite the cited successes, there remain challenges for which there are as yet no good solutions. For example, it is important to ***propagate the uncertainty quantification between the codes.*** While there is some early work in this area, such as quality of service or guaranteed accuracy of numerical libraries, more needs to be done to understand how to efficiently and accurately include this information as part of the exchange of data between codes.

3.4.2 Parallelization

Few of the legacy codes used for nuclear facility design and safety have been parallelized. These codes, developed by the nuclear industry, the national laboratories, and universities for various parts of the nuclear fuel cycle, were largely designed and developed in the 1960s, 1970s, and 1980s before the advent of modern high-performance computing methods and platforms and focus predominantly on LWR technology as opposed to fast sodium reactor technology. Nevertheless, they represent the primary repository of a vast amount of scientific knowledge applicable to nuclear facilities. On the other hand, numerous general-purpose codes scalable to thousands of processors have been developed for CFD, structural mechanics, and other basic science and engineering applications, but these codes generally lack specialized capabilities for treating certain phenomena necessary for simulation of nuclear facilities.

Current Status

Clearly, high-performance computing capabilities must be married with the physics captured in these legacy codes. A fundamental tension exists among those who advocate incremental extension of the capabilities of legacy codes, including parallelization, those who advocate extension of general-purpose codes to include nuclear-specific phenomena, and those who advocate starting from scratch using pieces of codes from both arenas.

Needs

Parallelization is often required to provide efficient access to larger memories in order to improve resolution and accuracy as well as to reduce the time-to-solution. While some codes in use already scale to hundreds to thousands of processors, others are still sequential codes. No codes appear to be ready for hundred- to thousand-way parallelism. There are both tools and techniques that can be applied to ***parallelize existing codes and to enhance the scalability of parallel codes.*** Several of the SciDAC projects have

addressed these issues (including the APDEC, PERC, TOPS, and TSTT projects). It is important for parallelizations, particularly scalable ones, to be developed with careful attention to the mathematical abstractions. Software tools that aid in managing distributed data structures, including those for materials properties, will be required for the massively parallel, processor-rich (and hence relatively memory-poor) systems.

3.4.3 Advanced Frameworks in GNEP

The potential of advanced frameworks in GNEP is both revolutionary and evolutionary. Evolving legacy codes and programmers into modern software engineering practices preserves the valuable code base in NE and will improve portability and code verification.

Current Status

While some advantage may be gained in using commercial or open source tools generically, the DOE toolkits developed specifically for scientific performance have the most potential. ASCR tools for profiling and source analysis (e.g., TAU, Rose, Jumpshot) already made available by DOE researchers can improve, sometimes vastly, the performance of existing codes.

Armed with a better understanding of the location of performance bottlenecks, NE researchers can gain clearer insight into where parallelism and HPC will benefit their simulations. A joint collaborative program between ASCR and NE with goals for moving NE code into the high-performance computing arena will realize most of these goals.

Needs

A long-term possibility is to transform the current NE code library of separate simulations into a ***single framework with interchangeable code modules.*** In this conception the components of the nuclear plant would be rendered as replaceable software parts along with numerics, I/O, and so forth. The current NE code base could be drawn upon to create these modules. Verification and certification could be done on a module basis rather than the whole code so that the NE simulation code base as a whole supports both certified simulations and innovative test runs. Not only would power plant/fuel cycle understanding and design benefit from a comprehensive simulation, but regulatory agencies could draw on the same code base from which to make safety assessments. Because separately developed simulation codes each must replicate much of the same infrastructure, moving to a common code base will save the cost of that development and improve code verification. To (loosely) quote one NE researcher: "Everyone has his own version of thermal transport in a cylinder; if we could all use a verified standard, our lives would be easier." (For a discussion of algorithm injection as a step toward this goal, see Section 3.1.)

Moving to such an integrated framework must be done incrementally, as has been successfully demonstrated by the Community Climate Model. A single modular simulation evolves, first by linking disparate codes together by files in a workflow-like script, then by connecting them running simultaneously through a software coupler. Along the way scientists must negotiate schemes for connecting their codes and preserving the fidelity of the physics.

Bringing best practices to building new NE software and maintaining legacy simulations will improve software quality and reliability generally. The use of existing ASCR-developed tools will improve performance and help simulations yield higher-fidelity results through the use of HPC platforms. Moving the current code base of separated simulations for different power plant physics to an integrated modular multiphysics framework will improve cost-performance and reproducibility of the results.

3.5 Computing Facilities, Data, and Networking

The current capability of facilities used by the nuclear engineering community is limited. Within the United States, a small number of commodity clusters are in place at national laboratories and in industry for reactor simulation and seismic analysis. These clusters are typically well under a teraflop/s of peak computing power. Nuclear engineers outside the United States have regular access to more computational power. In France a 4 TFlop/s (peak) system is used, and in Japan scientists have access to a 13 TFlop/s (peak) system, on which they recently completed a five-day seismic analysis run. Addressing the key fundamental and design problems for GNEP requires multiple systems with 10–1000 times as much capability, deployed over time.

3.5.1 Current Status

Advanced simulation and integrated experiment and modeling activities clearly have the potential to make a great impact on the GNEP objectives. High-fidelity simulations will require orders of magnitude more computer power than what is used today. A staged approach would satisfy the key objectives with a coordinated software and facilities effort. At each stage, computing facilities would support production use of the current generation of codes, configured to provide the maximum range for those codes. At the same time development would proceed on the next generation of codes, which require scalable development systems and at least one instance of a system with the capabilities of the next generation of production systems. Data storage, networking, and support services also would be scaled to meet the GNEP research and design workload.

3.5.2 Making an Impact

The ***early period*** (years 1–4) would focus on evolving existing codes to make use of current computational technology. The existing code base ranges from single-processor codes to codes that exhibit modest parallelism. Most existing codes were developed quite some time ago; where practical, these codes would be optimized for modern processor technology and expanded in scale. At the same time, there would be an effort to design and develop a new generation of codes that use modern methods and are capable of using high degrees of parallelism to achieve higher fidelity and resolution. This first stage would include introducing new mathematical methods and new algorithms as well as state-of-the-art physics. The codes developed during this stage would focus on discrete components within the GNEP program: different reactor types, different fuel processing methods. Further, a set of tools and interfaces must be developed to support the integration of the new codes. This framework would allows a whole community of developers—teams discipline scientists, computational methods experts and computer scientists—to contribute to the development of a suite of codes. This period would involve several activities: development and debugging the new generation of codes, engineering design runs using today's (evolved) codes, and conducting limited "hero" calculations using new codes to address high-impact previously considered intractable problems. Other activities would focus on outreach: training a new cadre of nuclear engineers in advanced computational methods and concurrently familiarizing computational scientists with GNEP problems.

The ***middle period*** (years 5–10) would see the replacement of the existing code base with those codes produced in the first stage. The new codes would have state-of-the-art physics and would be able to harness the full capability of the computational and data systems through parallelism (ranging for 10,000 to 100,000 CPUs). This period would include development and debugging of the next-generation codes with increasing levels of system and physics integration, validation and verification of the early period codes in engineering design runs, and large numbers of production runs to support design activities. During this period also, the codes and frameworks for the later period would be defined and developed. Data analysis and assimilation would occur for the demonstration projects and other experiments.

The ***later period*** (years 11–20) would see the wide use of the codes and framework developed in the middle stage. The codes used during this period would have state-of-the-art physics and multiscale and multiphysics features and would be closely integrated to provide integrated analysis of multiple components. These codes would be able to use millions of compute elements simultaneously to harness the full capability of the computational and data systems. The activities during this period would include validation and verification engineering design runs, parameter studies to explore engineering margins, and a significant number of "hero" calculations to address high-impact problems previously considered intractable. Data analysis and assimilation would occur for the demonstration projects and other experiments and could include ongoing operational data from systems and plants.

3.5.3 Needs

We discuss below five specific areas where research and development are needs: computing resources, data management, networking, codes and frameworks, and advanced services.

1. Computing Resources. At every stage of this work, multiple computational needs define the capabilities of the computer systems and their supporting infrastructure:

- Production runs of existing science and engineering codes must be supported, where the production system architectures and configurations support ***very large capability runs*** with the available software applications, and they support high numbers of capacity runs for parameter studies. The number of systems and their configuration should be determined by analyzing the workload.
- ***Simulation code development*** must be supported at scale, for both application development activities and early science and engineering runs. This work requires at least one system that has the full capabilities and other characteristics of what will be used as production systems for the next generation.

During the next 15 years there is an opportunity for the nuclear energy community to exploit computer, data storage, and networking generations that would provide cost-effective resources to the GNEP program. Table 3.5.1 provides initial estimates of the computing capacities and capabilities needed to take advantage of this opportunity, based on what is known about present and next-generation application requirements, together with experience in facilities deployment in other science and engineering domains. A more comprehensive analysis should be performed as science and engineering needs are determined and ranked.

2. Data Management. The scale of the GNEP data systems must be balanced with the scale and number of computations and experiments being performed. For experimental data, there is a need not only to accumulate past data and make it more broadly available but also to provide ample metadata to make it useful for future researchers and engineers. Therefore, elements of the community or some other body must be charged with the ***long-term curation*** of the important experimental datasets. To date, the aggregate data requirements are not well understood, but existing data and experience with similar simulations in other fields provide the initial estimates in Table 3.5.2. Here we used 50–100 bytes of on-line storage per sustained flop/s for simulation computations and 1,000–2,000 bytes per sustained flop/s for experimental data analyses.

Table 3.5.1
Initial estimates of the computing capacities and capabilities needed by GNEP

Period	Production Science and Engineering Computing Facilities	Development and Early Science and Engineering Computing Facilities
Years 0-4	• Multiple systems in the 1-10 teraflop/s (sustained) range to support production design studies and experimental data analyses	• System in the 10-100 teraflop/s (sustained) range to support development of new applications, algorithms and tools • System in the 100-1,000 teraflop/s (sustained) range for early use of the new applications
Years 5-10	• Multiple systems in the 500 to 10,000 teraflop/s (sustained) range to support large numbers of production runs for design studies and V&V studies • Multiple systems in the 100 teraflop/s (sustained) range to support experimental data analyses	• System in the 1-10 petaflop/s range (sustained) range to support development of new application, algorithms and tools • System in the 10-100 petaflop/s (sustained) range for early use of the new applications
Years 11-15	• Multiple systems in the 10-50 petaflop/s (sustained) range to support large numbers of production runs for design studies and V&V studies • Multiple systems in the 1,000 teraflop/s (sustained) range to support experimental data analyses	• System in the >100 petaflop/s (sustained) range for development of new applications, algorithms and tools and early use of the applications

Table 3.5.2
Initial estimates of the online and archival data capacities needed by GNEP

Period	Capacity of Online Data Systems (petabytes)	Capacity of Archival Data Systems (petabytes)
Years 0-4	• Simulation Data = 110 • Experimental Data = 20	• Simulation Data = 2000 • Experimental Data = 400
Years 5-10	• Simulation Data = 13,000 • Experimental = 200	• Simulation Data = 260,000 • Experimental Data = 4,000
Years 11-15	• Simulation Data = 130,000 • Experimental Data = 2,000	• Simulation Data = 2,600,000 • Experimental Data = 40,000

3. Networking

GNEP networking requirements need to support the effective ***use of multiple computational and data facilities*** by a nationally and internationally distributed science and engineering community; see Table 3.5.3.

Both ***local area networks (LANs) and wide area networks (WANs)*** are vital to the GNEP computational facilities. LANs link the high-performance computers, online storage, and archival storage. High-performance systems in all three categories have many network connections; hence, LANs have evolved into fabrics whose performance may by characterized by the cross-sectional bandwidth, nominally between the high-performance computer and its storage systems. WANs connect GNEP computing and data resources to scientists, engineers, and regulators at their home sites around the world, easily hundreds of sites for the GNEP effort. WAN connections also knit the various GNEP computing and data resources into an overall GNEP infrastructure. Here is it appropriate for the computing facilities to join the national and international network at speeds comparable to the network backbone.

Table 3.5.3
Initial estimates of LAN and WAN requirements for GNEP

Period	Local Area Network (cross-section gigabits/s)	Wide Area Network (gigabits/s to backbone)
Years 0-4	100-2,000	40
Years 5-10	2000-20,000	1000
Years 11-15	20,000-100,000	10,000

4. Codes and Frameworks. One of the strengths of the GNEP concept is the opportunity it provides to share simulation and analysis technologies in the form of applications and modules that interoperate with community model frameworks and numerical libraries. The computer facilities used by GNEP must then support the ***common frameworks and libraries*** needed by these applications. As more sites and data become available and information services become more uniform, there will be an opportunity to employ Grid-like services to move and manage data, to schedule workflow with stages at different sites, and to support end-to-end problem solving. Topical information and computation portals may become important for engineering community use.

5. Advanced Services. The move from desktop and work-group computers to large high-performance systems brings a greater need for ***expert user support***, including focused science team support, software support for libraries, tools and commercial codes, expert advice on libraries and tools, and assistance with computation and I/O performance optimization. Planning and optimization will grow to cover the whole computational campaign, including input data access from distributed sites, high-performance simulation, data analytics, visualization, and model comparison with other models and experiment.

Because some GNEP efforts may involve export-controlled or sensitive data, access control and security require extra effort. International credential arrangements may be needed for collaborators. It also remains to be determined whether security requirements will dictate specialized computational facilities for some work. Moreover, some computations may be used to make decisions about life-critical design parameters, adding significant requirements in areas such as licensing, certification, and change management The Office of Science has not done life-critical computing before, and such computations would add significant requirements if done on ASCR systems.

3.6 Data Analysis and Visualization

Effective tools for managing and understanding the myriad of experimental, design, and simulation data associated with the design and engineering of GNEP reactors and repositories are essential if we are to meet safety, performance, and cost goals. Nuclear data must be captured, managed, integrated, and mined from a wide range of sources to produce optimal designs. Data analysis and visualization will help engineers predict the reactivity of fuel and radiation source terms critical for efficient reactor and repository design.

3.6.1 Current Status

Data analysis and visualization tools must address the realities of enormous quantities of data, diverse information sources and formats, and distributed design teams.

Data Management. Data management encompasses the processes of capturing, annotating, tracking, integrating, and mining information. In GNEP, information sources will include observations, lab experiments, predictions from theory, and computational simulations. The scale of the GNEP data problem in terms of the number of sources, overall volume, sophistication of analysis techniques, and number of participants accessing information makes the data management problem challenging. Current formats, storage, and transmittal methods for data relevant to the advanced fuel cycle initiatives are nonexistent or insufficient for an integrated international project; there is no experience with the management of petabyte-scale data. GNEP researchers can, however, learn from the Evaluated Nuclear Data Files (ENDF/B) model formalized in the nuclear physics community and expand the scope to include multiphysics simulated data. GNEP can also benefit from ASCR efforts in scalable I/O, distributed data management, and distributed computing.

One GNEP objective is to produce a set of integrated multiphysics codes capable of replacing testing with high-fidelity simulation. Major challenges include the lack of standardized data formats and metadata; analysis and simulation methods; and capabilities to integrate, assess, label, and compare the quality of simulated data from multiple sources. Furthermore, such petascale simulations will generate terabytes to petabytes of data that have to be stored quickly into disk in parallel, moved reliably to

mass storage systems, and distributed to analysts. These technical issues amplify the challenge to harden the notion of a GNEP workflow and deliver it at scale.

Analysis and Visualization. As nuclear energy simulations strive for petascale resolution, extremely large datasets will be created. Computational explorations of different parameters, methods, and approaches will generate ensembles comprising millions of runs. For example, in repository modeling, Monte Carlo techniques are used to quantify uncertainty by generating many evolutions of a repository's performance over time. As another example, in order to understand how a reactor will perform, thousands of variables must be considered in a design simulation; many simulations may be required to identify combinations of parameter values that satisfy cost or safety constraints. Identifying how these variables affect these constraints is critically important to the NE community.

A common technique for analyzing such huge datasets is visualization. Processing and displaying results of such datasets, however, are tasks that typically overwhelm existing postprocessing, networking, and display systems. Moreover, general-purpose analysis and visualization tools frequently require extensive customization to NE problems, for example to trace diffusion of waste following water intrusion in a repository. Compounding the difficulty of visualization is the breadth of visualization and analysis products and usages. For example, different types of visual analysis are required for regulators, program managers, and scientists. (cf. the discussion in Section 2.3). Clearly, visualization remains a major issue. Developing the right tools can enhance the productivity of scarce design talent and thus both improve design quality and reduce risk.

3.6.2 Needs

The following three R&D activities address the data management and visualization needs:

- A ***GNEP data center*** is needed to collect, format, manage, and disseminate observational, experimental, theoretical, and computer-generated data related to program goals. Center activities would include community participation both at the national and international levels in the standardization of critical data formats, including sufficient metadata formalism with the goals of assisting in validating and improving data accuracy and consistency. This work would have a high impact in the medium and long term.
- A ***GNEP distributed data environment*** is needed to handle the GNEP-related data, most of which will be produced, and in many cases permanently located, at different sites. A distributed data environment would allow discovery, access, analysis, and movement of this data. This environment would be essential to the infrastructure of the GNEP collaboration and the construction of the GNEP data center, design, and visualization and analysis environments. There already exist technologies (such as developed in the Grid community) that integrate geographically distributed hardware and software efforts to enable disjoint but

related research efforts to be brought together. Japanese nuclear engineers have expressed interest in unifying their GNEP-related efforts to the U.S. efforts through such technologies. This work would have a high impact in the medium term.

- ***GNEP design and analysis environments*** are needed to enable GNEP engineers to work with ASCR computer scientists in using state-of-the-art analysis and visualization tools and techniques. Such environments would require production analysis and visualization staff, visualization software, and hardware resources support for the GNEP community. This work would have a high impact in the short term. In the longer term, the NE community could be supported with custom NE design and analysis environments that provided direct support for the definition, analysis, visualization, and manipulation of NE objects of interest.

Research and development work will be needed to support and inform these efforts. Such efforts ideally would include the involvement of the university community.

- ***Hardware and software technologies****,* to support metadata management, to manage a petascale storage space on demand, to permit data searches and mining, and to deliver (optimized) robust and secure data collection and distribution. A process for delivering the same capabilities for controlled data is also needed. This work would have a high impact in the medium term.

- ***Uncertainty visualization and analysis****,* including efforts on sensitivity analysis to determine the change in a computed result due to a change in input parameters used in a calculation. This work would have a high impact in the long term.

- ***Comparative and quantitative visualization,*** supporting the measurement and the visual and analytical comparison of the differences between ensembles of data. Techniques and tools are just beginning to emerge to address this issue. R&D resources focused on this area would have a medium impact in the long term.

- ***Large-scale visualization and analysis,*** supporting the ability process the extremely large scientific datasets generated by petascale computational resources. This effort would have a medium impact in the long term.

- ***Workflow architectures*** for different GNEP functions, capable of leveraging the GNEP program's information content. The goal is to automate the data processing and data movement between multiple physics codes, the analysis, and visualization. A fundamental issue in realizing such an objective is the definition of a data model that forms the basis for all workflow components in GNEP. Ideally, the process of defining and refining formats and metadata standards would be coupled to the identification of essential features to be marked for such purposes. The high impact of GNEP workflow capabilities are long term in scope and will require close collaboration of NE and SC/ASCR engineers and scientists.

4. Conclusions, Findings, and Recommendations

By bringing together nuclear energy researchers and computer scientists and applied mathematicians—groups that ordinarily simply "pass in the night" —the GNEP Modeling and Simulations Workshop encouraged the sharing of ideas and problems in bringing the GNEP vision to reality.

In addition to providing insight into the needs of the nuclear energy community, the workshop provided a forum for identifying new mechanisms for improved software sharing and for exchanging information about areas for future research.

4.1 Conclusions

The researchers in both the computing sciences and nuclear energy communities recognized that the current code base used for advanced nuclear systems lacks the predictive ability needed to achieve the goals of GNEP. Many, likewise, recognized the opportunity offered by advanced modeling and high-performance computing to improve designs of future reactors, reduce uncertainty in facilities development and construction costs, improve safety, and reduce development times of new fuel types needed to close the nuclear fuel cycle.

Nevertheless, **significant research challenges** remain. A clear need exists for better tools for ***uncertainty quantification*.** The validation process is key to engineering applications; in essence it consists of providing demonstrated uncertainty evaluations to all predictions. Currently, validation techniques deployed by the nuclear engineering community span from empirical approaches to science-based approaches using sensitivity analyses and statistical methods. Better error estimation is sorely needed in simulations. The separations chemistry group, for example, cited the need for uncertainty quantification across the entire plant; the neutronics group noted the need for improved energy discretization techniques critical to achieving predictability and estimating uncertainty; and the reactor core group cited the need for a new simulation systems that included assessment of margins, qualify, validate, and optimize designs

A second major challenge is ***coupled modeling***. Multiphysics coupling is needed, for example, to link neutronics to fluids and heat transfer algorithms, structural mechanics, and fuel behavior. Enabling effective code coupling will require development of second-order (at the least) in time coupling methods, as well as new coupling approaches that support sensitivity analysis, data assimilation, and PDE-constrained optimization. A new software architecture will also be needed to treat the coupled problems, enabling researchers to plug in new physics modules to study different phenomena more efficiently.

Related to the need for coupled systems is the question of **optimization strategies.** Both unconstrained and constrained optimization will be critical for parameter identification, design, and control. Currently, several efforts are under way to develop general geometry

modification and derivative computation tools for design optimization needs. Others are developing tools for I/O performance optimization. We anticipate that GNEP optimization needs will grow to include input data access from distributed sites, high-performance simulation, data analytics, visualization, and model comparison with other models and experiment. Moreover, optimization strategies will be needed beyond linear programming for complex systems varying in time; and these strategies must be coupled with the data management and archival strategies.

Visualization will be a key tool in data analysis and presentation of the vast datasets expected from GNEP research. Feature extraction will be needed in order to provide quantified measures of key characteristics. Distributed visualization, with automated integration of large 4D datasets distributed across multiple storage sites, will also be critical. Even further, different users (e.g., policy planners, researchers, designers) will require different mechanisms to view and interpret large data sets.

Finally, a significant number of researchers felt that increased emphasis should be placed on **modular software environments**. Researchers cited the need to be able test different components or models, for instance for reactor core design. "Plug-and-play" techniques such as those used by the Community Climate Model are needed to efficiently treat coupled problems. Similarly, high-fidelity assessment of chemical environments requires coupling multiphysics solutions across domain boundaries. a modular software infrastructure would facilitate the necessary collaborative efforts in parallel meshes and efficient PDE solvers.

4.2 Findings

The workshop participants identified several areas for improving the effectiveness of the nuclear energy program. We begin with the findings of the NE group and then turn to those of the computing sciences group.

4.2.1 Nuclear Engineering Findings

Globally, we have confirmed that because of the absence of a well-defined project over many years, the nuclear engineering community that specializes in the key GNEP technologies has suffered from an almost total lack of investment and is significantly behind the state of the art in simulation-aided design. Four specific issues became apparent during the workshop:

1. Requirements-driven Specification Process. The nuclear engineering community is capable of expressing, for each simulation area of relevance, the limits of its current tools and to some extent the accuracy desired for future tools. Nevertheless, the definition of that future objective is often focused on individual disciplines and does not integrate the deep coupling between disciplines needed to analyze these advanced systems. What is

needed is a process that, starting from the specification of GNEP objectives, defines in a rational manner specifications for each tool and the physics data they rely on.

2. Integration of Advanced Simulation Capabilities. The nuclear engineering community is also capable of expressing an incremental path to improving its tools. This is sometimes defined as solving the same simplified model somewhat faster and with finer resolution. Again, because of the absence of a well-defined project that would focus the efforts, this approach sometimes ignores the shift in paradigm that is now possible with advanced computing and simulation tools, where quasi-first-principles models can be used to provide accurate predictions.

3. Validation of Simulation Tools. The validation process is key to engineering applications; in essence it consists of providing demonstrated uncertainty evaluations to all predictions. We have found that the validation techniques currently deployed by the nuclear engineering community range all the way from empirical approaches (i.e., comparison of calculations to "representative" experiments, followed by expert judgment for generalizing the observed biases) to science-based approaches making use of sensitivity analyses and statistical methods for information treatment. It seems critical that more formal validation processes be developed and used for all disciplines.

4. Development Process. This workshop was focused on the technical contributions that simulation and modeling can bring to advanced energy systems. It did not address key elements that are required for a complete picture:

- There is a clear need to define a development process where needs are well specified, and priorities are established taking these needs into account
- The development of new tools must proceed in parallel with the development of strategies to use these tools, particularly in the design and licensing areas.

The most important contributions expected from modeling and simulation are as follows.

- ***Separation plants and repositories****:* Accurate process models can help both to guide the R&D process and to predict loss mechanisms. Such models could be coupled for a complete plant. Accurate waste form models would help to predict waste behavior for a variety of scenarios, ranging from local handling and transportation to temporary storage and long-term geologic disposal.
- ***Fuels****:* The development of predictive fuel behavior models (during fabrication and during irradiation) could shave years off a purely experimental approach.
- ***Fast reactors****:* High-fidelity coupled neutronics, thermo-hydrodynamics, and structural models could reduce margins without compromising safety and confidence, and hence could reduce cost and facilitate licensing demonstrations.

While some of the required technologies are available "off the shelf," others are in their infancy. In particular, long-term research is needed to (1) develop and implement a validation methodology for the suite of codes to be employed in a predictive sense in GNEP and (2) devise a means for coupling component models to produce whole system models—a process that demands both deep engineering insight into what interactions and

scales must be represented and flexible and powerful software tools to capture and balance them.

4.2.2 Computer Science and Applied Mathematics Findings

Components of the GNEP research program where simulation must be improved include materials and fuels properties, reactor modeling and design (structural, hydrodynamical, thermal, and transport), reactor control and operational envelope evaluation, fuel (re)processing and separation, repository modeling, and infrastructure modeling (systems analysis, security, and economics).

The ***mathematical simulation techniques*** required to support this program include CAD-to-mesh, solution adaptivity, mesh partitioning, discretizations of virtually all types, solvers, stiff integrators, kinetic and particle methods, unconstrained and constrained optimization (for parameter identification, control, design, etc.), uncertainty quantification, sensitivity analysis (both statistics-based and derivatives-based), multiscale methods, homogenization, and reduced-order modeling.

Computational techniques underlying this agenda include parallel programming models (MPI, multithreading, etc.), dynamic load balancing, language interoperability, componentization, high-performance I/O, performance monitoring/debugging, data archiving, visualization, automated discovery and data mining tools, assimilation and fusion of experimental data with simulations, workflow description, and codification.

GNEP represents a rare and ripe opportunity for developers of the enabling technologies in applied mathematics and computer science to demonstrate a ***paradigmatic shift*** that they have envisioned for years. Since the current code base for GNEP technologies is antiquated in many ways, it will have to be substantially rewritten. This substantial task can be accomplished while preserving key code assets at low levels, such as physical property data bases and software that evaluates constitutive properties (in its original language), but the connective and control code and the majority of the means of interchange of data between code components will need to be completely rewritten or written for the first time to take advantage of modern software practices and high-performance parallel architectures. Virtually all large-scale data structures in existing codes will have to be replaced with distributed versions. As the software infrastructure is rebuilt, due attention can be given to extensibility, reusability, object orientation, componentization, portability, performance portability and tuning, code self-description and self-monitoring, and the construction of multilayered interfaces that enforce correct usage.

Escaping the world of "spaghetti code" confers several benefits on the GNEP software universe beyond the immediate practical scientific advantages, in terms of debugging, correctness, and efficiency. With modularity, export control and intellectual property restrictions can be applied with finer granularity, enabling greater sharing without compromise of security or company propriety. In addition, for that subset of the GNEP research software infrastructure that is useful in the federal regulatory process (licensing

or certification), streamlined approvals may be possible through reuse of approved components.

4.3 Recommendations

Here we summarize the principal suggestions offered by the workshop participants, and—equally important—we propose a mechanism for implementing each suggestion.

Suggestion: A significant number of **multidisciplinary teams** should be supported. Special attention should be given to teams comprising experts in applied mathematics, computer science, nuclear engineering, materials science, chemistry, and advanced software engineering.

Mechanism:

- Begin developing next-generation simulation codes based on ***models closer to first principles***. Deployment should be realized within the five- to ten-year time frame.
- Task these teams with the explicit goal of developing ***open source community codes*** that will be used for next-generation design of nuclear fuels, power plants, separation plants, and repositories.

The SciDAC and ASC experiences offer confidence that this goal can be achieved, as well as offering much software to be leveraged.

Suggestion: Existing codes within the nuclear engineering community should be enhanced **to take advantage of modern computing resources**.

Mechanism:

- Port existing codes to **modern platforms** in the near term.
- Integrate the codes into **modern engineering workflows** so that they can be used to support near-term design and engineering.

To achieve this goal, teams of software engineering and parallel computing experts should work with the established nuclear engineering community to parallelize and enhance existing codes.

Suggestion: A scientifically demonstrated **validation process** should be developed in order to provide sufficient assurance of the predictive capabilities of simulations.

Mechanism:

- Establish a requirements-driven process that will enable the community to define accuracy and validation goals for each computation tool and for an integrated simulation system

Such an effort can begin by focusing first on validation of components and the ultimately on integrated systems. The objective is to ensure that stakeholders beyond the technical realm will be able to rely on simulation to support capital investment and national and international policy making.

Suggestion: A long-term research program should be established that is aimed at **advancing cross-cutting issues**.

Mechanism:

- Explicitly fund **new approaches to uncertainty quantification** and error estimation, multiscale and scalable algorithms, and development and validation of coupled multiphysics codes.

Such funding should be provided for a mix of university and laboratory research and at a level that permits rapid acceleration of research.

Suggestion: New incentives should be developed to ensure the availability of the **next generation of computationally oriented nuclear engineers and scientists.**

Mechanism:

- Fund university programs and laboratory ***internships*** for training in related disciplines needed to support the long-term redevelopment of nuclear energy in the United States and the world.

4.4 The Promise of the Future

Arguably, a significant investment in human and computational resources will be required to realize the potential of such technologies in the Global Nuclear Energy Partnership program. One can expect, however, that this investment will be dwarfed by the savings relative to a purely experimental program and should begin paying off much earlier—perhaps a decade or more.

Appendix A: Charge for the Workshop

"Conduct a workshop to obtain community input on the role of computational science and high performance computing in the advanced fuel cycle initiative. Explore the entire spectrum of opportunities, both short and long term. Ensure close coupling of the workshop discussions and activities to the science and engineering needs of the Office of Nuclear Energy (NE). Reference the workshop findings and recommendations to both those NE needs as well as to current and expected future capabilities of the Office of Science, and in particular, its Office of Advanced Scientific Computing Research (ASCR). Prepare a preliminary letter report within one week of workshop completion and follow with a full report within 30 days of workshop completion."

Appendix B: Agenda

August 15, 2006

Plenary Session

Introduction – *Vic Reis*

Charge – *Michael Strayer*

Goals of the Meeting

Modeling and Simulation Needs for Advanced Nuclear Systems – *Phillip Finck*

GNEP Technology Demonstration Program – *Kathryn McCarthy*

European Perspective on Reactor Core Simulations – *Massimo Salvatores*

Breakout Sessions

1. Reactor core simulation (Pino Palmiotti (ANL), Neil Todreas (MIT))
2. Materials and Fuels (Jim Tulenko (Univ of Florida), Bill Corwin (ORNL))
3. Separations Chemistry (Terry Todd (INL), Dave Dixon (Univ of Alabama))
4. Repository Modeling (Robert MacKinnon (SNL), Paul Wilson (Univ of Wisconsin))
5. Seismic/structural/balance of plant (Dave McCallen (LLNL), Christophe Dellis (CEA))
6. Validation (Phillip Finck (ANL), Kathy McCarthy (INL))

August 16, 2006

Direction of ASCR – *Michael Strayer*

Overview of ASCR Computational Mathematics and Software – *David Keyes*

Overview of ASCR Computational Facilities and Networking – *Rick Stevens*

Breakout Sessions

1. Mathematical and Geometrical Modeling (Phil Collela (LBNL) and Lori Diachin (LLNL))
2. Validation, Verification, and Uncertainty Analysis (William Oberkampf (SNL) and Alyson Wilson (LANL))

3. Scalable and Multiscale Algorithms (George Fann (ORNL) and Paul Fischer (ANL))
4. SW tools and SW engineering (William Gropp (ANL), Rob Armstrong (LLNL))
5. Computing Facilities, Data and Networking (Ray Bair (ANL), Bill Kramer (LBNL))
6. Data Analysis and Visualization (Jim Ahrens (LANL) and Ken Roche (ORNL))

Appendix C: Participants

Adams, Marvin – Texas A&M University
Ahern, Sean – Oak Ridge National Laboratory
Ahrens, James – Los Alamos National Laboratory
Aidun, John – Sandia National Laboratories
Anitescu, Mihai – Argonne National Laboratory
Armstrong, Robert – Sandia National Laboratories
Azmy, Yousry – Penn State University
Bair, Ray – Argonne National Laboratory
Berry, Ray – Idaho National Laboratory
Bertrand, Fred – Department of Energy
Besmann, Theodore – Oak Ridge National Laboratory
Bethel, Wes – Lawrence Berkeley National Laboratory
Bielak, Jacobo – Carnegie Mellon University
Bland, "Buddy" S. – Oak Ridge National Laboratory
Bowman, James – GE Energy, Nuclear
Bulatov, Vasily – Lawrence Livermore National Laboratory
Burrow, Richard – U.S. Department of Energy
Candy, Jeff – General Atomics
Carlson, Donald – Nuclear Regulatory Agency
Caro, Alfredo – Lawrence Livermore National Laboratory
Cary, John –Tech-X Corporation and University of Colorado
Cattaneo, Fausto – Argonne National Laboratory
Chalk, Christine – U.S. Department of Energy
Chiu, George – International Business Machines Corp.
Chauliac, Christian – French Atomic Energy Commission
Clarno, Kevin – Oak Ridge National Laboratory
Colella, Phillip – Lawrence Berkeley National Laboratory
Collis, Scott – Sandia National Laboratories
Corwin, William – Oak Ridge National Laboratory
Corones, James – Krell Institute
Corwin, Bill – Oak Ridge National Laboratory
Day, Marc – Lawrence Berkeley National Laboratory
D'Azevedo, Eduardo – Oak Ridge National Laboratory
de Almeida, Valmor – Oak Ridge National Laboratory
de Jong, Wibe "Bert" – Pacific Northwest National Laboratory
Dellis, Christophe – French Atomic Energy Commission
Diachin, Lori – Lawrence Livermore National Laboratory
Dixon, David – University of Alabama
Dorr, Milo – Lawrence Livermore National Laboratory
Downar, Thomas – Purdue University
Dunn, Michael – Oak Ridge National Laboratory
Dzodzo, Milorad – Westinghouse
Ecker, Lynne – Brookhaven National Laboratory
Endres de Oliveira, Cassiano – Georgia Institute of Technology
Estep, Donald – Colorado State University

Finck, Phillip – Argonne National Laboratory
Fischer, Paul – Argonne National Laboratory
Fitzsimmons, Timothy – U.S. Department of Energy
Foster, Ian – Argonne National Laboratory
Garaizar, Xabier – Lawrence Livermore National Laboratory
Gehin, Jess – Oak Ridge National Laboratory
Gianoulakis, Steven – Sandia National Laboratories
Glimm, James – Stony Brook University
Goldner, Frank – U.S. Department of Energy
Goodwin, Dave – U.S. Department of Energy
Gougar, Hans – Idaho National Laboratory
Gropp, Bill – Argonne National Laboratory
Hansen, Glen – Idaho National Laboratory
Hansen, Charles – University of Utah
Hardin, Angela – Inside Energy
Harrison, Robert – Oak Ridge National Laboratory
Hendricks, John – Los Alamos National Laboratory
Ingersoll, Daniel – Oak Ridge National Laboratory
Ishikawa, Makoto – Japan Atomic Energy Agency
James, Scott – Sandia National Laboratories
Johnson, Gary – U.S. Department of Energy
Johnson, Peter – U.S. Department of Energy
Kahn, Ehsan – U.S. Department of Energy
Kaji, Yoshiyuki – Japan Atomic Energy Agency
Kale, Laxmikant – University of Illinois at Urbana-Champaign
Kennedy, Ken – Rice University
Keyes, David – Columbia University
Khalil, Hussein – Argonne National Laboratory
Kikuchi, Shin – Embassy of Japan
Kim, Seokho – Oak Ridge National Laboratory
Kirby, Robert – University of Utah
Kneisly, William – International Business Machines Corp.
Knepley, Matt – Argonne National Laboratory
Knoll, Dana – Idaho National Laboratory
Kothe, Doug – Oak Ridge National Laboratory
Kouzes, Richard – Pacific Northwest National Laboratory
Kramer, William – Lawrence Berkeley National Laboratory
Kugo, Teruhiko – Japan Atomic Energy Agency
Levendahl, Kirk – U.S. Department of Energy
Long, Kevin – Sandia National Laboratories
MacKinnon, Robert – Sandia National Laboratories
Mailhiot, Christian – Lawrence Livermore National Laboratory
Martin, Dan – Lawrence Berkeley National Laboratory
Martin, William – University of Michigan
Martineau, Richard – Idaho National Laboratory
McCallen, David – Lawrence Livermore National Laboratory
McCarthy, Kathryn – Idaho National Laboratory
Meakin, Paul – Idaho National Laboratory
Meredith, Jeremy – Oak Ridge National Laboratory
Minato, Kazuo – Japan Atomic Energy Agency
Mompean, Federico – Organization for Economic Cooperation and Development

Morel, Jim – Texas A&M University
Morgan, Hal – Sandia National Laboratories
Morgan, Dane – University of Wisconsin
Mousseau, Vincent – Idaho National Laboratory
Nakajima, Norihiro – Japan Atomic Energy Agency
Negrut,Dan – University of Wisconsin
Ng, Esmond – Lawrence Berkeley National Laboratory
Nichols, Jeffrey – Oak Ridge National Laboratory
Nowak, David – Argonne National Laboratory
Nukala, Phani – Oak Ridge National Laboratory
Oberkampf, William – Sandia National Laboratory
O'Leary, Patrick – Idaho National Laboratory
Ott, Larry – Oak Ridge National Laboratory
Ougouag, Abderrafi – Idaho National Laboratory
Palmiotti, Giuseppe – Argonne National Laboratory
Pannala, Sreekanth – Oak Ridge National Laboratory
Papka, Mike – Argonne National Laboratory
Parks, Cecil – Oak Ridge National Laboratory
Parsons, Ian "Dennis" – Lawrence Livermore National Laboratory
Pasquali, Matteo – Rice University
Pernice, Michael – Los Alamos National Laboratory
Peters, Mark – Argonne National Laboratory
Pieper, Gail – Argonne National Laboratory
Pierpoint, Lara – U.S. Department of Energy
Ragusa, Jean – Texas A&M University
Ray, Jaideep – Sandia National Laboratory
Reardon, Bradley – Oak Ridge National Laboratory
Reed, Phillip – U.S. Nuclear Regulatory Commission
Regalbuto, Monica – Argonne National Laboratory
Roche, Kenneth – Oak Ridge National Laboratory
Salari, Kambiz – Lawrence Livermore National Laboratory
Salvatores, Massimo – French Atomic Energy Commission
Samulyak, Roman – Brookhaven National Laboratory
Schraad, Mark – Los Alamos National Laboratory
Schwartz, Peter – Lawrence Berkeley National Laboratory
Sekine, Yukiko – U.S. Department of Energy
Shadid, John – Sandia National Laboratory
Shephard, Mark – Rensselaer Polytechnic Institute
Shoshani, Ari – Lawrence Berkeley National Laboratory
Siegel, Andrew – Argonne National Laboratory
Simon, Horst – Lawrence Berkeley National Laboratory
Simos, Nikolaos – Brookhaven National Laboratory
Simunovic, Srdjan – Oak Ridge National Laboratory
Smith, Barry – Argonne National Laboratory
Sood, Avneet – Los Alamos National Laboratory
Spada, Mary – Argonne National Laboratory
Stan, Marius – Los Alamos National Laboratory
Stevens, Rick – Argonne National Laboratory
Stocks, Malcolm – Oak Ridge National Laboratory
Stoller, Roger – Oak Ridge National Laboratory
Strickland, James – Sandia National Laboratories

Summers, Randall – Sandia National Laboratories
Takase, Kazuyuki – Japan Atomic Energy Agency
Tang, William – Princeton Plasma Physics Laboratory
Tautges, Timothy – Sandia National Laboratories
Todd, Terry – Idaho National Laboratory
Todreas, Neil – Massachusetts Institute of Technology
Tulenko, James – University of Florida
Turinsky, Paul – North Carolina State University
Turner, John – Los Alamos National Laboratory
Uddin, Rizwan – University of Illinois at Urbana-Champaign
Urbatsch, Todd – Los Alamos National Laboratory
VanderHeyden, William – Los Alamos National Laboratory
Wagner, Albert – Argonne National Laboratory
Wagner, John – Oak Ridge National Laboratory
Wilson, Alyson – Los Alamos National Laboratory
Wilson, Paul – University of Wisconsin
Wojtkiewicz, Steve – University of Minnesota
Wolf, Dieter – Idaho National Laboratory
Worley, Patrick – Oak Ridge National Laboratory
Yoder, Graydon, Jr. – Oak Ridge National Laboratory
Zachmann, David – Colorado State University
Zidel, Cheryl – Argonne National Laboratory
Ziebarth, John – Krell Institute
Zinkle, Steven – Oak Ridge National Laboratory

Bibliography

- The Path to Sustainable Nuclear Energy – BES Workshop Report (Sept. '05) – *http://www.sc.doe.gov/bes/reports/files/PSNE_rpt.pdf*
- Advanced Simulations: A Critical Tool for Future Nuclear Fuel Cycles Workshop – Livermore (Dec. 2005) – *http://eed.llnl.gov/nuclear_workshop*
- SCaLeS – *http://www.pnl.gov/scales*
- SCaLeS 2 – *http://www.mcs.anl.gov/~gropp/bib/reports/scales2-2005.pdf*
- International Workshop on Advanced Computation Materials Science: Applications to Fusion and Generation-IV Fission Reactors (March 31-April 2, 2004) – *http://www.csm.ornl.gov/meetings/SCNEworkshop/DC-index.html*
- GNEP Site – *http://www.gnep.energy.gov/default.html*
- Whitepaper on Modeling and Simulation in Support of GNEP – *http://www.mcs.anl.gov/anes/smanes/NE Needs in Modeling and Simulation.pdf*
- Simulation – Based Engineering Science – Revolutionizing Engineering Science through Simulation, May 2006 Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science – *http://www.ices.utexas.edu/events/SBES_Final_Report.pdf*