

1.0 Modeling and Simulation in Support of GNEP

Modeling and simulation has always been a key tool in nuclear engineering. From the earliest times primitive computers were used to obtain predicted quantities through interpolation of experimental data. More recently, computer based analyses have been used to predict in detail quantities that could not be readily measured *in situ*, for example the aging of structures, power distributions in cores, transient safety behavior, etc. Until the early 80's nuclear engineering was at the forefront of computer applications, making massive use of the largest machines available at the time. Nevertheless, these machines remained very limited when compared to the requirements for an explicit modeling of key phenomena in a reactor. Thus, the codes developed at the time were rather simplified, using lumped parameter models for predictions of neutronics, thermohydraulics, and structural mechanics quantities. These codes were validated on a very large experimental database, developed over the years for specific projects. The validation process used at the time was coarse, as it could only compare macroscopically measured data and macroscopically calculated quantities. Frequently the validation process consisted of simply comparing these experimental and calculated quantities as the tools and techniques available for a more formal validation process were missing.

These same tools are the ones available for the GNEP project today, and constitute the starting point for design activities. We expect that their use will lead to significant negative consequences for the projects. There are three principle reasons for this assessment -- first, the validation process needs to be repeated with more formalism, even though this might not be possible due to the disappearance or lack of documentation for the experimental data. Furthermore, these tools are embedded with many approximations and uncertainties that eventually lead to significant cost increases for the projects. Finally, modeling tools available for researchers in critical areas, in particular for the development of advanced fuels, are not predictive, and force a research approach that is largely empirical, and therefore expensive, lengthy, and extremely risky. There is a broad consensus that a project guided by good science embedded in modern simulation tools has a much higher probability of success.

Preliminary evaluations of the critical areas where modern simulation tools are required for the success of GNEP have been undertaken over the past few months, in particular during workshop held December 2005 at LLNL. The following list, while it is not exhaustive, provides key priorities:

- Core simulation tools (neutronics, thermohydraulics, structural mechanics) need to be updated and validated to give accurate and trustworthy predictions of plant behavior during normal, incidental, and accidental conditions.
- Fuels and materials behavior models need to be build to enable acceleration of the research process in these two critical areas, and significantly increase the probability of success.

Subsequent discussions have also identified the need for organizing a staged development process, whereby critical needs would be met in a timely manner to satisfy project needs in the short, medium, and long term.

The GNEP simulation plan below includes a detailed list of the major simulation goals of the project together with a framework for identifying and prioritizing specific simulation targets during the course of the GNEP program. This section is organized as follows: 1) a background

and overview of the opportunities presented by advanced simulation; 2) a methodology and framework for prioritizing simulation activities; 3) GNEP simulation goals, and 4) a list of additional domain-specific simulation opportunities within the GNEP framework. This will be done in close collaboration with the DOE's Office of Science.

1.1 Opportunity

Computer simulation addresses critical needs of the GNEP program in providing the tools necessary for safety calculations, design activities, cost, and risk reduction. Existing tools based on a large experimental database are likely to be insufficient. For most of the technologies related to the three major GNEP demonstration technologies, testing is an extremely expensive, protracted, and in some cases unfeasible process. Furthermore, the existing experimental database is insufficiently documented to support a modern validation process. Complementing or replacing testing with high-fidelity computer simulation will make it possible to collect simulated data that can, in conjunction with sound experimental validation program, be used to understand fundamental processes that affect facility efficiency, safety, and cost. One can, for example, imagine virtual prototyping of reactor cores yielding data that leads to more accurate identification of design margins, allows early experimentation with novel design concepts, and ultimately significantly reduces plant certification timelines. In other areas, such as advanced fuel fabrication, atomistic fuel simulations could ultimately make it possible to target a small subset of promising candidate fuel types for further experimentation, greatly reducing the number of experiments to be performed.

Such simulation-based methods are within the reach of modern supercomputers, which currently are approaching a peak theoretical performance of one petaFLOP/s, about five orders of magnitude faster than a standard desktop computer. In fact, other related industries, such as automotive, airline, chip manufacturers, etc. have demonstrated the effective use of high-fidelity modeling (viz. computational fluid dynamics) as an integral part of the conceptual design and optimization process. Related industries are making remarkable progress in reducing experiments in favor of high-end simulation – e.g. pharmaceuticals, engine design, turbines, etc. It is clear that we have only scratched the surface of what is possible in the application of advanced simulation to nuclear engineering.

Of course, over the past twenty five years, simulation tools have been in common use among nuclear engineers in a wide range of applications. However, as discussed, most of these can be considered legacy tools that were conceived and developed over twenty years ago, when available computer power that was approximately five orders of magnitude less than current state of the art. Equally importantly, over that period significant advances have been made in enabling technologies to more easily leverage this performance. With the tremendous computing power currently available in the form of modern supercomputers (e.g. IBM BG/P, Cray XT3), radical new approaches can be taken that were previously unthinkable. In many cases, leadership class computers can be used to calculate first-principles-based physics on very fine meshes, yielding results with accuracies much greater than current techniques, or with the ability to predict new scenarios that have not been directly tested. In other cases (e.g. molecular dynamics simulations), it is possible to implement completely new techniques now that were inconceivable or impractical twenty years ago. A detailed discussion of the simulation opportunities is given in Section 6.4.

1.2 Organization

While it is possible to identify early candidate simulation projects with high potential payback (see introduction and next section), the detailed process of downselecting and prioritizing will need to be done in the early phases of the project, in close collaboration with the facilities leads,

and to some degree dependent on funding levels. For this reason, we have devised a methodology whereby simulation effort will be organized as a close collaboration between the engineers designing the GNEP facilities and computational scientists, computer scientists, and applied mathematicians who are experts in various aspects designing numerical software and large application codes for leadership class supercomputers. This will be an iterative decision-making process. Facilities designers formulate short and long-term simulation goals to directly address areas that would greatly impact their engineering and scientific goals. Computational modellers help identify barriers to performing such calculations and assist in prioritizing simulation goals, identifying potential “low-hanging fruit”, and articulating specific short and long-term scientific and engineering target problems. For longer-term, more fundamental R&D on the target problems will include significant advancements in underpinning technologies, include helping to define next-generation computing architectures in support of GNEP, scalable numerical methods and algorithms, advance visualization, i/o, data management, in addition to more scientific and modelling challenges (see below). For shorter-term goals the strong emphasis will be on immediate validation and verification of results, definition of supporting experiments, and channeling results into particular GNEP technologies. An absolutely critical component of this model is the formation of a team responsible for ensuring that all development efforts, on whatever timescale, feed into particular GNEP facilities needs and timelines, and therein clearly demonstrate improvements in the above-mentioned areas. Furthermore, while the tools initially will be used for facility designers, as they mature a process will need to be developed of knowledge and technology transfer to appropriate certification agencies for ultimate adoption and incorporation into their process.

In the following section we prioritize our simulation needs based on overlapping short, medium and long-term goals.

1.3 Objectives

Within this framework, the emphasis will be placed on the components most directly supporting the ESD, ABTR and AFCF facilities. Since one of the overarching goals of the simulation program is the development of a suite of software tools that will enable quantification of margins of uncertainty to aid and accelerate the licensing of new reactor systems, the simulation program will engage and collaborate with the research branch of the Nuclear Regulatory Commission at an early stage to position the program for appropriate levels of engagement in the future.

1.3.1 Short-Term Objectives

The short-term goal of the Modeling and Simulation activity is to advance the development of the three major GNEP demonstration facilities, the ESD, ABTR, and AFCF. Improved engineering simulation tools, based on existing modeling codes, software infrastructure and knowledge discovery (e.g., visualization, feature identification) applications, will be created via the integration of existing capabilities and focused on advancing the deployment of the facilities. Tool specifications will be developed in close collaboration with the leads for the three major demonstration projects to ensure that the resulting suites will benefit the development of the facilities. Existing capabilities will be examined, and the most promising will be chosen for integration. Tool development will look to utilize the advances in computing technologies as well as leveraging previous work from programs such as ASC, SciDAC, and TeraGrid. The need for new numerical algorithms and other enabling technologies will be assessed in terms of the facility needs to provide guidance for the intermediate and long-term objectives. It is also important to begin initial development of a GNEP enterprise level planning tool. While this tool will lack

maturity in the early stages of GNEP development, it nevertheless will provide useful direction to the overall program.

The leads for each of the demonstration facilities will determine the modeling applications upon which they will rely for the successful construction of their facilities. The work processes of the participants in each activity will be carefully examined to obtain an accurate workflow description of the modeling activities. Traditionally, this is a series of independent operations that the analyst must individually combine. The examination will cover the specifics of which applications require input from others, in what formats, and how the data is currently transmitted. There will also be an analysis of the manner in which the suite of applications is used (e.g., multiple flux calculations being performed on a given geometry, or different geometries examined with similar fuel loadings). The end-to-end analysis process will then be examined, looking for opportunities for efficiency improvement. Many of the data transmission steps, sensitivity analyses via parameter variation, model input construction steps, and results analyses will lend themselves to modernization capabilities that have been developed and implemented by other programs. Once the steps of the process and work flow are understood, efficiency and performance optimization will be examined to determine which will provide the greatest benefit to the facility construction process.

For the ABTR, the priorities have been determined to be the thermal hydraulics and structural mechanics components. The ESD requires the current modeling code to be fully integrated with minimally a static, but preferably a dynamic, plant model in order to accommodate non-equilibrium events within the facility. ESD also desires a substantial improvement in the usability of the ESD modeling suite. An equivalent analysis with the AFCF lead will provide a similar set of facility-oriented priorities. These priorities will drive the efforts in the workflow analysis and process improvement.

A formal validation process also needs to be established within the GNEP project to bring the full benefits of modern simulation capabilities to the design and safety of the facilities and the research and development process. The purpose of the validation process is to provide for each calculated quantity an estimated uncertainty that takes into account all possible sources of uncertainties in the analysis, and integrates them for each particular situation.

Several approaches have been used in the past in the nuclear area; they range from the very rudimentary to the somewhat sophisticated:

- The rudimentary approach has historically consisted of taking a code – developed to whatever level of sophistication – and compare its output to data from a set of representative experiments. The uncertainties are then estimated on the basis of the comparison. This process does not distinguish the origins of uncertainties and biases, and gives only a vague definition of the domain of validity.
- More advanced approaches have been developed, for example in neutronics and structural mechanics, where reference codes (that provide exact solutions to the basic equations) exist and can be used to estimate numerical biases; uncertainty propagation techniques have been developed, and have been used to estimate the final uncertainties due to nuclear data or mechanical properties. Finally, formal statistical processes have been developed to formally compare integral experimental data and predictive results.

These processes are not satisfactory, as they do not provide absolute confidence in uncertainty predictions. Furthermore, it seems likely that the experimental database currently available is insufficiently documented to support a formal modern validation process. Finally, it is also likely

that this database is incomplete and does not contain sufficient experimental data to validate codes capable of very detailed modeling of key phenomena.

Modern methods need to be developed in the very short term that incorporate tools such as formal uncertainty propagation techniques, statistical analyses of experimental data, and reference codes that minimize the effects of modeling approximations. Additionally, GNEP will need to acquire and analyze a complete experimental database for validation of the new or updated analysis tools. While these experimental needs have not yet been determined, a formal process will be put in place to do this, and this will include as a first step the analysis of the existing database.

1.3.2 Intermediate-Term Objectives

In addition to the codes adopted within the short-term objectives described previously, an analysis will be performed for other existing codes that may provide value but are not currently in general use within the nuclear industry. In particular, these codes could serve to bring additional functionality to the short term efforts without having to rely on the results of the longer-term research activities. Limitations of the existing nuclear code suite will be used to identify possible candidates for inclusion. Once these codes have been identified, verification and validation activities will then define the breadth and depth of possible inclusion into the Modeling and Simulation activity.

There are several possible candidates for this activity already identified by the ABTR and ESD facility leads. The ABTR could utilize higher fidelity thermal hydraulics simulations than those currently achievable using commercial CFD applications. These commercial codes do not scale to the levels required by nuclear reactor models simply because there is currently little market for such applications. Hence, replacing the commercial thermal hydraulics code with one capable of greater spatial resolution and execution in a modern HPC environment would bring greater confidence to the simulation results. Structural mechanics is another area of the ABTR modeling where the capabilities of existing commercial codes are too limiting. Replacement of these commercial codes with those from the DOE community would again contribute to higher confidence in simulation results. Finally, the ESD design work would benefit from the coupling of the existing model with a dynamic plant model that would calculate the effects of transients with the facility. The ESD would also benefit from greater ease-of-use, another straightforward application of modern computing experience.

The integration of the previous model assessment and development work will define the intermediate-term goal to establish an efficient “end-to-end” modeling architecture. Consistency of cross-model assumptions, data, and approaches will be essential for the success of the long-term, large-scale modeling efforts. This is especially true when data and models address phenomena across vastly different scales, with the results of one calculation becoming the input of another. A set of sub-model requirements based on physical constraints, prediction accuracy, and technical and computational consistency within an integrated approach will be defined.

1.3.3 Long-Term Objectives

The long-term goal for the simulation program is the development of an architectural model that will facilitate modeling the entire fuel cycle from mining through final disposition of waste material, taking into account interacting factors that are key to the ultimate success of GNEP (e.g., market forces, socio-political effects, technology risk). This will facilitate the implementation of a comprehensive suite of simulation tools for the design, analysis and engineering of next-generation nuclear energy systems with enhanced safety, reduced environmental impact, optimal deployment of facilities, and reduced construction cost. To

achieve this long-term goal, the GNEP simulation program must address the following areas of research and development:

- Integrated 3D reactor core simulations with rigorous propagation of uncertainty
- Coupled thermal hydraulic and primary loop simulation
- Advanced fuel design and performance
- Fuel behavior engineering
- Advanced secondary loop and balance of plant engineering and analysis
- Advanced fuel cycle design
- Separations facility engineering optimization
- Repository design including seismic, geological, chemical, and thermal modeling and simulation
- Overall nuclear energy systems model development suitable for alternative economic analysis.

1.4 Fuel Cycle Elements

This section provides further details on the specific simulation opportunities and challenges that exist for each component of the fuel cycle.

1.4.1 Material Properties

Simulation of basic material properties is the area with the greatest potential for progress and return on investment. Simulations that cover the full fuel cycle will require the ability to treat a wide range of materials and material behaviors across the full range of scales from atomistic to reactor system. Material properties, including nuclear (e.g., reaction cross sections), thermophysical (e.g., thermal conductivity, multi-component phase diagrams), mechanical (e.g., tensile properties, fracture toughness), and chemical (e.g., corrosion rates), must be determined under static, transient, and accident conditions and after irradiation (e.g., radiation-induced hardening, swelling, and embrittlement).

The fuel selection process is an example that illustrates the possible gain. In the design of a reactor, fuel definition along with the choice of coolant is always the first step that then determines the subsequent components of the system. The traditional approach requires fabrication of samples or pins of the new fuel, measurements of physical and mechanical properties, and finally neutron exposure to high fluence under relevant operating conditions with subsequent characterization. This approach requires a great investment of money and time (several years). In some cases, the choice of fuel may have become obsolete or irrelevant as a result of programmatic considerations before the experimental evaluation is complete. A similarly long process is required for the structural materials involved in the fuel pin cladding and other critical in-core components. Modern methods and powerful computing tools are expected to speed the evaluation and selection of advanced fuels and structural materials.

Use of several materials simulation methods will be essential. For example, first principles methods such as quantum density functional theory (DFT) can now realistically be used to determine fundamental material properties, augment experimental information on the phase diagram of multi-component actinide alloys and compounds, predict chemical reactivity and material compatibilities, and support the development of new interatomic potentials that can be used in Molecular Dynamics (MD) simulations involving millions of atoms. The MD simulations can then be used to study defect properties and to determine parameters such as the atomistic reaction rates that are required in coarser scale simulations of degradation mechanisms that take

place over long periods of time. These parameters can be employed in reaction rate theory or Kinetic Monte Carlo (KMC) models of microstructural evolution. MD-based dislocation dynamics simulations can also provide the fundamental dislocation-defect interaction parameters required for continuum 3D Dislocation Dynamics (DD) simulations. The 3D DD simulations can then be used to obtain needed information on the constitutive behavior of the materials which is required for use in macroscopic methods such as finite element models of defect interaction and long term defect stability, as well as simulation of behavior under irradiation. Taken together, this family of multi-scale simulations can provide predictions from the atomistic and microscopic through to the mesoscopic and macroscopic levels.

Initial goals will be to determine the set of material properties and behaviors of concern, along with the range of conditions under which these need to be known, and to establish the required degree of accuracy and practical limitations at each level of simulation. This will provide a basis for predicting the expected impact of an advanced simulation program to reduce both the absolute development time and the related uncertainties as part of the overall fuel and materials development effort. The initial technical objectives should include a strategy for determining the best approach for integrating the various multi-scale components (i.e., when to use parameter passing and when models should be more tightly coupled). Verification and validation steps will need to be an integral part of this strategy.

1.4.2 Fuel Behavior

Fuel performance modeling places an emphasis on the detailed understanding of the thermal, mechanical, physical, and chemical processes governing fuel rod behavior during normal reactor operation and under accident conditions. Fuel rod performance codes are used extensively in research, by fuel vendors, and by licensing authorities for the prediction of fuel and cladding performance.

A fuel performance code should consist of a clearly-defined mechanical-mathematical framework into which physical models can be easily incorporated. In addition to its use for fuel rod design, the code will be utilized for a wide range of different situations such as the simulation of under-normal, off-normal, and reactor accident conditions. The time scale of the problems may range from milliseconds to years.

All important physical models will be included in the fuel performance code, including models for thermal and irradiation-induced densification of fuel, fuel swelling due to solid and gaseous fission products, fuel creep and plasticity, pellet cracking and relocation, fission gas release, oxygen and plutonium redistribution within the fuel, volume changes during phase transitions, formation and closure of center void and treatment of axial forces (between the fuel and cladding), cladding creep and cladding/coolant interactions (such as oxidation), etc.

Additionally, the code must have access to a comprehensive material database for oxide, mixed oxide, carbide, nitride, and inert matrix fuels, and Zircalloy (and advanced zirconium alloys) and steel cladding (with the capability to add new fuel forms and advanced cladding). Also, interfaces must be available for thermal hydraulic and neutronics feedback to the fuel performance models.

Code verification and validation (V&V) of the mechanical-mathematical framework will be accomplished by comparing code output to exact solutions and by comparing results from different solution techniques. Other assessments will include validation of single-physics models, code-to-code comparison benchmarks, and comparison with experiment for multi-physics validation.

1.4.3 Neutronics

The scope of applications for future neutronics modeling will need to address all reactor physics aspects related to the design, operation and fuel cycle management for reactor systems developed under GNEP. Many computational tools exist for performing stand alone analyses of core reactivity, power production, fuel burn-up, shielding design, and ex-core criticality safety. The challenge is to address each of these analyses in an integrated, self-consistent framework.

The analysis of neutronics for complex systems requires a very high degree of sophistication for the description of the geometry and for physically realistic representation of the energy dependence of neutron cross section data used for modeling. The availability of accurate cross sections and their temperature dependence is necessary for modeling the various aspects of neutron transport and interaction within highly heterogeneous reactor cores. An assessment of pertinent cross section data available through ENDF (Evaluated Nuclear Data Files) and other sources should be performed to determine additional needs for experimental and theoretical nuclear physics work to support the establishment of an adequate nuclear data base for GNEP applications. A comprehensive assessment would also include photonuclear reaction cross sections and cross sections for relevant charged-particle interactions.

Neutronics modeling has traditionally relied on both stochastic (Monte Carlo) simulations and deterministic transport and diffusion theory approaches. Monte Carlo techniques incorporate the basic physics at the level of stochastic particle tracking with the general system geometry and material cross sections governing the particle track histories. Monte Carlo offers the strong conceptual advantage of keeping a close (essentially exact) correspondence between computational and physical geometric and cross section energy dependence models. Nevertheless, Monte Carlo can become computationally impractical for several different classes of problems. These include calculations of small reactivity coefficients, some types of sensitivity/uncertainty propagation studies, time-dependent solutions, and some types of burn up calculations.

For these applications, as well as for several other aspects of neutronics analysis, computational advantages can be achieved with deterministic transport and diffusion theory approaches that complement the Monte Carlo approach. The two basic computational methods, taken together, can provide a much more comprehensive picture of the neutronics aspects of nuclear reactor system behavior than either method alone. The deterministic approach may also be favored by the need for coupling the neutronics models with other deterministic models (e.g., thermal hydraulics system models) with which data is dynamically shared, and in fact neutronics models are ideally organized from the outset to take advantage of inherent couplings of neutronic behavior to the thermal hydraulic, structural, and possibly the radiochemical behavior of the reactor system. Existing and improved stand alone models should be adapted to ultimately serve as sub-models within a multi-physics, multi-scale, and probably multi-processor approach. The goal is to provide reactor concept design tools that can predict the overall impact of the neutronics on the system as a whole (e.g., plant operations, safety analysis, economics and efficiency) by computing a coupled multi-physics simulation of the underlying behavior with all relevant feedback mechanisms taken into account.

1.4.4 Thermal Hydraulics

Existing reactor core thermohydraulics codes use the traditional single-channel or sub-channel approach to model reactor core heat transfer. This is clearly inconsistent with the goal of a first principle type of methodology that this project is pursuing. The advantage of a more first-principles based approach is the ability to generate data for a much greater range of conditions

than is possible with empirically based codes. The latter depend greatly on using empirical correlations of global quantities that are valid only for the specific designs for which they were tested – that is, they have very little true predictive capability. A general thermal hydraulics tool has to be capable of treating both single-phase and multi-phase fluid flows in coolants ranging from gas to liquid metal. For the purposes of the ABTR, in normal operating conditions single phase incompressible fluid models are adequate, but these must be augmented with multiphase and free convection models for accidental scenarios (coolant exposure, pump shutdown, etc.). Additionally, both steady state and transient solutions are required for the full range of phenomena to be studied.

Computational fluid dynamics (CFD) is the general terminology for the numerical solution of the Navier-Stokes equations. If solved using direct numerical simulation (DNS), the Navier-Stokes equations can represent all regimes of flow from laminar to fully turbulent. Since even the largest and fastest computers available today are not capable of solving the full range of energy transferring scales in a fully turbulent flow, some degree of physics approximation is still required even with this technique, and thus some experimental insight for modeling and validation is needed. A CFD approach can, however, be adopted to achieve the degree of accuracy and confidence that are essential parts of the scopes of this project, provided that the computational burden stays reasonable and that results obtained with this methodology can be physically validated.

For a better understanding of the physics behind the single-phase operational mode of reactors, we can couple high performance stochastic and deterministic neutronics tools to coupled incompressible flow and thermal transport tools. The goal is to model in three dimensions, with fine resolution, the local- to global-scale effects for a representative reactor core rod bundle in operational mode. For the simple channel flow of a rod bundle, the code structure of choice may be a structured grid with adaptive mesh refinement. For more complex geometry and piping, an unstructured grid CFD tool may be preferred.

The analyses of accident scenarios pose additional challenges. An accident scenario in a liquid-cooled reactor usually results in boiling or voiding of the coolant and condensation of liquid on cold structures. The excess temperatures and voiding of coolant can cause melting of fuel and cladding. All of these processes are transient, have strong, nonlinear feedback effects on fluid displacement, and the whole process can occur in seconds. The current approach to the analysis of accident scenarios is through the use of semi-empirical tools with adjustable parameters and models determined from experiment. An analysis based on first principles would require multiphase, multi-component fluid dynamics with variable core geometry and the characteristics of the fluid dynamics would vary through initiation to the final stages of the accident.

There are a number of research challenges that must be addressed to design an efficient and accurate modeling tool. The current capabilities for solving incompressible and compressible flow must be extended to the regimes that exist in nuclear reactors with large temperature variations. The high-order-accurate solution of the Navier-Stokes and heat transfer equations in fluid regimes can be coupled to high-order-accurate solution of heat transfer in solid regimes. These schemes can be extended to use adaptive mesh refinement, and the coupled scheme must be scalable on parallel computers. The coupling of the flow and heat transfer models to the neutronics tools will require research into ways to couple these models which are solved on different grids and evolve at different time scales. Considerable work will be required to develop effective techniques to verify and validate the approach. Through the use of structured and unstructured grids and high-order accurate methods resulting schemes will be very efficient and will allow the rapid evaluation of various design and accident scenarios.

1.4.5 Structural Mechanics

Structural mechanics software development has been driven by a breadth of applications over the last thirty years which include aerospace, national defense, civil infrastructure, and, in the 70's and 80's, nuclear reactor technology. These developments have led to a number of finite element based computer programs that have mature element technologies and solution algorithms.

Existing software that has application relevance in the nuclear fuel cycle area can generally be divided into three categories: linear finite element programs, implicit time integration nonlinear finite element programs, and explicit time integration nonlinear programs. In addition to the general-purpose structural mechanics software just mentioned, the nuclear power industry has a unique need to incorporate soil-structure-interaction (SSI), whereby the coupling between massive concrete containment systems and the surrounding supporting soil is accounted for in earthquake response simulations. Special purpose linear, frequency domain programs were developed in the 70's specifically to simulate SSI effects, and these programs are still the standard tools today. The existing SSI programs typically must idealize the nuclear plant superstructure with very simplistic structural models in order to arrive at reasonably executable models.

In terms of future advancements, 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 should address the effects of high radiation levels, extreme temperatures, and chemical interactions on material behavior. Advanced materials models should account for the fully 3D, multi-axial states of stress both at low strain rates (normal operations), and at high strain rates (accident scenarios). The development of macroscopic, continuum based phenomenological models must progress in parallel to fundamental materials science research aimed at understanding microscopic material behavior in extreme environments. It is essential that the materials science community work hand-in-hand with the structural mechanics community to ensure that constitutive models represent an appropriate balance between characterization of material behavior and numerical efficiency and stability in finite element implementations.

Recent developments in solid/structural mechanics have moved towards a merging of capabilities from traditional solids hydro-type codes, which have pushed the computational technologies for representing extreme deformations and flow of materials, with traditional structural type elements. Such codes have been developed in frameworks that prevent mesh tangling at extreme ranges of response. This has begun to open up substantially the types of problems that can be modeled for extremely nonlinear accident scenarios. Pushing these developments towards a logical conclusion, it would be very desirable to move towards a single program that can solve multiple problems associated with slow (static and quasi-dynamic) phenomenon associated with operations, slow accidental events like earthquakes, and also accurately simulate extreme accidents associated with very rapid transients such as pipe breaks.

Direct coupling of multi-physics codes can result in more realistic representations of actual behavior and eliminate the need for grossly-approximated hand-offs between codes representing different physics. There are two areas where coupling of structural mechanics codes can enhance existing capabilities. In reactor analysis, vibrations induced by fluid structure interactions can be a problematic design issue. Explicit coupling of CFD and structural mechanics codes would be useful in rigorously modeling and addressing this issue. Coupling between neutronics and structural mechanics codes would also permit the effects of radiation on materials to be explicitly represented for various structural components. The neutronics coupling would allow direct, time-dependent integration of the effects of radiation on the embedded materials models.

With the advent of high performance computers, a rigorous, fully coupled simulation of a combined soil-structure system is within our computational grasp. With appropriate development of an interface model between the soil and the structure foundation, it would be feasible to execute a time domain simulation, including nonlinearities in the soil and superstructure, with a fully 3D detailed model of the superstructure. Such an analysis would bypass the coarse idealizations of the superstructure system currently embedded in typical SSI simulations.

1.4.6 Balance of Plant

Balance of plant (BOP) modeling (e.g., piping, valves, heat exchangers, pumps, power conversion units, and reactor containment systems) is required during the plant design in order to determine system operating parameters and performance, as well as to perform overall reactor system design optimization. Reactor control system design and development must also include simulation of the balance of plant systems. Finally, reactor safety analysis must include a balance of plant simulation in order to provide appropriate boundary conditions to the reactor core during transient events.

Traditionally, the codes used to perform these simulations have been independent, with minimal overlap of component simulation algorithms. An overall objective of this task is to develop high fidelity balance of plant simulations that can be used for both design and safety analyses and that can be easily used to investigate multiple design options. BOP simulations will require the capability of modeling multi-dimensional fluid flow, natural circulation, and transients in order to effectively simulate BOP performance. The application must be capable of using code and input uncertainties to quantify uncertainties in reactor limits, and it must have a complete validation and verification package developed. Longer-term requirements include those discussed above, plus the capability of investigating multiple BOP and power conversion system types, highly-detailed component simulations, the ability to operate on next generation computational platforms, multi-physics interfaces, and the ability to verify and validate the algorithm.

Near-term objectives focus on supporting the ABTR deployment effort and include the development of a requirement set for BOP simulation, evaluation of existing BOP simulation methodologies, component models, etc., and a down-selection of the most appropriate methodology or methodologies. Intermediate-term objectives include development of appropriate interfaces with the design/optimization, instrumentation and control, and safety codes, integrating the BOP methodologies into this code or codes, identifying existing data to benchmark BOP simulations, outlining additional data that is required to complete benchmarking, and developing a validation package for the BOP simulation to use in ABTR licensing arguments. Long-term objectives include developing a fully integrated BOP simulation package that can be used across all technical areas that is flexible enough to incorporate multiple high fidelity process designs (e.g., Rankine cycles, Brayton cycles, multiple heat exchanger designs, and multiple control designs), porting to high performance parallel computational platforms, developing interfaces with other design physics codes, and developing a validation package appropriate for licensing applications. This effort will support reactor system design, instrumentation and control, and safety analysis, providing a more consistent and high fidelity analysis package that will be effective across multiple disciplines.

1.4.7 Separations Processes

Modeling of a separations process involves many complicated steps, each of which requires knowledge of several areas of physics, chemistry, or engineering. Fuel disassembly involves mechanical processes (chopping, and filtering) and/or chemical dissolution in strong acid. The fuel solution is then passed through many stages of solvent extraction in order to separate several

fission product and actinide streams. Several separate, solvent extraction processes are required to accomplish this separation, each using different additives and components in the organic phase, as well as different acid concentrations in the aqueous phase. Safety considerations require monitoring of volatile fission product and organic gaseous releases, careful evaluation of component inventories in each stage and even in piping, to avoid costly shutdowns or repairs which must be performed remotely, strict attention to nuclear criticality safety in actinide solutions with widely varying component inventories, and control systems which are based on realistic models of processes, not generalizations or even intelligent assumptions. The hazards of plant operation involve radioactive materials, toxic materials, strong acids, highly flammable materials, and highly volatile materials. Thus, detailed accounting of all components through all process stages is of utmost importance.

Current reprocessing models provide only qualitative descriptions of process behavior. Empirical models of chemical behavior for major components are used to provide overall descriptions of various reprocessing strategies. These empirical models are based on benchtop experiments, and usually assume chemical equilibrium conditions are met instantly. Even then, current models are unable to answer many questions involving phase equilibria, such as precipitation from solution or determining oxidation states, where multiple possibilities exist. Very few reaction rate constants are known, and wherever transient conditions are simulated, they are usually just assumed or selected heuristically.

Hence, in order to support both detailed design and safe operation, the improvement of models for separations processes requires improved chemistry modeling, including both equilibria and kinetics. New fuel materials and requirements arising from nonproliferation concerns demand the use of modern sophisticated modeling tools for the design and optimization of a process consisting of several major steps, each of which presents its own chemical and physical complexity. None of these steps is adequately simulated in a production sense, and some require experimentation to understand or confirm their chemical behavior. Advanced simulation can be used to help understand and optimize these processes, as well as integrate their behavior into the overall model. Added value can come from the optimization of the fuel cycle as a whole, and the possibility of detecting diversions, criticality problems, or possible effluent composition deviations outside specifications.

In addition to improved chemistry, additional elements of separations systems must be modeled which are currently not even considered. Fluid dynamics must be considered in piping as well as in process equipment. Effects of control systems on component inventories, and vice versa, are necessary to adequately understand inventories throughout the plant. Interfaces with nuclear criticality calculations are important for both design and safe operation. Balance-of-plant modeling (such as volatile releases to the environment) must be included. It is essential that computer codes be flexible, adaptable, and modular. They must not only be compatible with other codes which perform related or concurrent calculations, but they must be designed to function within larger systems of codes.

1.4.8 Repository Modeling

The success of the GNEP initiative will mean that a very different incoming waste stream will be sent to a geologic repository than the waste stream (mostly commercial LWR spent fuel) currently planned. This new waste stream, consisting mainly of fission-product wastes from recycling, will ultimately require that the repository be analyzed for the purposes of compliance with NRC regulations, and perhaps have its design updated to take advantage of the significantly

reduced loadings (heat loading, mass loading, and much shorter overall half lives) that the new waste stream will represent.

If one postulates that the spent fuel in the current incoming waste stream is replaced by reprocessed fission-product waste in glass (or another solid waste form), the opportunity arises for a redesign of the repository. If the new approach to the repository were simply to substitute, waste-package-by-waste-package, the reprocessed waste for the commercial spent fuel that it came from, with no other changes, then the new analysis would be simple (and for compliance purposes almost unnecessary), because showing compliance would be far easier. However, a central tenet of moving to reprocessed waste forms is the desire to reduce the volume within Yucca Mountain that will be occupied by the new waste. This suggests an updated repository design may be appropriate, offering the opportunity for development of advanced, multi-faceted simulations that can more effectively capture the major processes for a suite of new design concepts. This will allow optimization of the safety (represented by dose to a human receptor on the surface in the distant future), the cost, and the repository volume within Yucca Mountain.

For a new design, the opportunities for improvement are many. They include the configuration of tunnels within the mountain, the configuration of waste packages within each tunnel, and the waste loading per package. Difficult analyses such as the structural performance of the system under seismic loads, the interactions of incoming water with the drift walls including capillary forces, and fracture flow and transport, are all amenable to advanced simulation that analysts would not have considered even a decade ago, because the computer power to execute such analyses was far beyond what was available. Now those barriers can be overcome, allowing for more mechanistic process models.

1.5 Crosscutting Technologies

Modeling and simulation of advanced nuclear fuel cycles will require a hierarchy of models of vastly different physical systems across a wide range of space-time scales, from detailed molecular dynamics of new materials to systems level simulation of the entire cycle. The final goal will be optimization in the presence of modeling and input uncertainty in order to design safe, reliable, economical, and socially acceptable end-to-end solutions for nuclear energy production. While there have been many advances in fundamental enabling technologies in mathematics and computer science in the past, additional research and development will undoubtedly be required to tackle a problem of this scale. This will be done in close collaboration with the DOE's Office of Science

At each level, new enabling technologies will be required in order to enhance predictive capability, understand and propagate uncertainties, model unresolved physics, and couple multiple physical models at a wide range of space-time scales. Likewise, new research and development is required to analyze, visualize, and optimize the results of such large simulations and to do so in a way that is useful to designers and decision makers who must be fully aware of the limitations of the computational predictions and the uncertainties inherent in the simulated results due to the inevitable uncertainties of input parameters and modeling assumptions. Associated with this is the stringent need to establish careful protocols for simulation code verification (are you solving the model correctly?) and validation (does the model represent reality?). These tools must be uniformly accessible within an integrated computational environment that reduces time-to-simulation, provides compatible geometry representations, and allows for a hierarchy of model fidelity running on workstations to state-of-the-art parallel computer architectures.

Finally, continued research and development of new high performance computer architectures and systems software are required to meet the future needs of this initiative where first-principle simulations of fuel cycle elements are combined for system-level simulation and optimization under uncertainty.

1.5.1 Multi-physics Coupling

Predictive simulation of each process within the GNEP fuel cycle requires accurate solutions to multiple, simultaneous nonlinear physical processes. Traditional simulation approaches to this problem involve segmented solution techniques whereby the simultaneous physics are assumed to proceed in a sequential, loosely-coupled manner. Such a solution approach is not nonlinearly consistent, is prone to numerical errors (particularly sensitive to time step size), and in some cases does not even converge (exhibits zeroth order errors). Such an approach is in general not predictive. A fully-coupled, nonlinearly-consistent multi-physics time integration algorithm, such as that offer by Jacobian-free Newton-Krylov algorithms, solves this problem. Multi-physics coupling efforts will also provide common computational tools and interface structures, through executables and/or modules, to unite the varied temporal and spatial discretizations of each physics package to provide a consistent basis for analysis and information propagation. These products and interfaces will be used by facility designers to integrate multiple state-of-the-art physics simulation packages to provide a generalized coupling. The extensive R&D results conducted in the DOE ASC and DOE/NSF SciDAC programs will be examined and may provide a coupling mechanism for facility-specific research. This work will not only payoff in more accurate, predictive simulation results, but in many cases result in increased efficiency (time to solution) by virtue of being able to take a larger integration time step per given level of desire temporal accuracy.

The algorithmic and software coupling of multiple physics modules and codes will provide analysis capabilities for the design, construction, and operation of near-term facilities (short- and intermediate-term objectives) and must integrate the current best-in-class, qualified simulation tools. However, utilizing high-performance computational systems, high-fidelity simulation packages may be tightly-coupled to provide a fully-integrated facility simulation that will provide substantial impact on the viability of commercial-scale facilities. Associated strategies for Multi-physics Coupling include:

- Utilizing and developing advanced computational algorithms for fully-coupled, nonlinearly-consistent multi-physics time integration techniques
- Providing the improved algorithms via standardized software interfaces for the communication of information from each physics package
- Developing generalized interpolation, integration, extrapolation routines to ensure compatibility of solution with different geometric representations and time-scales
- Integrating tightly-coupled physics packages into a unified module to provide an efficient solution on high-performance computing architectures.

1.5.2 Optimization and Confidence Analysis

Sensitivity analysis is used to determine the change in a computed result due to a change in some input parameter used in the calculation. When this sensitivity information is combined with knowledge of input data uncertainties, the standard deviation in the computed result can be determined. Sensitivity and uncertainty (S/U) analysis will be an important component in the Modeling and Simulation program, not only for performing methods/data V&V studies, but also for certifying that a proposed system design satisfies all performance and safety specifications.

This is especially significant for GNEP because the proposed reactor and fuel processing/reprocessing systems have not been previously characterized by measurements. Specifically, S/U methods can provide the following types of information:

- Improved physical insight into the underlying phenomena governing the system of interest, by indicating relationships between variables. This is often useful for guiding design modifications and interpreting hypothetical accident scenarios.
- Realistic, best-estimate design margins that can reduce the tolerances obtained from bounding-analysis.
- Quantitative ranking of important modeling/data parameters that impact the calculated results. This analysis can identify major sources of uncertainties and can determine the required measurement accuracy in the input data necessary to achieve a desired accuracy in the computed results.
- Rapid (but approximate) evaluation of how design perturbations affect computed output parameters. This can be coupled to a system optimization algorithm.

Although developed most extensively for criticality safety and reactor physics analysis, sensitivity techniques can also be applied to other types of calculations needed in the overall GNEP program, including shielding evaluations for reactors, reprocessing, and transportation systems, fuel depletion studies of actinide burning, core lifetime, and proliferation indicators, ex-core fuel cycle parameters such as source term activities/decay heat, and safety analysis involving reactor kinetics with thermal hydraulics feedback.

Several techniques have been previously developed for S/U analysis of the above types of calculations. Among these are deterministic methods based on perturbation theory or automated differentiation methods, and stochastic techniques based on perturbation theory or statistical sampling of the model. The different approaches each have advantages and disadvantages, so that in practice a combination of the methods may be necessary for a given application. Regardless of the approach, a number of significant challenges must be addressed. The S/U methods should be able to address 3D system designs, possibly with multi-physics coupling. Time-dependent problems for core burnup and kinetics, as well as radioactive waste transmutation, must be addressed. Nonlinearities can cause problems with first-order perturbation theory methods. An efficient technique to address distributed output parameters (in space or time) must be developed. A realistic collection of uncertainties in data describing neutron and photon interactions, radioactive decay/emission, thermal hydraulic properties, and possibly mechanical properties must be assembled. In spite of these serious difficulties, the required S/U methods for the simulation and modeling program should be tractable, since considerable expertise has been gained through previous work.