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Requirements for Advanced Simulation of Nuclear Reactor and Chemical Separation Plants

Nuclear Engineering Division

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by
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Abstract

This report presents requirements for advanced simulation of nuclear reactor and chemical processing plants that are of interest to the Global Nuclear Energy Partnership (GNEP) initiative. Justification for advanced simulation and some examples of grand challenges that will benefit from it are provided.
An integrated software tool that has its main components, whenever possible based on first principles, is proposed as possible future approach for dealing with the complex problems linked to the simulation of nuclear reactor and chemical processing plants. The main benefits that are associated with a better integrated simulation have been identified as: a reduction of design margins, a decrease of the number of experiments in support of the design process, a shortening of the developmental design cycle, and a better understanding of the physical phenomena and the related underlying fundamental processes.
For each component of the proposed integrated software tool, background information, functional requirements, current tools and approach, and proposed future approaches have been provided. Whenever possible, current uncertainties have been quoted and existing limitations have been presented. Desired target accuracies with associated benefits to the different aspects of the nuclear reactor and chemical processing plants were also given. In many cases the possible gains associated with a better simulation have been identified, quantified, and translated into economical benefits.

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I Introduction

In this report we provide functional requirements for advanced simulation of a nuclear reactor plant, targeting the Advance Burner Test Reactor (ABTR), and ABR, and a chemical separation and processing plant, with the Engineering Scale Demonstration (ESD) and the Advanced Fuel Cycle Facility (AFCF) as special cases. These plants are of interest to the Global Nuclear Energy Partnership (GNEP) initiative. In the introduction, we first provide a justification and motivation for advanced simulation followed by a list of challenging problems that would benefit from it. Finally, the functional requirements are specified on a per-domain basis in Section II to XI.

I.A Case for Advanced Simulation

The current design process for nuclear energy systems leads to many inefficiencies that translate to significant costs as advanced systems are developed. Benefits from the improved design and performance of the nuclear fuel cycle can be readily identified: a decrease of design margins, a reduction of lengthy testing programs in support of the design process, and a shortening of the developmental design cycle. The decrease of design margin can be achieved only by reducing the uncertainty of the key parameters that characterize system performance through improved accuracy and validation of the models used in the design. The reduction of testing programs will be possible only when a solid and robust simulation tool can be used with confidence through experimental validation. The shortening of the developmental cycle can be accomplished by the use of more efficient and integrated design tools that would significantly reduce the engineering processing steps.

Current nuclear system simulation represents a conglomerate of tools that are uneven in terms of accuracy and validation and are only loosely coupled (often by human intervention). Most of these tools were produced many years ago (often thirty or more years ago). The basic methodology was to rely on bench-top experiments leading to prototype operation leading to full-scale demonstration. The role of costly testing was essential because of the lack of confidence in the simulation tools and associated parameters. Moreover, the approach lacked a rigorous, scientific-based methodology for evaluating sensitivities and uncertainty of the key parameters and validation of the data and models used in the design process. Conservative design margins were established a posteriori (i. e. after some operation of the full size system) or were defined through "educated guess" or "expert elicitation," rather than through a rigorous understanding of the underlying science.

Today, though, with the advances in modeling and computing we believe that technologies are mature enough to transition to a science-based approach in order to make a breakthrough in the way nuclear systems are conceived, designed, and operated. This could be fostered through a fundamental change in the way nuclear systems are modeled. Historically, scientific research has been carried out in two main ways: modeling based on theory and experimentation. With the advent of computers, simulation has found a role as a third complement to the historical approach. The triad of modeling,

simulation, and experiment is quickly becoming the new backbone of the R&D process. The progress achieved in computing power allows numerical simulations of complex phenomena that were unimaginable not long ago. As a consequence, predictive science has progressed as a complement to empiricism, with key experiments as the essential instruments to validate the models and simulation tools. Because of the high cost and long time associated with experimentation, simulation has gained more ground in the scientific research process. In particular for nuclear systems, the improvement in understanding of fundamental processes and the progress in simulation capabilities through integration and multi-physics and multi-scale approaches, when linked to the huge advances in computational power, make significant technological breakthroughs achievable.

The ultimate goal is a design that has as low as possible uncertainties. There are two major sources of uncertainties. One is related to input physical data. Among them we can list nuclear cross sections. physical characteristics of materials (e. g. heat capacity, thermal conductivity, viscosity, etc.), fabrication data, chemical reactions rates, etc. In general these quantities can be improved either by measurements or by a better industrial process (fabrication data), but often a limit exists in the level of improvement that can be achieved. The other source of uncertainty is related to modeling stemming from approximations made in the computational methodology used in the design process. Here is where advanced simulation can provide a major benefit. In principle one can hope to reduce to the smallest amount the impact of uncertainties coming from the modeling of the physical processes. In this report, some examples of existing uncertainties will be provided with indications of possible improvements thanks to a better, advanced, simulation. On the other hand a consistent approach, based on a more rigorous and scientific basis, which allows a reliable propagation of uncertainties among the different components describing the multi-physics aspect of the phenomena to be simulated, will insure a correct evaluation of the impact of the first source of uncertainty coming from the input data. In the past a very conservative approach on uncertainty propagation has lead often to margins that are far too conservative.

The proposed simulation methodology is to compute, to the greatest extent possible, high-fidelity, physics-based solutions of the governing fundamental equations on very fine computational grids. Where our fundamental understanding of a process is insufficient or where key physical property data are lacking, first-principle modeling must be coupled with phenomenological modeling until a more sophisticated methodology is available. The fundamental modeling level has the greatest potential for advancement over the simulation capabilities that exist today. The use of first-principle-based methodologies (e.g., molecular dynamics, direct computation of turbulence, microscopic fuel behavior models, etc.) will allow, on the one hand, the elimination of recipes that lower the degree of accuracy, require greater safety margins, and limit model applicability, and, on the other hand, the possibility of exploring new phenomena that lack the benefit of extensive experimental data (e.g., related to new classes of materials or design concepts). Phenomenological modeling embodies all the experimental information that is available and can be employed either for cross-checking of fundamental modeling

or as a replacement when fundamental modeling is not available or too complex to be adopted.

It is quite difficult to perform a precise cost/benefit analysis for advanced simulation, but the final goal, as previously indicated, is to be able to design a system with highly decreased margins of uncertainty, reduced number of supporting tests, and shorter design development time. Of course, all these, if achieved, would translate into huge economic savings, but, as the famous commercial says, there are things that are priceless and in our case this is represented by the gain we will achieve in better understanding the physical phenomena and the related underlying fundamental processes.

I.B Challenging Problems That Will Benefit from Advanced Simulation

Today, several issues exist that need to be resolved in order to ensure the technical and economical viability of nuclear energy systems and fuel cycles that are envisaged in the GNEP program. We provide here a series of examples of challenging problems that will benefit from advanced simulations and help toward the goal of the viability of those nuclear energy systems. This is not an exhaustive list, but it provides a good illustration where action is needed for solving the problems.

I.B.1 Safety Case for Sodium Cooled Fast Reactor

As is well known, the proposed ABTR for the GNEP program, and in the following the ABR, are reactors with a fast neutron flux energy spectrum and cooled by liquid metal, specifically sodium. The choice of the fuel has not been made between metal and oxide types. In the following we will relate more on the case of the metal fuel case, but it is worth noting that similar simulation challenges exist for the safety analysis of the oxide fuel. For the metal fuel reactor it has been claimed that passive reactivity shutdown can be achieved for any type of unprotected whole-core accident. But even in the case this cannot be demonstrated, the safety behavior has to be benign in response to a series of several types of initiators, e. g. unprotected loss of flow (LOF), unprotected loss of heat sink (LOHS), unprotected rod runout transient overpower (TOP). There are several references [1-4] that deal with this issue and what is illustrated in the following is mostly taken out from these references.

The coolant mixed mean outlet temperature reached asymptotically upon passive shutdown in each of these unprotected events is a useful figure of merit for assessing reactivity shutdown effectiveness. These asymptotic temperatures are found to depend on ratios of reactivity feedbacks and for the TOP on a ratio of burnup control swing to reactivity feedbacks. It is important to observe that the reactivity feedback coefficients are very small. In contrast to the multiple tens of dollars of shutdown reactivity embedded in control rod scram, the passive shutdowns bring the core to zero power by balancing off reactivities in the range of cents or several tens of cents. We now briefly

illustrate the sequence of physical phenomena involved in these types of accident scenario in order to show how complex could be their simulation.

An unprotected LOHS accident is postulated to start with a loss of heat rejection at all steam generators with the primary and intermediate loop pumps continuing to run. It is also assumed that control rods fail to insert so that the reactor power changes only in response to thermal reactivity feedbacks. As the core inlet temperature rises in response to the loss of heat sink, radial core expansion introduces a negative reactivity of several tens of cents, causing the power to be reduced to near zero. The coolant temperature rise collapses to a small value, and the final asymptotic state is achieved when the positive reactivity introduced by bringing the power to zero is balanced by the negative reactivity introduced by raising the core average (nearly isothermal) temperature.

In the case of an unprotected LOF accident the initiator is assumed to be the total loss of offsite power in conjunction with a failure of the reactor scram. As the rate of flow through the core drops, the outlet temperature of the coolant rises. With this temperature increase, the thermal expansion of the above-core structure spreads the core, increasing the axial neutron leakage, his makes the reactivity negative, reducing reactor power. Feedbacks from decrease in coolant density, axial expansion of the fuel and control rod drivelines, and Doppler effect in the fuel superimpose on the feedback from radial expansion of the core. The net effect of all these passive feedbacks, none of which exceeds a few tens of cents, is negative.

The hypothetical incident of a transient overpower accident TOP involves unprotected runout of a single control rod with no control rod scram and all pumps continue to run. The rod runout reactivity increase causes the power to increase, raising fuel and coolant temperature. The course of the accident is determined by the amount of reactivity added to the core, the reactivity feedbacks caused by the high temperature, and the capability by the balance of plant to absorb the power generated. In the case of the Integral Fast Reactor (IFR) design, it was further assumed that the steam generator's output to the turbine remains constant, so the power increase raises the temperature of the cold leg of the secondary coolant loop, and thus the inlet temperature of the primary coolant. The latter increase introduce negative reactive feedbacks through radial expansion of the core, which counters the rod withdrawal reactivity and brings the power back into balance with the available heat rejection once the rod withdrawal is completed. When rod motion terminates, removal and production of heat are in balance, with the entire system at a higher temperature than under normal operating conditions, but still within safety margins.

All these examples illustrate the complexity and interrelation of events that have to be represented in these accident scenarios. Multi-physics representation must necessarily include neutronics, thermal-hydraulics, and thermo-mechanics. Besides the geometrical complexity, the time scales are different for the phenomena to be described, including 10^{-7} s or higher for the prompt generations of neutrons, 10^{-4} s to minutes for thermal-hydraulics, seconds to minutes for delayed neutrons and mechanical events (e. g rod ejections), and minutes and hours for complete description of accidents (e. g. LOHS).

Additionally to the complexities, one has to consider uncertainties. Table I.I (Reference 3) illustrates uncertainties on reactivity coefficients coming from the approximations and data uncertainties from different fields (neutronics, thermal-hydraulics, thermo-mechanics). Even if often these uncertainties can cancel out, one has to be very careful in treating them correctly. In the end all these uncertainties translates in ad hoc factors (e. g. hot channel factors for hot spot determinations) and safety operating margins that penalize the overall economics of the plant. Typical hot channel factors for sodium cooled reactors can add up to 1.5 and safety operating margins of 115% are often adopted. It is indubitable that for the safety case, advanced simulation can on the one hand help to better understand the phenomena in play giving a more robust case in front of the safety authority, and on the other hand help to reduce the safety margins. Even 1% reduction, when compared to the total fleet of reactors can translate into savings of billions of dollars.

TABLE I.I

Uncertainty Assignments in Reactivity Coefficients Used in ANL Risk Assessments of Advanced LMR Concepts*

Reactivity Feedback Mechanism	Metal (%)	Oxide (%)
Doppler	20	15
Sodium density	20	20
Fuel axial expansion/contraction	30	25
Neutronic	20	15
Thermomechanical	20	20
Net radial expansion		
($P/F > 0.8$) (including bowing)	20	20
Neutronic	15	15
Thermal hydraulic	10	10
Structural	10	10
($P/F < 0.8$)	50	50
Neutronic	15	15
Thermal hydraulic	15	15
Structural	50	50
Control rod expansion	20	20
Neutronic	10	10
Thermal hydraulic	<20	<20
Pre-clad failure, in-pin, molten fuel relocation	Not evaluated	Not evaluated
Vessel axial expansion	Not evaluated	Not evaluated
Core support structure expansion	Not evaluated	Not evaluated

*Values shown represent 1-σ deviations from the mean of a normal distribution expressed as percentages of the best estimate reactivity coefficient. "Subeffect" contributions are statistically combined to develop the five major short-term reactivity feedback uncertainties, which are rounded to the nearest 5%.

I.B.2 Fuel and Structural Materials in Reactor Operating Conditions

It will be essential for the ABTR (and ABR) project to qualify a new fuel form in a reasonable amount of time, establishing a firm basis for fuel reliability with specifications that are valid, not only at the time of fabrication, but also during operation and of normal conditions. This is especially true for new fuel forms that have yet to be subjected to irradiation tests. For these advanced reactors, this includes fuels that will contain a non-negligible amount of minor actinides resulting from the multiple recycling in reactors.

The traditional design and implementation approach, of the so called "cook-and-look" type, involves fabrication of samples or full pins of the new fuel, measurements of physical characteristics under a few potential operating and off-normal conditions (temperature, stress conditions, interactions with coolant and cladding, etc.), and finally long-term, high-fluence neutron irradiation to study degradation and failure. This approach requires a large amount of money and many years. When irradiation results are finally available, the new fuel under study may already be obsolete because of considerations that may be unrelated to the fuel design itself.

Using modern methods and powerful computing tools, it might be possible to screen proposed fuels without component testing. For example, molecular dynamic (MD) simulation has the potential to predict thermo-physical behavior, study defect problems, and provide insights into local, microscopic-scale degradation mechanisms. Kinetic Monte Carlo (KMC) and dislocation dynamic (DD) simulations can also be used to supply insights into defect interaction, long-term defect stability, and irradiation behavior. These simulations could provide the transition from the microscopic to the mesoscopic scale. Fundamental modeling may also give insights into migration of fission products and interaction of fuel with cladding and coolants, but would likely need to be supplemented by phenomenological modeling at this time to describe these complex, non-linear processes.

Advanced nuclear reactors, like the ABTR, will demand advanced materials for which little physical, mechanical, and thermodynamic data exist. As with nuclear fuels, structural materials under extreme temperatures and radiation fields represent a modeling challenge that will be overcome only through a better understanding of their behavior. Structural behavior of irradiated metallic alloys, for instance, depends non-intuitively on temperature. Non-equilibrium, multi-component, multi-phase systems evolve over time in ways that can promote creep and crack propagation. Dislocation microstructures are poorly understood. Similarly, the interaction of vacancies and interstitials with minor alloying ingredients and decay products are inadequately modeled today. Data are non-existent for modern engineered materials such as nano-scale coatings and composites.

Fuel and structural materials designed with improved performance under normal and transient conditions, combined with improved core designs, can reduce temperature peaking in the reactor, which can allow higher average operating temperatures, improved thermal efficiency for electricity production, and reduced safety margins. The modeling and simulation approach does not eliminate need for experimentation, but it allows for a more judicious selection of expensive and time-consuming experiments that would need to be performed.

I.B.3 Chemical Separation and Reprocessing Plant

Disposal of spent fuel, proliferation concerns, and lack of a closed fuel cycle are principal impediments to the future viability of the nuclear energy option. The pyrochemical technology or proliferation-resistant variants of aqueous solvent extraction options such

as UREX+, the one proposed for the Engineering Scale Demonstration (ESD), can play an important role in reducing the hazards of spent fuel by separating uranium and the transuranic actinides, which in turn may be transmuted in a fast reactor. The most efficient way to accelerate the development of the two processes to a commercial scale is to formulate physical models of the underlying chemical and transport processes. Complex, 3-D, time-dependent mixing and electric currents representing multi-component fluid-dynamics, chemical reactions, and electromagnetic effects must be assessed to confirm and optimize the treatment process. Again, an integrated multi-physics simulation offers a radically different approach to designing, testing, and implementing these processes.

Over the past decades, ANL has developed a pyrochemical process for treatment of spent nuclear fuel and demonstrated its feasibility for treating metallic fuel from EBR-II. Over this and next decades, the challenge will be expanding this technology for treatment of commercial spent fuel in a much greater scale. Efforts in designing past and current generation electrorefiners have been almost exclusively based on experiments. The design of next generation continuous-throughput electrorefiners and oxide reduction devices with greater capacity, improved economics, and better performance will require sophisticated computational tools based on first-principles. By bringing the advanced computing capabilities together with historical chemical technology and analytical process modeling expertise, the design cycle for such advanced systems can be reduced to several months, as opposed to decades.

The results of a typical simulation of current generation electrorefiners are shown in Figure I.1. In general, the throughput (cell current) is determined by the cell configuration, operating conditions (mixing, applied voltage), and the chemical state of the electrorefiner. The ion current in the bulk electrolyte requires knowledge of electric potential distributions in the cell. The concentration overpotentials near the electrode surfaces require 3-D analysis of mixing and mass transport. The electrode kinetics requires empirical and analytical knowledge of exchange current density and parameters for deposition and dissolution of ions. Although these pieces of the process can be solved individually with existing computational tools, their integration in a comprehensive electrorefiner model to address their interdependency is yet to be accomplished. Simultaneous solution of the equations representing these individual phenomena based on first-principles requires substantial modeling effort, large scale computing power, and expertise on the phenomena.

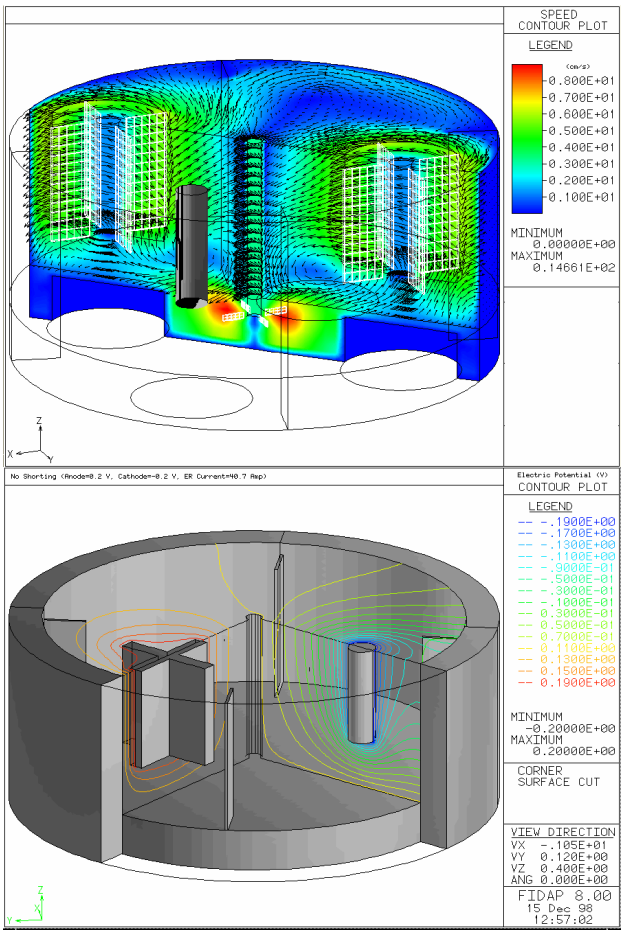


Figure I.1. Integrated 3-D transient analysis of ANL electrorefiners: (a) Mixing and species transport under "mass transport limited" conditions, (b) corresponding electric potential field and tertiary current distributions between the electrorefiner components.

To address this multi-physics, multi-scale process modeling challenge on a much larger scale, it will probably be necessary to adopt non-traditional techniques, i.e., particle methods, Monte Carlo simulations and molecular dynamics, for solving electrochemical problems involving concentrated solutions. Starting from the basics of interactions among ions and potential energy diagrams for elementary charge transfer reactions, the focus could be on statistical simulations of molten salts with electrode reactions as subgrid scale solutions that could then be used as source terms for device scale models. This type of approach could radically change the way electrochemical processes are developed in the industry and at research institutions. It could allow use of limited, bench-scale, fundamental laboratory data to design processes and equipment suitable for commercial practice without resorting to extensive testing at intermediate scales.

Under the Department of Energy's AFCI, ANL is leading development of the UREX+ aqueous separations, a multi-step process for separating out the high-risk elements of

spent nuclear fuel. ANL has successfully demonstrated the entire process in hot cells and gloveboxes and is preparing for scale-up demonstration.

The use of a multistage centrifugal contactor is an important element in the development of the UREX+ processes. The device is a cylindrical rotor surrounded by a mixing bowl. The spinning rotor acts as a mixer, a centrifugal settler and a pump. The liquid waste and solvent enter the bowl from opposite directions, and the rotor mixes them, allowing the solvent to extract the material to be removed. The liquids enter the hollow spinning rotor, and centrifugal forces 100 to 400 times gravity separate the liquids, which leave through separate ports at the rotor's top. The simulation needed for improving and optimizing the centrifugal contactor unit has to involve multiphase treatment (aqueous, organic, and air), and surface science (such as liquid surface tension, coalescent properties, micelle and reverse micelle properties, etc., for each of the liquids involved). In addition to predicting hydraulics properties, it is essential to include the understanding of the actinide mass transfer process as well as the thermodynamic properties necessary to calculate partitioning of the elements present in both aqueous and organic phases (i.e. distribution values). These are the key variables that determine the degree of separation that can be achieved in the process. A clear understanding of the hydraulic and mass transfer mechanisms will provide valuable information that can be used to design units that are critical safe, highly efficient, and produce high throughput. In addition the understanding of operating condition that can prevent undesirable third-phase formation and precipitation will be invaluable for improving the range of safety operating conditions.

A separation plant, like the Engineering Scale Demonstration, includes several major processing steps. Once sufficiently cooled, the fuel must be disassembled and the elements chopped. In the case of aqueous reprocessing, the chopped fuel is dissolved in a concentrated nitric acid solution. Cladding and any undissolved solids are separated from the dissolved fuel solution for further treatment and eventual disposal. The dissolved fuel is treated in a series of solvent extraction processes to separate different components of the fuel. The products of the solvent extraction are streams containing specific components of the fuel in acidic solutions. Each component in solution is concentrated and solidified for further processing to generate a final product—either fuel or waste forms. Each of these steps is currently poorly simulated and in many cases recipes are applied with testing providing confirmation of chemical rates or losses. Advanced simulation of these processes, based on a deeper understanding of their underlying science, will benefit their optimization. Accurate modeling has the additional value of detecting diversions, criticality hazards, or possible effluent composition deviations outside specifications.

I.C Characteristics of a Future Advanced Simulation Tool

A new system can be conceived taking advantage of progress made in theoretical understanding of physical phenomena, numerical modeling, algorithm efficiency, high performance computing and data visualization. Use of basic science adopting a first principle approach, together with the advances in both hardware and software tools, will

make it possible to put together a new simulation system with extraordinary capabilities. This will result in:

- An integrated high-fidelity system of software tools that will describe the overall nuclear plant behavior taking into account coupling among the different systems and physical phenomena during reactor operations ranging from neutronics to fuel behavior, from thermal-hydraulics to structural mechanics.
- The ability to derive basic data and static and dynamic (operating condition) properties from first principles based methodologies and fundamental experiments.
- 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.

A modernized suite of software tools would enable:

- A predictive ability for any new component conceived or proposed for improvement of performance or new plant capabilities (e. g. new fuel forms, new materials, new reactor configurations, new power conversion devices, new processes) without the use of very expensive "mock up" type experiments.
- Bridging multi-scales from the microscopic (atomistic) to mesoscopic (fine grain) and finally to the continuum level in order of deriving from an elementary level the basic properties of materials under operating conditions (high temperature, neutron irradiation, mechanical stress etc.)
- Execution of sensitivity and uncertainty analyses with the goals of assessing margins and qualifying the validity of the assumed approach and the data used, and make possible an accurate optimization of all aspects of the design process.

Figure I.2. shows how the future software tool should be structured with the link (coupling) among the different components (building blocks). The coupling could be strong (e. g. the coupled calculation of the reactor core), weak, as in the case between the core and the balance of plants, or very weak as between the reactor and the reprocessing plant. Given these characteristics for the future software tool, in the following chapters we present the requirements that are needed for each individual building block that include:

- Material Properties
- Neutronics (Core and Fuel Cycle)
- Thermal-Hydraulics
- Structural Mechanics
- Fuel Behavior

- Balance of Plants
- Safety Analysis
- Chemical Separation and Reprocessing
- Sensitivity and Uncertainty Analysis
- High Performance Computing Enabling Technologies

In general for each item, background information are first provided, then functional requirements are specified, current tools and approach are listed, and finally proposed future approaches are indicated. Whenever possible current uncertainties are quoted and existing limitations are presented. Desired target accuracies with associated benefits to the different aspects of the reactor and chemical processing plant designed are also given.

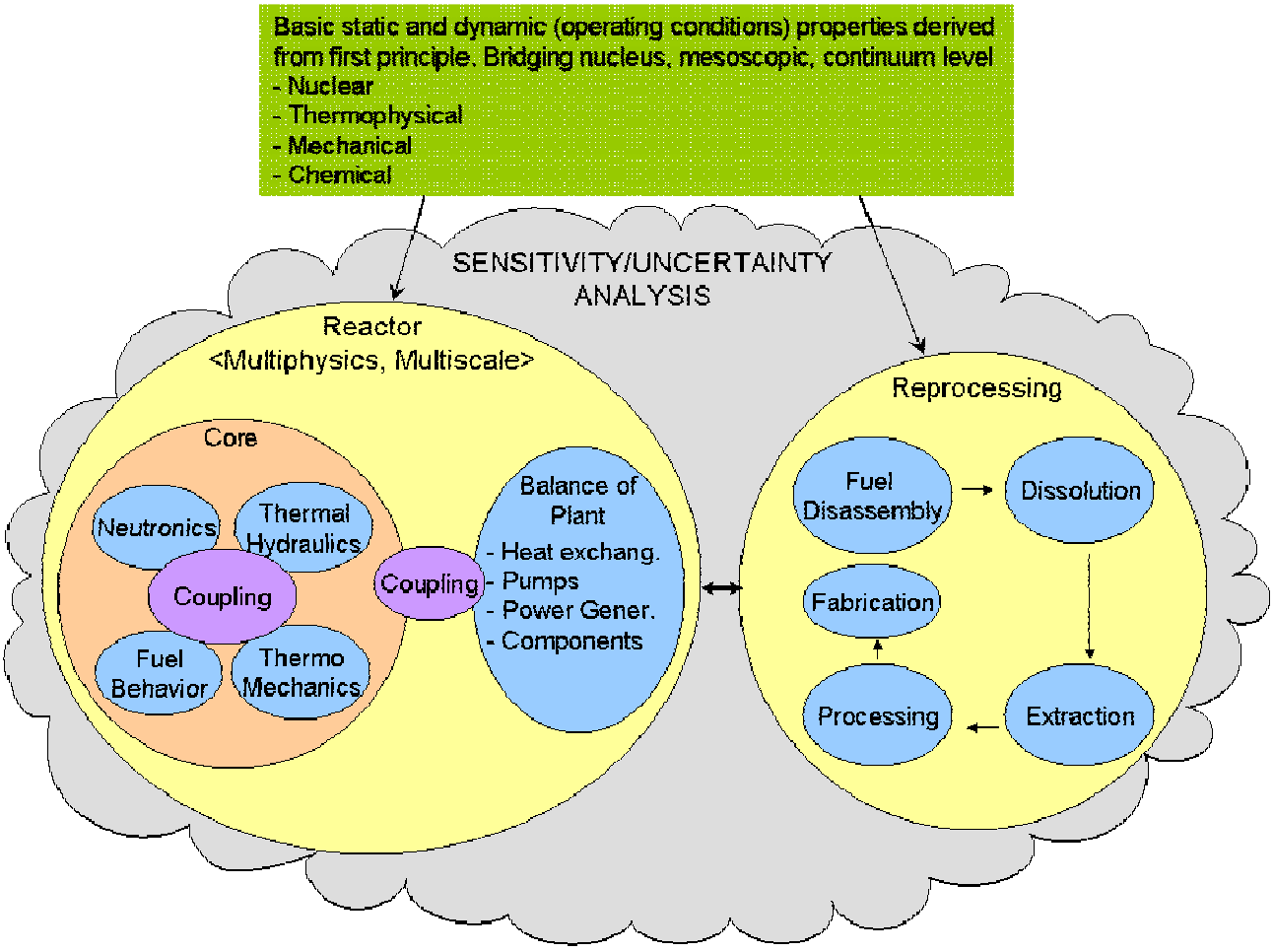


Figure I.2. Proposed structure for future advanced simulation tool.

II Material Properties

II.A Background

Better understanding of basic physical properties represents the area where probably the most progress can be made and where the biggest potential payoffs exist for advanced simulation. Properties including thermophysical (e.g., thermal conductivity and phase diagrams), mechanical (e.g., elastic moduli, ductility), and chemical (e.g., corrosion and reaction rates) have to be determined under static and dynamic conditions.

Materials science of nuclear fuel elements studies structures, properties, and applications of nuclear materials in future power plants. Nuclear materials include functional, structural, and fuel materials. Materials science is based on physics, chemistry, and mathematics; and for that reason, it has no general governing equations. Computational materials science (CMS) studies materials at an electronic, atomic, and at macroscopic levels. Molecular Dynamics (MD) and Monte Carlo (MC) are the most powerful methods of CMS that are capable of studying the materials' properties at a time scale of one atomic vibration, 10^{-12} s. MD and MC simulations of nuclear fuel materials properties require an interatomic potential that represents the energy and forces associated with a configuration of atoms. To be usable for complex geometries and/or statistical averages, the potential needs to be computed rapidly.

Many interatomic potential functions have been developed and are reported in the literature, but none are necessarily adequate for simulation of the wide range of properties required for reactor materials. With pair-wise interactions some are necessarily wrong. With many-body potentials (such as glue, Finnis-Sinclair, embedded atom, modified embedded atom and effective medium theory potentials) many can be fitted, provided that "correct" values are available. These types of potentials have been the "state of the art" for twenty years.

The most efficient potentials in materials research are based on the Effective Medium Theory (EMT) which closely resembles the Density-Functional Theory (DFT) approach. As DFT represents exact solution of the quantum mechanics equations, EMT is helpful to directly derive a potential as from first principles. However, many potential functions only obtain the functional form from EMT, while in practice they are constructed purely by fitting to a vast set of experimental data.

- Metal EAM potentials

The most widely used method is called the Embedded-Atom Method (EAM) [5-9]. EAM typically consists of two terms which are the attractive many-body part and a repulsive pair-wise potential.

$$\mathbf{E_{tot}} = \sum_{\mathbf{i}} \mathbf{F_i}(\mathbf{n_i}(\boldsymbol{R}_\mathbf{i})) + \frac{1}{2}\sum_{\mathbf{ij}} \mathbf{\Phi_{ij}}(\boldsymbol{R}_\mathbf{i} - \boldsymbol{R}_\mathbf{j}),$$

$$\mathbf{n_i}(\mathbf{R_i}) = \sum_{\mathbf{i}\neq\mathbf{j}} \mathbf{n_a}(\boldsymbol{R}_\mathbf{i} - \boldsymbol{R}_\mathbf{j}).$$

EAM is similar to EMT and DFT. Φ typically are obtained by fitting to a large set of experimental data, such as lattice parameter, sublimation, vacancy-formation energies, elastic constants, and energy difference between BCC and FCC lattices. F is a universal function and it also works for alloys. Here $n(R)$ is the total electron density, and is obtained as a rigid superposition of the atomic densities of the neighboring atoms.

EAM potentials are excellent models of metallic bonding for simple (closed-shell) metals, such as copper or gold, and have been used extensively since their creation in 1984. Excellent potentials exist for several FCC metals (e.g. *Cu*, *Ag*, *Ni* and *Al*).

- Materials for which the EAM potential was developed:

1. FCC metals - *Ni, Cu, Pd, Ag, Pt, Au, Al* and all alloys *Cu, Ti* and their alloys; *Ni, Cu, Rh, Pd, Ag, Ir, Pt, Au, Al* and *Pb*. The big exception is surfaces, which require a longer-range interaction.
2. HCP-metals – i) *Hf, Ti, Mg* and *Co.* ii) *Be, Y, Zr, Cd* and *Zn.* iii) *Ti, Zr, Co, Cd, Zn* and *Mg.* iv) *Mg, Ti* and *Zr.*
3. BCC-metals - *Fe, V, Nb, Ta, Mo* and *W. Li, Na, K, V, Nb, Ta, Cr, Mo, W* and *Fe*.
4. Metal-hydrogen potentials: *H-Ni*
5. Covalent solids: *Si, C, C-H*, Oxygen
6. Actinides: *U, Pu, Np, Am*, Oxides, Nitrides
7. Lanthanides: *La*

- Modified EAM (MEAM)

A new Modified EAM (MEAM) potential approach has been recently developed by M. Baskes and co-workers at Sandia [10, 11]. The main difference from EAM is that MEAM depends on the orientation angles between two and three neighboring ions, and that makes it similar to other "cluster" potentials, like Brenner or Tersoff potential functions for silicon and carbon.

- Metal-Oxide Fuel Potentials [12-19]

Oxides have more complicated potentials than metals. The most successful potential contains partially-ionic inter-ionic terms with additional covalent forces was introduced for *U, Pu* dioxide model by Kawamura et al.. [16].

- MD simulation of fuel and structural materials properties

The motivations to study properties of nuclear fuel and structural materials by classical MD have increased in view of the fact that ab-initio MD methods failed to reproduce the Pu phases, which instead were obtained by the Modified EAM potential developed for plutonium by M. Baskes [10].

This is important since Pu will be present in expected fuel material to be used in future generations of fast spectrum nuclear reactors.

In MD, the classical equations of motion are integrated to obtain dynamical evolution of a system of atoms. Accurate integration requires time steps in the femto-second range, limiting the total simulation time to less than a microsecond on today's processors. Direct MD is a powerful tool, giving the exact dynamical picture of a many-body system with an interatomic potential which should be known beforehand from other theoretical or experimental sources.

It provides almost experimental quality materials properties; and often MD predicts material properties at the atomic scale. It also offers a benchmark for more macroscopic methods such as Kinetic Monte Carlo (KMC), Dislocation Dynamics, Chemical Transition State rate theory that can be used for their verification.

Advances in interatomic potentials shows that more often MD simulations can be compared directly to experiment. Although there are exceptions for light atom (such hydrogen or helium) where the diffusion coefficients below room temperature are difficult to calculate by MD, they can still be studied by classical MD with quantum corrections introduced e.g. by Ab-initio methods.

All fuel oxides have ionic crystalline structure of the CaF_2 structure type. Typically simulation is performed with N=324 ions (108 cations, 216 anions). Large-scale simulation is highly demanded (M. Baskes, 10^5 ions [11]).

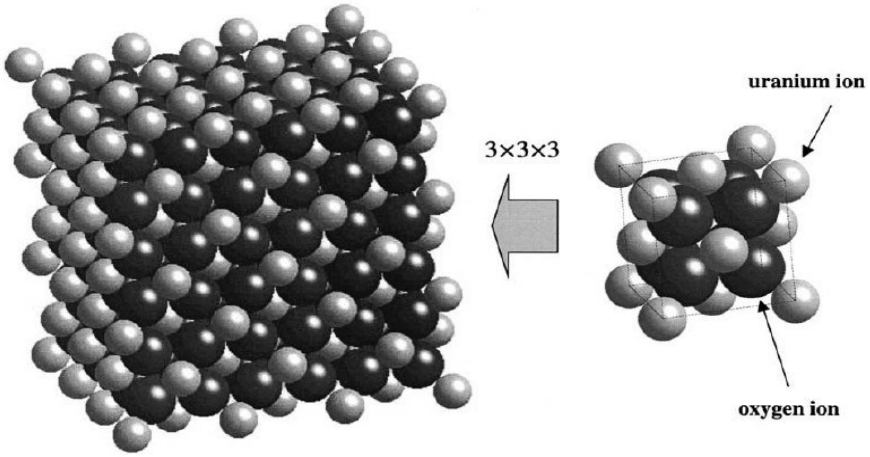


Fig. II.1 MD cell for UO_2 [from [17] K.Kurosaki et al (2001)]

- Transport properties of (*U, Pu*) O_2, *Zr* by Molecular Dynamics calculations

Table II.I summarizes the results of MD simulation studies of oxide nuclear fuels and structural materials obtained in [10-19].

Table II.I Nuclear materials properties obtained by MD simulations

UO_2	$Pu\ (U)\ O_2$	AmO_2, NpO_2 (minor actinides)	Zr	Radiation defects
- Heat capacity - Thermal conductivity (Lattice parameter was used to adjust the potential) - Thermal expansion coefficient, - Density & compressibility - Viscosity - Super-ionic conduction of oxygen ions - Bredig transition - Peak in heat capacity	- Molar specific heat - Thermal conductivity - Bredig transition (anomaly in spec. heat) - Vegard's Law	T=300-3500K - Lattice parameter - Thermal expansion coefficient - Compressibility - Heat capacity - Thermal conductivity	- HCP(α) – BCC (β) phase transition - Defects - Surface - Displ. Thresh. for properties of a-Zr	- Vacancy formation energies (anionic, cationic) - Interstitial formation energy - Frenkel U, O pairs formation energy (MEAM for Pu) - Schottky energy

- Comparison of MD results for UO_2 with experiment (Fig. II.2).

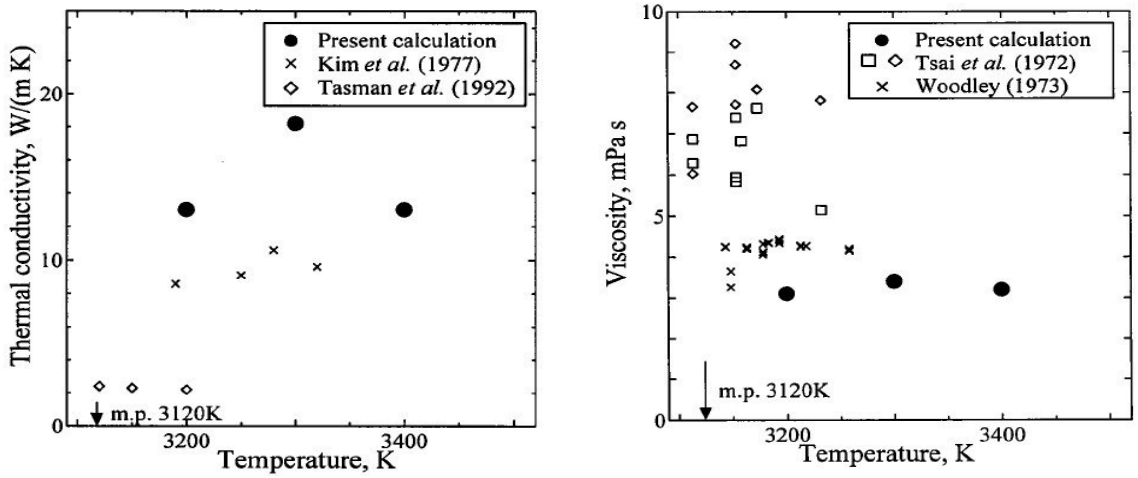


Fig. II.2. Comparison of thermal conductivity and viscosity obtained by MD with experiment

The followings are the advantageous features of atomistic simulations of nuclear fuels. MD is capable of calculating with a high accuracy many parameters. The following parameters have been obtained: viscosity, thermal conductivity, compressibility, heat capacity of UO_2 (MD – solid symbols). However, there are still unresolved problems and

limitations of this method. For example, MD still needs adjusting to a lattice parameter, MD simulations have been done mainly for single crystalline materials, although the experiments use polycrystallines and that could be a source of simulation errors.

Grain boundaries (GB) are internal interfaces formed when two crystals that misoriented relative to each other are brought into close contact. Atomistic studies of GBs are very important to materials science and engineering as in reality all materials are poly-crystalline and their mechanical properties such as strength, ductility, fatigue, and fracture, and their kinetic properties such as diffusion coefficients are mainly defined by the GB structure.

II.B Functional Requirements

As described earlier, advanced simulation could provide a screening tool for candidate fuels and materials using techniques such as molecular dynamics, kinetic Monte Carlo, and dislocation dynamics. Basic property simulation needs to focus on establishing the degree of accuracy and the practical limitations among the possible levels of simulation (e.g., fine grain, mesoscale, atomistic) and the impact that advanced simulation has on predictive capabilities and reduction of uncertainties. An approach that combines phenomenological and fundamental modeling will be necessary in cases where the basic science needs to be better understood. Regardless, modeling of basic properties is prerequisite to the development of an integrated software tool of the type proposed in this report.

There are several phenomena that represent real grand challenges for simulation in treating nuclear fuels and structural materials. These include:

- Structural transformations, swelling, fracture, damage, and properties in structural materials (alloys, carbides, nitrides, composites) caused by radiation-defects and helium and link of these properties with the overall fuel integrity
- Phase transformation and decomposition under reactor irradiation
- Fission gas transport and chemical reactions
- Development of *ab-initio* based methods for generating computationally efficient and robust interatomic potentials
- Development of hybrid methods for coupling Ab-initio, atomistic MD, kinetic Monte Carlo, and mesoscale methods
- Development of method for fracture and corrosion models
- Close relation and inter-exchange of the materials science data with the fuel performance codes.

The atomistic simulation tasks should be separated in two classes:

- Short-term tasks, providing basic properties of metal fuels

- Create a database of nuclear fuel properties and a library of existing atomistic codes (coupling with fuel performance tasks)

♦ Long-term tasks: properties of alloys/oxides/nitrides, studies at high-temperature and pressure; coupling of the database (see below) with fuel performance codes, for enabling integrity and safety of the high burn-up fuels, etc.
  - Develop multiscale/hybrid codes for predicting fuel properties (Ab-initio, MD, kinetic MC, mesoscale code, finite elements)
  - MD study of chemical reactions between fission gases and cladding material
  - Visualization of computational results (POV, AtomEye)

Phases for atomistic simulation tasks:

In figure II.3 a road map indicates the short and long term goals for the material properties simulation activity. The multiscale aspect of the material simulation problem can be presented by two major phases that can be identified for the atomistic simulation tasks.

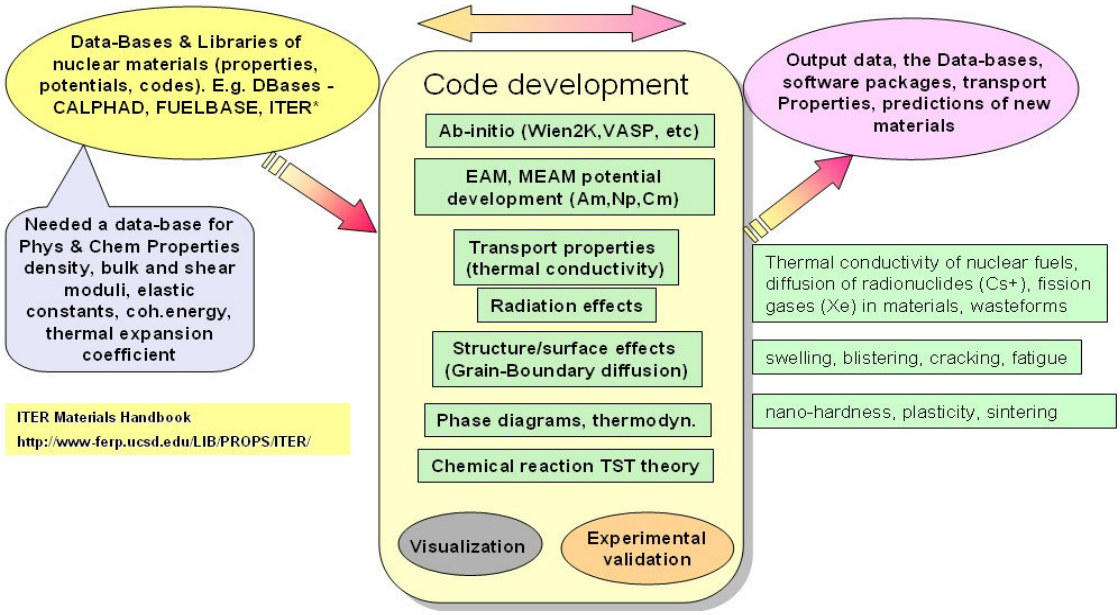


Fig.II.3. Materials properties roadmap shows short- and long-term goals for materials research for advanced nuclear fuels, tasks for code development and the ultimate goal of the project – prediction of new properties for fuel performance/integrity.

First Phase

- Data-Bases & Libraries of nuclear materials (properties, potentials, codes). E.g. DBases - CALPHAD, FUELBASE
- Interatomic potential development (EAM, MEAM, ADP, ab-initio) – there is a need for a Data-Base for the materials properties: density, bulk and shear moduli, elastic constants, lattice parameter, linear expansion coefficient, cohesion energy, vacancy formation energy. Among the first-principle MD codes (~ 10), Wien2k may be helpful for solving actinide problems. All other existing codes cannot be applied to actinides. Existing Ab-initio, EAM, rigid ion interatomic forces need to be improved – various methods exist based on taking into account polarization, angular dependence etc, and enabling accurate potentials.
- Kinetic MC, meso-scale approach
- Build a large-scale MD code

Second Phase

- Radiation effects: (defects: local, extended, cascades) in nuclear materials: swelling, cracking, fatigue, creep, etc...
- Calculation of transport coefficients (diffusivity, thermal conductivity) of nuclear materials by Non-Equilibrium MD (NEMD) method, as the accuracy of the equilibrium MD is low. There is a controversy with the simulation methods: EMD vs. NEMD as Coulombic forces should vanish as ~ r^{-5}. Diffusion of radionuclides (Cs+), fission gases (Xe) in materials, wasteforms. Thermal conductivity of nuclear fuels, Diffusion of radionuclides (Cs+), fission gases (Xe) in materials, and wasteforms
- Interaction of fuel with cladding which includes simulation of transport of the rare earth isotopes to the cladding, and possible C depletion in the cladding material
- Structure/surface effects: 3-d mesoscale code for polycrystalline solid fuel, with radiation defects and energy release, GB-structures, polycrystalline materials, dislocations, hardness, plasticity, and sintering of fuels. Nanocrystalline materials with open surface (thermodynamics, interaction with liquid solutions).
- Phase diagrams: high-T, P ?? equation of state
- Electronic properties/Chemical reactions: Ab-Initio and Transition-State Theory for radionuclides.
- Output data, Benchmarking, Data-Bases, software packages, transport (2010), Visualization packages, Experimental validation

Mesoscale approach to polycrystalline nuclear fuels

The polycrystalline microstructure consists of interconnected grains for which typical polygons can be generated by a Voronoi construction, with periodic boundary conditions. An original 2-D approach developed in Ref. [23] should be extended to a 3-D case.
It is assumed that GB migration is governed by the so-called dissipated-power functional Π ($\boldsymbol{v}$; $\boldsymbol{r}$; ϕ) that can be formulated in terms of the velocity field $\boldsymbol{v}$ of all the grain-boundaries and triple-point nodes

As a global minimization procedure for finding the velocity field requires inversions of a large sparse matrix at each time step, this restricts the method to the study of small systems. Therefore, to extend the size of the system to a realistic size, a stochastic approach based on the Velocity Monte-Carlo method developed by Cleri [21] to minimize the variational functional can be used. [21, 22]

Estimate of the computation task

A feasible atomistic simulation of a polycrystalline surface should consider modeling of at least 5×5×2 = 50 grains. The grain sizes of metals and oxides widely used in nuclear fuels, materials and industrial applications are as follows: *Fe, Ni, Cu,* U_2O, and Pu_2O – 10-100 μm [20]. A direct fully-atomistic MD simulation of such systems is unrealistic in a foreseeable future. Previous atomistic studies of granular systems show that the grains as small as 20 nm still allows one to get the most important properties of the system. Each grain with a volume of 20×20×20 = 8000 nm^3 and contains ~ 10^6 atoms. 50 grains contain 50 million atoms, which are needed for the realistic advanced nuclear fuel cycle.

The time scales of fuel irradiation phenomena include shock-wave (SW) generation, SW propagation, amorphization, decay of amorphous material, thermal relaxation; crystallization, these processes would take at least 10 ns. Comparable to this is the time for defect formation, defect accumulation, fission gas emission, void and cavity formation, bubble nucleation. After a single energetic impact, these processes are followed by viscous flow, melting, diffusion, and re-crystallization processes of the irradiated surface area.

However, the estimated simulation time of 1-10 ns for the grain-boundary evolution is much longer. Therefore, the overall computing time should be ~ 10 ns. For an MD time step of 1 fs, such atomistic MD simulation would need 10 million time steps.

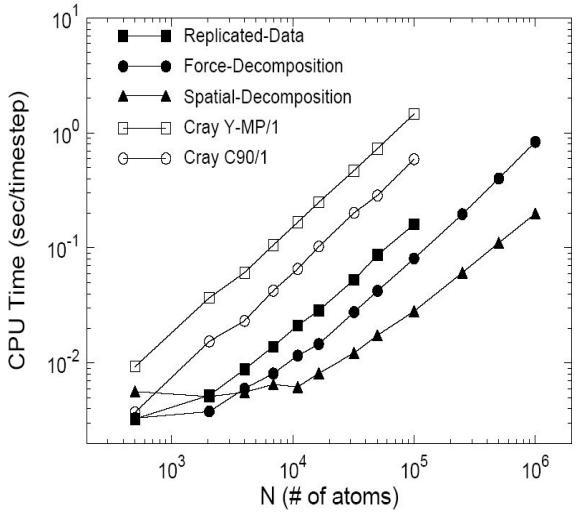


Fig. II.4. CPU time (sec/ MD-time step) for three parallel algorithms on 1024 processors of the Intel Paragon for different problem sizes. Single-processor Cray Y-MP and C90 timings are also given for comparison.

A real physical CPU-time for such computing could roughly be estimated by assuming a full parallelization, which is applicable to the MD codes that use short-ranged interatomic potentials. Fig. II.4 shows the CPU times per MD-time step for three parallel MD algorithms: the replicated data, force-decomposition, and spatial-decomposition algorithm; the latter gives the shortest time for the 1024 processors Intel Paragon system [24].

Assuming that the execution time is linear to the number of atoms, we could estimate the CPU execution time for 50 million atoms as ~ 40 sec. If the number of processors in a future Petaflops machine could be increased by a factor of 1000, one would have 40 milliseconds per MD-time step, for a system of 50 million atoms. Such simulation would run 100 hours on a petaflop machine. The MD simulations are realistic for existing Teraflop computer simulation tools like Blue Gene with the record high performance of 280.6 Teraflops. This task would take ~ 3000 hours or 4 months of Earth-Simulator [25].

The MD simulations of realistic advanced nuclear fuels and materials irradiated with neutrons would need development of better algorithms, optimization and they are well suited the computing power of the future large-scale supercomputers.

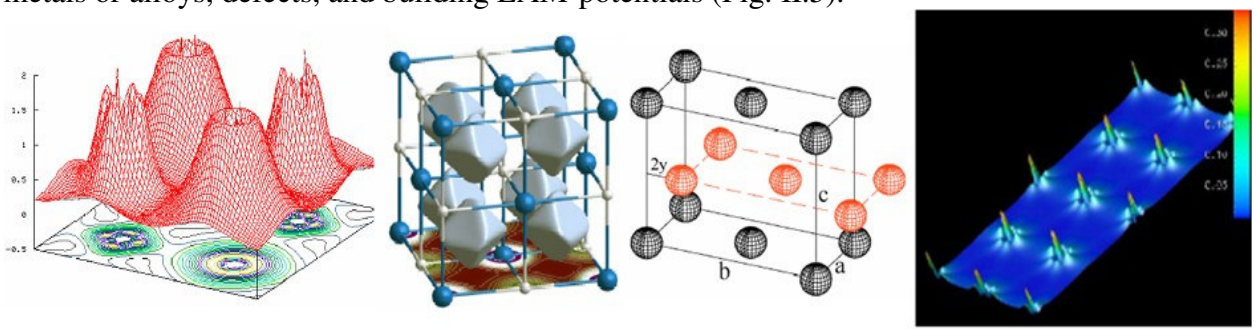
II.C Current Tools and Approach

Ab-Initio Tools

Numerous ab-initio tools that are applicable to solving various problems of crystalline materials are available. Among the AB-Initio packages we can mention: VASP, FLAPW, Paratec, PEscan, PEtot, PWscf, Siesta, WIEN2K, ABINIT, AL_CMD, CHARMM, DL_POLY, NWChem, and TBMD. Most of them are commercial, such as Wien2k, VASP.

WIEN2k Computational Physics and Chemistry Software

This package allows performing electronic structure calculations of metal compounds or alloys using density functional theory (DFT). It is based on the linearized augmented plane-wave (LAPW) + local orbitals (lo) method. [26]
Wien2k can be used for the DFT study of the surface electronic behavior of actinide metals or alloys, defects, and building EAM-potentials (Fig. II.5).



Electron density of TiC in [110] plane and 3D electron density

α-uranium structure and the spin density in the outermost plane

Fig. II.5. Ab-Initio simulation of basic properties of nuclear materials by Wien2k package

The Wien2K software package can be also used for ab-initio calculations of the interatomic EAM potentials and of the defect fine-structure in actinides and other nuclear materials. Testing and purchase of the VASP ab-initio software package which has a better interface than Wien2K will be planned. Ordering of the visualization packages such as BALSAC and XCrysDen that work with Wien2k will facilitate the overall productivity of simulations.

The calculations of the diffusion coefficients of a polycrystalline metal, for various types of twist grain boundaries, with and without an open surface are useful for the fuel performance and integrity codes.

Quantum Chemistry: Gaussian, LAMMPS, LSMS,

Quantum chemistry codes use simulation methods for studying the diffusion-controlled chemical reactions in dense media. This is essential for the high-temperatures and pressure conditions in the fuel core. Moreover, these codes enable simulations of the chemical reactions of nuclear fission gases with the cladding materials.

Classical EAM MD: HyDyn, Moldy, NAMD, Monte Carlo

The hybrid MD code HyDyn consists of two main blocks and is applicable for studying radiation effects in solids. The inner part relies on MD simulation, while the outer one, using a finite difference description of a continuum, allows correctly taking into account boundary effects. This methodology allows to achieve very significant gain in total computing time.

II.D Proposed Future Approach

The simulation tasks for nuclear fuel material's development and problems are very important and very broad. A plan can be defined to complete short- and long-term tasks, to build a nuclear property roadmap, and a feasible time-schedule for the tasks

Short term plans

- Create a DataBase of nuclear fuel properties and a library of existing atomistic codes (coupling with fuel performance tasks)
- Modeling the basic properties of actinides and actinide alloys
- Kinetic MC for defect studies
- Develop a Kinetic MC code that will be more advanced than existing codes.
- Mesoscale GB models of poly-crystalline materials
- Computational Grand Challenge - Large-Scale MD computation for Advanced Nuclear Fuel Cycle. Multiscale codes for predicting fuel properties.

The reasons for utilizing large-scale computing are manifold. The aim is to gain better understanding of the basic physical properties of single-, poly-crystalline, and liquid fuels

and surfaces under intense neutron and ion irradiations. It will be necessary to study effects of interfacial strains and microstructural constraints; comparison of the kinetics versus thermodynamics for amorphous vs. crystalline fuels; effect of interfacial strains, thickness, microstructure and composition on thermo-mechanical, transport and electrical properties.

Long term plans

- Radiation defects. This include: radiation effects: defects, damage, fatigue, and aging problems of nuclear fuels and high-temperature structural materials.
- Benchmarking
- Parallel implementation
- Incorporate dislocations into GB mesoscale model.
- Incorporate electronic properties into the classical MD: the potential functions will be corrected "in-fly" during the work of the main MD code. Electronic properties of GB for polycrystalline materials [27-29]

- Grain-boundary and surface scattering are known to increase the electrical resistivity of thin metallic films and wires. The length scale at which these produce appreciable effects is of the order of the electronic mean free path. The total resistivity of a metal can be calculated from a model in which three types of electron scattering mechanisms: scattering due to phonons and point defects, scattering due to a distribution of grain boundaries, and scattering due to the external surfaces.
- MD study of chemical reactions between fission gases and cladding material
- Visualization of computational results: Terabytes of data generated by MD (POV, AtomEye, RasMol)

III Neutronics (Core and Fuel Cycle)

III.A Background

Neutronics is the discipline devoted to the analysis of the main physics process of a nuclear reactor. The governing equation for neutronics is the differential-integral Boltzmann equation for neutron transport, which is a linear equation requiring the treatment of six independent variables, three in space, two in angle and one in energy, for time-independent problems. The difficulty in obtaining accurate solutions for problems in reactor core physics, shielding and related applications is further aggravated by a number of factors. The nuclear data (i.e. the neutron cross sections) frequently fluctuate rapidly over orders of magnitude in the energy variable. The neutron population is often sharply peaked in a particular angular direction, and those directions may vary strongly in space and energy. Finally, the geometric configurations that must be addressed are complex three-dimensional configurations, with many intricate interfaces resulting from arrays of fuel rods, coolant channels, and control rods, as well as reflectors and shielding penetrated by ducting and other irregularities. A great deal of effort has been expended in developing computational methods to deal with these problems. They fall into two classes: Monte Carlo and deterministic. Each has its advantages and limitations.

Monte Carlo methods follow individual neutrons, using random numbers to generate distances between collisions, and energy transfer and direction change at the collision sites. These methods are able to utilize directly cross section data that is continuous in energy, and they are able to treat complex three dimensional geometries. For geometrical configurations that can be treated by deterministic methods, Monte Carlo calculations tend to be substantially more expensive, however, and historically have been the method of last resort for geometric configurations too complicated for deterministic methods to treat. While Monte Carlo methods can calculate in a reasonable amount of time integral quantities (e. g. the multiplication factor), a major weakness is related to the difficulties in obtaining large enough statistical samplings of neutron histories, to calculate detailed distributions of neutron populations in space and energy with adequate precision. Such distributions are essential for determining detailed spatial distributions of power, fuel depletion, actinide buildup, temperature feedback are other phenomena that are essential to the design and operation of power reactors. A similar argument can be applied also for major safety related reactivity coefficients (control rods, Doppler coefficient, local coolant void, etc.) where very small variation of the fundamental eigenvalue has to be calculated. For similar reasons, burnup calculation is quite challenging (difficulty to propagate local variances of density variations) and time-dependent calculation with thermal feedback is impractical when performed with a stochastic methodology.

Furthermore, while the Monte Carlo codes allow treating the energy variable in a continuous way (a clear advantage over the multigroup approach), they have the drawback that they cannot calculate an adjoint solution (except in a multigroup mode) needed for sensitivity analysis, that are today so important for the reactor designer to perform uncertainty evaluation or optimize design parameters. Finally, the major disadvantage of the Monte Carlo method is associated with its stochastic approach that

disallows establishing any systematic extrapolation, while with deterministic codes a hierarchical approach permits establishing trends and deducing theoretically correct results.

Deterministic methods utilize finite elements, quadrature formulae, spherical harmonic expansions, collocation and a variety of other techniques to reduce the Boltzmann equation to sets of very large algebraic matrix equations, which have complex sparse structures. With advances in computing capability deterministic transport methods have progressed for treating one- to two- to three-dimensional configurations, and likewise the treatment of angle and energy have been refined. Nevertheless, to obtain the detailed distributions of power, fuel depletion and other quantities not obtainable by Monte Carlo methods, deterministic methods must rest on a sequence of approximations, often of questionable validity, that involve homogenization in space and collapse of the continuous data in energy into a manageable number of energy groups.

The ad-hoc assumptions in such methods have been fine-tuned against experiments and operating experience to obtain acceptable results for existing reactors. However, they are prone to error particularly when neighboring fuel rods or fuel assembles have significantly different compositions, and are sometimes even less reliable as new reactor designs are considered.

The difficulty in obtaining solutions to this artificially simplified reactor problem with a coarse treatment of energy and a quite limited spatial domain points to the how far current reactor physics computational methods are from the ideal. In the deterministic case, that ideal is the elimination of the need for group collapse and spatial homogenization approximations, and the treatment of the entire space-angle-energy phase space with sufficiently fine grained levels of discretization to obtain accurate results.

III.B Functional Requirements

The most important parameters that a neutronic code has to calculate are the main eigenvalue, called also the multiplication factor, and the associated neutron flux distribution that is subsequently used to evaluate in a post treatment several other quantities of interest like power distribution, damage rates, specific reaction rates etc.

Typical classes of neutronic calculations include:

- Core calculations
- Reactivity coefficients and kinetics parameters calculations
- Shielding calculations
- Burnup calculations
- Kinetics calculations
- Out-of-Pile and Fuel Cycle (Decay Heat) related calculations

The last three are time-dependent calculations. The burnup and out-of-pile calculations could however rely on the static calculation using different types of quasi-static

approximations. For the burnup and out-of-pile calculations the solution of the Bateman equation is required. In general this equation, when considered over a specific domain (averaged rates) does not represent a challenge for its solution.

Other particular needs are related to the calculations of reactor start up configurations where external sources are present. In this case the neutron transport equation to be solved is inhomogeneous. Finally, adjoint solutions are needed, using both classical and generalized perturbation theory, for sensitivities studies and reactivity coefficient calculations.

Table III.I indicates a set of target accuracies (1σ) for different neutronic parameters of interest of fast reactor design. Two separate cases are considered, the viability case to be used for a preconceptual phase, and a performance case to be used in the final design phase.

Table III.I Target Accuracies (1σ) for Fast Reactor Neutronic Parameters Design

	Viability	Performance
Multiplication factor, k-eff	<0.5%	<0.2%
Relative Power density		
Peak	~3%	~1%
Distribution	7%	3%
Control rod worth		
Element	10%	5%
Total	5%	2%
Burnup reactivity swing (of reactivity value)	3% or 0.5%Δk	<2% or 0.5%Δk
Breeding gain	0.05	0.02
Reactivity coefficients		
Large effects	10%	5%
Small effects	20%	10%
Kinetics parameters	5%	2%
Local nuclide densities		
Major constituents	5%	1%
Minor constituents	10-20%	2-5%

In general, it is believed that the major source of uncertainty is to be attributed to the cross section data used in solving the neutron transport equation. Indeed sensitivity and uncertainty analysis confirm that current estimates of uncertainty on cross sections lead to large uncertainty values on many neutronic parameters. For instance in the case of the multiplication factor one can easily obtain an “a priori” uncertainty of more than 1% for

the case of a sodium cooled reactor [30] based on current cross section uncertainty estimates. In the past, heavy use of integral experiment has lead to the use of bias factors or adjusted cross sections that drastically reduce the "a priori" uncertainties.

For the purpose of reducing in a considerable way the use of integral experiments and relying on simulation for providing better estimates for the neutronic parameters, one has to improve both the basic nuclear data and the methodology for calculating those parameters. Cross section evaluation use both measurements and nuclear models for producing their data. For this reason, it appears that there will be a limit to the maximum improvement that can be achieved on cross section data (e. g. 1% on a fission cross section). On the contrary, there is hope in solving the neutron transport equation to attain a very accurate solution.

A possible target could be an uncertainty, coming from the solution method, of 50 pcm on the multiplication factor, and 0.2% for the power distribution. For this latter quantity, it is worthwhile to note that from Ref. 30 only 0.5% could be attributed to uncertainty on cross sections, therefore a significant improvement in method accuracy can produce a major gain for this very important parameter. For other parameters similar considerations can be made especially from the fact that they derive from neutron flux calculations (distribution rates, densities variation due to burnup, etc.).

For what relates to reactivity coefficients, that are essential for safety analysis, it is noteworthy that the 50 pcm uncertainty on the multiplication factor will be a systematic value for deterministic calculations, so that it cancels out when taking a difference between two eigenvalues. On the other hand, for Monte Carlo calculations, due to the stochastic nature, it will be very difficult to account for such small reactivity difference.

III.C Current Tools and Approach

There are two main aspects to be considered. One relates to the processing and generation of cross sections and the other is related to solving the neutron transport equation. The first aspect concerns the treatment of the energy variable in the governing equations. As mentioned before, the neutron cross sections vary very rapidly (for instance see Fig. III.1 for ^{238}U capture cross section) over the energy domain. Therefore, the treatment of the energy variable leads to one of the most cumbersome calculational procedures in neutronic computation: the multigroup cross section generation that have to be subsequently used in whole-core calculations. The multigroup cross section generation can be a source of uncertainty larger than that associated to the basic data. Two different methodologies (suite of codes) of cross section processing can lead to difference ranging from 0.5% to 1% on the multiplication factor of a fast reactor.

The generation of multigroup cross sections involves several steps (depending on the type of neutron spectrum of the reactor, thermal, epithermal, or fast) that have to take into account several calculational approximations including: resonance self-shielding (both in energy and space), energy group collapsing, and spatial homogenizations. Invariably the first step involves generating so called "multigroup libraries" processing the differential

cross section data measured or evaluated for each individual isotopes and reaction (e. g. fission, radiative capture, elastic/inelastic scattering, etc.) and putting in a multigroup form by weighting the data with spectra that are typical of the reactor to be studied. The number of groups of these libraries varies from several thousands for fast spectrum reactors, where the presence of the structural materials and the treatment of unresolved and resolved resonances require a large number of groups, to a few hundred for thermal spectrum reactors.

Then, an accurate calculation (integral transport) is performed but only over a small spatial subdomain – referred to as a pin cell – with approximate boundary conditions. For such calculations, the energy dependence of the neutron population is reduced by weighed averaging to produce a set of multigroup cross sections. The resulting group cross section data for fuel, coolant and other materials are then employed in a lattice calculation over a fuel assembly. An assembly typically consists of hundreds of fuel rods. The two-dimensional lattice calculation is performed with a high-order angular approximation, and an explicit treatment of the spatial interfaces between fuel coolant and other materials. The boundary conditions at the edges of the fuel assemblies, however, are approximate, assuming an infinite array of identical assemblies. From these lattice calculations, a set of few energy group cross sections are obtained, which are spatially homogenized over the fuel assembly. Finally a few energy group (typically of the order of thirty for fast reactors) three-dimensional whole core calculation is performed. Since the homogenization procedure wipes out much of the effect of the angular variation in the neutron population, the whole core calculations are performed using low-order angular approximations. Once the results for the homogenized assemblies are obtained, then the local spatial distributions from the lattice calculations are melded the whole-core results though the use of additional approximations to obtain an estimate of the power distribution in each fuel rod. Clearly, all these procedures are sources of approximations or possible misuse of methodology depending on the physical phenomena that has to be taken into account.

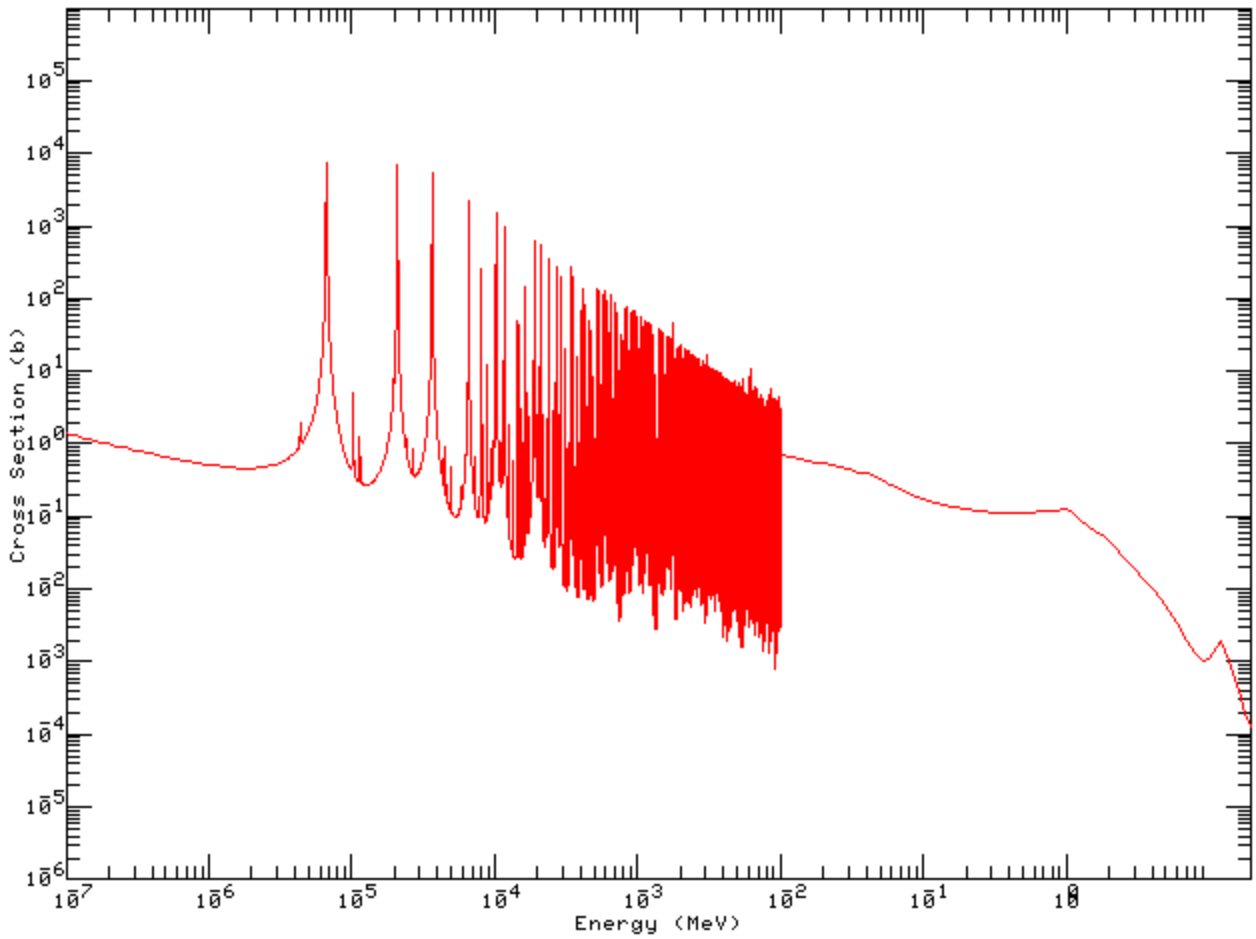


Fig. III.1 ^{238}U capture cross section

Among the codes used in the fast reactor community for implementing this procedure, NJOY [31], from LANL, is widely use for processing the differential data obtained from the basic data libraries (ENDF/B, JEF) to the multigroup form. ETOE-2 [32] is used at ANL to this purpose. Then the most established cell (lattice) codes for fast reactor applications are MC^2-2/SDX [32] at ANL and ECCO [33] in Europe.

For the whole-core calculation, the starting point for deterministic methods is a sufficiently fine-grained multigroup discretization that ensures that significant error is not introduced into the energy dependence of the cross sections. As a result thousands of coupled equations each of the form [34]:

$$\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\hat{\Omega})+\sigma(\vec{r})\psi(\vec{r},\hat{\Omega})=\int d\Omega'\sigma_s(\vec{r},\hat{\Omega}\cdot\hat{\Omega}')\psi(\vec{r},\hat{\Omega}')+s(\vec{r},\hat{\Omega}), \qquad \text{(III.1)}$$

must be solved over space, angle and energy. Here $\vec{r}$ and $\hat{\Omega}$ are the space and angle variables and $\psi(\vec{r},\hat{\Omega})$ is the neutron flux, defined as the speed times the density

distribution, and $\sigma_s(\vec{r},\hat{\Omega}\cdot\hat{\Omega}')$ is the macroscopic differential scattering cross section. The equations are coupled through the group source given by

$$s(\vec{r},\hat{\Omega}) = \sum_{g'\neq g} \int d\Omega' \sigma_{sgg'}(\vec{r},\hat{\Omega}\cdot\hat{\Omega}')\psi_{g'}(\vec{r},\hat{\Omega}') + S_{fg}(\vec{r})$$

g designates the group under consideration, $\sigma_{sgg'}$ represents scattering from group g' to g, and S_{fg} includes fission as well as known external sources.

Deterministic methods are classified by the treatment of the spatial variable; Eq. (III.1) is a first order method. We may evaluate Eq. (III.1) at $\hat{\Omega}$ and -$\hat{\Omega}$ and combine the results to obtain a second-order even parity equation,

$$-\hat{\Omega}\cdot\vec{\nabla}G\hat{\Omega}\cdot\vec{\nabla}\psi^{+} + C\psi^{+} = S^{+} - \hat{\Omega}\cdot\vec{\nabla}GS^{-} \qquad \text{(III.2)}$$

Here the even- and odd- angular parity flux is defined by,

$$\psi^{\pm}(\vec{r},\hat{\Omega}) = \tfrac{1}{2}\left[\psi(\vec{r},\hat{\Omega}) \pm \psi(\vec{r},-\hat{\Omega})\right]$$

and similarly for the cross sections and groups sources. In the case of isotropic scattering the collision and scattering operators reduce to $G \to 1/\sigma$, $C \to \sigma - \sigma_s \int d\Omega$ and $S^{-} \to 0$

In integral methods Eq. (III.1) integrates back along the direction of neutron flight. Thus

$$\psi(\vec{r},\hat{\Omega}) = \int_0^{\infty} dR \exp\left[-\int_0^{R} dR'\sigma(\vec{r}-R'\hat{\Omega},\hat{\Omega})\right] q(\vec{r}-R\hat{\Omega},\hat{\Omega}), \qquad \text{(III.3)}$$

where q contains the right hand side of Eq. (III.1)

Equations (III.1), (III.2) and (III.3) have each been most closely associated with a particular form of angular approximation. Equation (1) is treated with discrete ordinates (or S_n) in which the angular variable is evaluated in a set of discrete directions that are the same as those used in quadrature formula to evaluate the angular integrals. With appropriate spatial discretization, the operator on the left is reduced to a triangular matrix and the equations can be solved with so-called marching schemes. Equation (3) is also evaluated in discrete directions, while the integrand on the right is taken to be piecewise constant in space. The resulting algorithms are referred to as characteristics methods. The second-order form, Eq. (III.2) is most often expanded in spherical harmonics in angle, although discrete ordinates may also be applied, and the spatial variables are treated using finite element methods. Equation (III.2) gives rise to symmetric positive definite matrix equations.

All three methods are capable of treating unstructured meshes, and discrete ordinate and spherical harmonics methods have been incorporated in three-dimensional production codes. The computational difficulties of extending characteristics methods from two dimensions to three have thus far impeded their use in three dimensional production

codes. For a number of reasons discrete ordinate methods have been favored for deep penetration calculations, such as in radiation shielding. However, in some problems they suffer from ray effects: these are unphysical wiggles in the spatial flux distributions that are attributable to the angular collocation. Among the most used and popular three-dimensional S_N codes are PARTISN (from LANL, with only structured grids) [35], TORT (from ORNL prevalently used for shielding application and with no unstructured mesh capability) [36], and ATTILA (a commercial spin off of a LANL unstructured mesh code) [37].

The Method of Characteristics (MOC) is very accurate but gives rise to quite dense nonsymmetrical coefficient matrices, impeding their use over large spatial domains. This method, because of its accuracy, is the preferred method used in the lattice (cell) calculation step but because of the dense solution matrix has been widely used only in two dimensions with some limited application for predetermined local (subassembly) three-dimensional geometry. This is the case of the Canadian DRAGON code [38] used for the treatment of specific CANDU problems. The French APOLLO [39] lattice code has been recently extended to subassembly three-dimensional geometries. Finally, the Korean DeCART [40] code combines a two-dimensional MOC solution with a 1D axial solution.

Even-parity spherical harmonics methods are more widely used for reactor core calculations, with the lowest order angular approximation – so called diffusion theory – being the most widespread for the whole-core calculations. The weak point of the second-order methods is the cross section in the denominator: this causes the operator to become poorly conditions in low density (e. g. gas) regions, and singular in total vacuum.

The EVENT [41] and VARIANT [42] codes are among the most widely used second order spherical harmonics codes for reactor physics calculations. They differ in that EVENT utilizes a fine mesh finite-element treatment of the spatial variables while VARIANT utilizes hybrid finite elements to divide the spatial domain into subdomains. Solutions are then obtained iteratively by tracking the passage of neutrons in and out of these subdomains.

Many of these flux solvers are integrated in code systems that provide full capability for neutronic design, including criticality searches, burnup calculations, with equilibrium density evaluations, and time-dependent kinetic calculations. Among the systems developed for fast reactor application we can mention REBUS-3/DIF3D [43, 44] at ANL and the French system code ERANOS [45]. It is very important to consider the flexibility and easy to use of these code systems for satisfying the needs of reactor designers.

Monte Carlo methods do not suffer, in principle, from the approximations related to the treatment of the energy variable, even if unresolved and resolved resonance treatments require appropriate methodologies. To this latter purpose codes like NJOY are used to preprocess the basic data libraries for subsequent use in Monte Carlo codes. In theory, with unlimited computing power, because of the flexibility in treating complex geometries, and with a rigorous continuous energy treatment of the energy variable, the

Monte Carlo codes should be able to achieve an extremely accurate solution. While this is true for a fixed source problem without multiplication, on the contrary for an eigenvalue problem, due to the stochastic nature of the algorithm, it seems that an intrinsic limit of accuracy exists, similar to the uncertainty on a measured k_{eff}. Moreover, when interested in local quantities, in order to achieve very low standard deviations, unreasonable number of neutron histories could be required.

In the realm of the Monte Carlo codes, the Los Alamos MCNP [46] is the widespread reference. VIM [47], from ANL, and the French Code TRIPOLI [48] are among other very well known Monte Carlo codes, while KENO [49] from ORNL is prevalently used in the criticality-safety community. Some of these codes have been linked to Bateman equation solvers (e. g. CINDER [50], ORIGEN [51]) for providing burnup calculations (e. g. MONTEBURNS [52], MOCUP [53], MCODE [54]) but in general they lack flexibility for performing general design calculations (e.g. control rod movements, equilibrium densities, etc.) Also the propagation of stochastic results on depletion calculations has not been, up to now, treated in a satisfactory way.

III.D Proposed Future Approach

In general both Monte Carlo and deterministic approaches need to be further developed for a better neutronic analysis of future fast reactor systems. Monte Carlo will be kept as reference methodology that can provide extremely useful validation. The main areas of development for Monte Carlo codes would be in eigenvalue (and associated flux distribution) calculations, and time-dependent problems (burnup and kinetics calculations).

For the eigenvalue calculations, improvements are needed for nuclear reactor configurations with a high degree of decoupling. Better strategies for efficient eigenvalue convergence need to be devised probably using information from some approximate deterministic solution. As aforementioned, a reliable technique for propagation of stochastic values in burnup calculations is needed, as well as geometrical modification flexibility for following operation of the reactor (e. g. control rod movements). Similar characteristics are needed for the development of a Monte Carlo kinetics capability. If developed, these features will contribute enormously toward adopting Monte Carlo for more systematic (parametric) design calculations. Finally, developing a continuous energy adjoint Monte Carlo will make possible adopting this methodology for sensitivity analysis.

On the deterministic field, one of the major leaps forward that could be done is the elimination of the multistep calculational procedure for the treatment of the energy variable. If, with the advances in both numerical and algorithmic efficiency in conjunction with significant progress in computing power offered by the use of several thousands of processors, one can afford to solve the neutron transport equation in a detailed three dimensional geometry with thousands of energy groups, the deterministic solution will directly compete with Monte Carlo methods with the clear advantage of

having a systematic approach and providing the capability of adjoint solution for the calculation of sensitivity coefficients.

Many variants to the "brute force" approach of performing systematically three-dimensional ten (or twenty) thousand energy group detailed geometry calculations can be foreseen. Specific libraries of two or three thousand groups (one for each type of reactors) can be used for different spectrum reactors (fast, epithermal, thermal). Also alternatively only few reference calculations to the ten thousand group level would be performed and the corresponding neutron flux solution could be used to rigorously derive broad energy group cross sections to be used for parametric design studies and sensitivities analysis.

A new code can be built in modular form such that differing combination of approximations in space, angle and energy can be explored. In order to give complete geometrical flexibility, unstructured meshing for three-dimensional geometry could be adopted. In a first phase, one could concentrate on creating an efficient massively parallel code based on the second order form of the multigroup equations, using finite elements in space and spherical harmonics in angle. However, also techniques for coupling different space-angle formulations across interfaces between spatial subdomains have to be developed. For example, one can couple second order methods, with characteristics or other forms of ray tracing across vacuum regions. Likewise, while the first implementation can include a very fine-grained form of the multigroup equations, other techniques may be attempted in dealing with the rapid fluctuations of data in energy.

The huge CPU and memory resources required to carry out high fidelity reactor computations points to the need for flexibility in the level of space-angle energy discretization. For example, there is no reason why the same order of angular expansion is needed in every energy group, or for the entire spatial domain, just as there is no rationale for having an equally refined finite element mesh over the entire spatial domain, or in every energy group. Building multiresolution into a new code would allow economy of computing by allowing the level of approximation to vary over the phase space; it should not be uniform but rather varied according to the physics of the problem.

Multiresolution by itself, however, is limited in improving computational capability, for it requires a great deal of insight on the part of the user in choosing how to vary the level of approximation, and that level of insight is rare quality indeed. Adaptive mesh methods have been very successful in solid and fluid mechanics in circumventing this problem in spatial variables by developing effective a posteriori error estimators for coarse mesh solutions. The meshes then can be automatically refined selectively until a specified level of accuracy is obtained. In the neutronics field, much remains to be done in this area. While some starts have been made toward adapting meshes in space or approximations in angle, the transport equations calls for coupled adaptivity, for example by coupling space and angle, or of angle and energy, or ultimately of all three in selectively refining the solution until a predetermined level of accuracy is reached. In parallel computing, of course adaptive techniques will strongly interact with dynamic allocation of processor resources.

All the previous indicated improvements should lead to a more accurate neutronic design, with perhaps a reduction in need for integral experiments that have been so heavily used in the past. Moreover, having access to more accurate solutions in shorter response time will speed up the developmental process with the additional benefit of possibly reduced margins. As an example, also mentioned in other sections, the reduction in uncertainty on power peak factor would lead to huge economical benefits, while the uncertainty reduction on safety reactivity coefficients, besides their impact on operation costs, will have the added value of extra confidence in the safety characteristics of the new reactor plant.

Another domain that will benefit from improved neutronics codes is the estimated inventory that will be the input for the reprocessing plant. With better estimates of the nuclide inventory at the end of irradiation in the reactors, fewer measurements will be needed for establishing the content of the spent nuclear fuel with consequent reduced costs. Also there will be a favorable impact on the proliferation considerations about the plant in addition to reducing margins that are taken for compensating the uncertainties on the heavy isotopes contents.

Finally, one can expect that with high-fidelity advanced simulation, achievable with the proposed improvements in the solution of the neutron transport equations to be implemented in the next five years, it will be possible to attain a level of uncertainty, coming only from the methodology approximation, of 50 pcm on the eigenvalue, 0.5% for the power distribution or other distribution rates (e.g. damage, rates for burnup calculation, etc.) For the reactivity coefficients two categories need to be considered. The first one regards small variations where systematic approximations can be assumed (temperature, single control rod, mechanical expansion, etc.) In this case an absolute uncertainty of less than 10 pcm could be achievable. The second category relates to variations that are results of large compensations of different components (e.g. coolant void). In this case, with exact perturbation theory used for their evaluation, relative uncertainty of less than 2% should be targeted.

IV Thermal Hydraulics

IV.A Background

Recent nuclear energy system development activities in the context of Gen-IV and GNEP initiatives indicate substantial interest and opportunity in the use of multi-dimensional CFD-based techniques particularly for design optimizations. The innovative design features to reduce investment and operating costs and increase safety margins will require demonstration of concepts' viability by credible high-fidelity analyses verified with experimental data.

For the current generation nuclear reactors, systems analysis codes (like RELAP, TRAC, RETRAN, SASSYS) have been used successfully but only after being validated extensively by the code developers and the user community at large. Limitations of 1-D thermal-hydraulic phenomenology embedded in these codes have been generally recognized in addressing certain types of fluid flow and heat transfer issues that are fundamentally multidimensional in nature. Also, the empiricism incorporated into these systems analysis codes often limits their validity to specific applications.

To accomplish the objectives of the new nuclear initiatives, formation of and participation in programs that focus on increasing the accuracy and extending the range of applicability of more mechanistic, multi-dimensional CFD as a thermal-hydraulic simulation method is essential. Considering the scope of GNEP, an exclusive focus on liquid metal coolants will be of specific importance. The historical LMR design and safety analysis expertise combined with the advanced computing capabilities can be leveraged to lead a comprehensive CFD model development and validation program for the liquid metal coolants.

IV.B Functional Requirements

The application of commercial CFD software to light water reactor systems by the vendors has shown reasonable success for characterization of the thermal-hydraulic performance for turbulent flow and heat transfer in complex rod bundle geometries (with or without spacer grids), flow distributions and thermal stripping in the inlet and outlet plena, boron mixing in the downcomer, etc… However, applicability of general purpose CFD software for different types of coolants and to a wider range of flow and heat transfer phenomena such as natural circulation, multiphase flow, free surface modeling, and moving boundaries need further verification.

CFD simulations can be important for a broad range of applications in a nuclear engineering enterprise from reactor design and safety to spent fuel treatment. A significant immediate impact could be as part of a whole-core analysis capability for integrated simulation of neutronic, thermal-hydraulic, and thermo-mechanical phenomena. This approach departs from the conventional coupled neutronic/thermal-hydraulic model development efforts through rigorous pin-by-pin representation of fuel

assemblies and surrounding coolant channels in the core. Feasibility of such an approach has been recently demonstrated by coupling a commercial CFD software with a discrete integral transport model for neutronics calculations.[55] By representing local heterogeneity explicitly at sub-pin level without any homogenization, a computation intensive but high-fidelity capability can be developed to address the operational and safety characteristics of next generation nuclear reactor designs.

As part of such an integrated scheme, the CFD techniques can be used to determine the coolant and fuel temperatures throughout the core, obtain the flow field and pressure drop in coolant channels, and resolve the effects of spacer grids and orifices on flow distributions and cross-flow between the coolant subchannels to avoid hot-spots. Various other nuclear plant simulations require thermal-hydraulic component models that extend beyond the core, including the reactor vessel (particularly for pool type reactors), heat exchangers, steam generators, steam dryers, shutdown heat removal systems, and spent fuel pool.

The use of CFD based simulation capabilities can also be extended to other aspects of the nuclear fuel cycle starting from aqueous and pyro-process simulations for spent fuel treatment to waste-form analyses for safe disposal. Simultaneous solution of Navier-Stokes equations in conjunction with energy and species conservation equations lends itself to easy integration with chemical kinetics models such as CHEMKIN for optimization of spent fuel reprocessing. Feasibility of using CFD for electrochemical pyro-process modeling has also been demonstrated recently by solving special forms of Maxwell equations for ionic mass transfer in conjunction with Navier-Stokes equations for flow field to obtain electric field and current density distributions including the effects of concentration and surface overpotentials.

As a result, basic functions of a new simulation tool should include most standard capabilities of a general purpose CFD software, including:

- Mesh generation using models created with common CAD packages
- Generating unstructured grids with selective mesh refinement using variety of cell types (hexahedral, tetrahedral, polyhedral, or hybrid)
- Adaptive mesh refinement
- Transient and steady state analysis
- Incompressible and compressible flow simulations
- Newtonian and non-Newtonian fluids
- Laminar and turbulent flows
- Lagrangian and Eulerian multiphase flow treatments
- Buoyancy driven flows
- Porous media modeling with provision for non-isometric permeability
- A range of boundary condition options (inlet, outlet, pressure, periodic, symmetry, stagnation, free stream, slip and non-slip walls, smooth or rough surfaces)
- Isothermal and non-isothermal flows with convective, conductive, and radiation heat transfer

- Conjugate heat transfer for solving the energy equation among the solid and fluid domains simultaneously
- Active and passive species conservation solutions linked with the transport processes
- Formulations to specify mass, momentum, turbulence, energy, and species sources and sinks
- A functional interface to incorporate user-defined algorithms for thermo-physical properties, source terms, initial and boundary conditions via user functions
- Implicit, explicit, or hybrid solution methods, or algorithms with predictor-corrector stages
- Conjugate gradient or multi-grid preconditioning schemes to accelerate convergence
- Various differencing schemes including variants of upwind and central differencing, and advanced schemes to reduce numeric diffusion (QUICK, GAMMA, MARS)
- Restart capability
- Parallel computing

IV.C Current Tools and Approach

The desired accuracy of CFD-based thermal-fluid models depends on the target application.
Solving the Navier-Stokes equations in conjunction with the continuity and energy conservation equations to simulate flow and heat transfer offers a mechanistic approach based on first-principles. Due to the scale of the problem, however, the field variables and Reynolds stresses are often expressed in terms of their ensemble averages that are linked to the mean flow field via turbulence closure models that consist of a set of additional differential or algebraic equations. The most commonly used turbulence models fall under the category of Reynolds Averaged Navier-Stokes (RANS) models. The k-ε model is based on solving two additional differential transport equations for the turbulence energy, k, and its rate of dissipation, ε. The standard k-ε model is based on solving the high Reynolds number forms of the k and ε equations using the linear eddy viscosity hypothesis for the Reynolds stresses to determine the local turbulent viscosity.[56] Most often, the standard k-ε model is used in conjunction with algebraic "wall-functions" that represent flow and heat transfer within the boundary layers. A low Reynolds number variant of the k-ε model is based on solving the transport equations for k and ε for the entire computational domain including the boundary layers.[57] A hybrid option is the double-layer approach based on solving the high Reynolds number forms of the k and ε equations in combination with the low Reynolds number forms to resolve the boundary layer.[58]

The anisotropic eddy viscosity relationship removes the assumption of turbulence isotropy by formulating a constitutive relation for the Reynolds stresses resulting in a finite tensor polynomial. The non-linear k-ε models are based on quadratic [59] and cubic

[60] constitutive formulations for the stress-strain relations. Other variations of RANS models include the renormalization group (RNG) version[61] and Chen's variant.[62] The more complex second-order closure models such as the differential Reynolds Stress Model (RSM) are based on exact transport equations for the individual Reynolds stresses as derived from the Navier-Stokes equations.[63] Other higher order turbulence modeling approaches, such as the Large Eddy Simulations (LES) and its hybrid counterpart Detached Eddy Simulations (DES), attempt to actually resolve the large scale eddies while modeling the small scale ones; but, due to their transient nature, these techniques are very time consuming and their implementation under the existing CFD software is often not robust enough. While the common empirical coefficients appearing in these closure models (some of them are functions of other variables themselves) are intended to be applicable to a fairly broad class of flow and heat transfer regimes, they are generally not validated for a wider range of fluids.

Commonly used commercial CFD codes (STAR-CD, CFX, FLUENT, FIDAP, SCTETRA, CFD-ACE, FLOW-3D, FLOTRAN) provide a wide array of simulation models based on finite element and finite volume solvers. Although each code and each method has its strengths and weaknesses for various types of applications and fluid systems, no single code or model can claim capability of doing everything needed in a reactor design effort. A comparison of the competing codes and alternative turbulence methods in the context of a particular application is needed (and this could be an extensive project in itself). A quantification of the accuracy and uncertainties of current generation CFD software is not trivial effort and the results depend on the application.

IV.D Proposed Future Approach

The design of next-generation nuclear systems with improved economics, safety and performance will benefit from and likely rely on CFD simulations based on first-principles to provide accurate predictions of system performance. Application of CFD simulations to the evaluation of system transients and accident scenarios will likely prove computationally burdensome and benefit, at least initially, from the use of one dimensional approaches as acceleration schemes for CFD simulations or as a simplified model of selected system components to focus computational effort on areas of greatest importance. Furthermore, viability of innovative design features needs to be demonstrated by credible analyses that are validated with appropriate experimental data.

A CFD tool tailored for nuclear engineering applications, and especially for liquid metal cooled fast reactor applications, would likely require advanced capabilities beyond the standard formulations. As one example, many new reactor concepts rely on natural convection for heat removal under emergency conditions or even during normal operation. While most CFD tools include solvers which are capable of simulating natural convection with conventional fluids (water and air), the codes are largely not validated for these flow regimes. Because the experiment database with liquid metals in turbulent natural convection is extremely limited, evaluations of license applications for these concepts by U.S. NRC will likely stall unless supported by an extensive CFD validation

program similar to those conducted for systems analysis codes like RELAP in previous decades. NRC will likely seek DOE leadership in this area. For ABR-type reactor designs, it is expected that natural convection will involve mainly turbulent and transition-to-turbulent flow regimes. Therefore, the assessment of various turbulence methods for liquid metal coolants under prototypical operating conditions encountered in nuclear energy systems will be important first step. Outcome of such an assessment will help identify the need for new turbulence model improvements.

Another area where significant improvements over existing commercial tools could be realized is transient system analysis. Current generation CFD tools with computational meshing conventions which allow accurate representation of realistic geometries typically use semi-implicit segregated solvers for transient simulation. All current generation commercial CFD tools are very sensitive to the user's specification of time step size. Commercial CFD companies are investing significant effort in the development of improved fully-implicit simultaneous transient solvers which provide more consistent transient simulation capabilities, but it is likely that these solvers will be optimized for larger markets such as the automotive industry where single phase air and water flows dominate. Solvers optimized for transient simulation of the working fluids and flow regimes expected in nuclear reactor systems are needed to allow extension application of CFD beyond steady state design to include transient analysis.

Finally, since the large scale CFD models would generally lead to prohibitively long computing times, and effective parallelization scheme that can distribute the model to massively parallel computer platforms will be important. The recent experience[55] with a whole-core model for integrated simulation of neutronic and thermal-hydraulic phenomena for explicit representation of individual fuel pins and surrounding coolant channels indicate that the number of computational elements (cells) in a coarse CFD model would be in the hundreds of thousands (much larger if the effects of the spacer grids are to resolved). Using fine-mesh CFD solutions in each coolant channel will be important for an integrated whole-core analysis capability to capture important feedback effects between the first-principles based multi-physics models. The conventional domain decomposition schemes as implemented in commercial domain CFD software have relatively poor scalability characteristics. Again, the experience shows that distributing a 60 million cell CFD model onto more that 200 processors does not translate to significant speed up in real time.

A comprehensive CFD model development and validation program as part of a new advanced nuclear simulation initiative can potentially achieve accuracies beyond the current generation commercially available CFD software for specific fluids and expand the range of its applicability. However, a much greater impact will come from a brand new modeling approach with flexible software architecture to enable multi-component, multi-physics, and multi-scale engineering simulations assuming near-term availability of petascale computing platforms. Such a project will have merits to justify the effort envisioned for this initiative.

V Structural Mechanics

V.A Background

The structural mechanics field is considered to be quite mature and for its simulation there has been a widespread code development effort mostly based on finite element techniques. In any case, the application of structural mechanics models to nuclear reactor design would special treatment of thermal effects. Additionally, ANL has developed codes that cover the full spectrum of applications from slow to intermediate and fast transients up to the case of large deformations, however these capabilities have not been incorporated into a single code. Work has to be done in order to produce a general purpose code that is applicable in different cases covering all type of reactors and that has geometry capability compatible with the other components of the simulation tool.

The governing equations of motion for the finite element model are of the form

$$[M]\{\ddot{u}\} + [D]\{\dot{u}\} + \left\{f^{int}\right\} = \left\{f^{ext}\right\}$$

where $\{u\}$ is the column matrix of nodal displacements, $[M]$ the mass matrix, $[D]$ the damping matrix, $\{f^{int}\}$ the nodal forces which are obtained from the resistance of the finite elements to deformation, and $\{f^{ext}\}$ the nodal forces arising from external loads. Superposed dots denote time derivatives, so $\{\ddot{u}\}$ are nodal accelerations and $\{\dot{u}\}$ are nodal velocities. Both lumped and consistent mass matrices can be employed. A lumped mass matrix possesses nonzero terms only on the principal diagonal, so it can be a treated as a column matrix, $\{M\}$, and is often called a diagonal mass matrix. Damping forces usually arise from material response and are treated as part of the element internal forces $\{f^{int}\}$; however they are treated separately because viscous damping forces can be treated in this way when damping is not within the a stress-strain material law or behavior. The internal force vector $\{f^{int}\}$ is assembled from the element internal forces and transferred to mesh nodes that comprise the element.

The typical types of problems solved by structural mechanics simulations for the nuclear industry include core internals, reactor vessels, containment structures, confinement structures and other non nuclear grade structures. These problems include solutions for highly transient solutions for accident analyses to quasi static solutions for design basis issues. In order to assure the structural integrity of nuclear structures, it is necessary to simulate their response to anticipated loadings, both from a design basis and a beyond-design-basis viewpoint. To properly treat some of the important structures, it is necessary to perform three-dimensional numerical simulations for which two-dimensional models cannot properly capture the mechanics. The above situation was recognized in the early seventies, and efforts were initiated to develop a three-dimensional finite element code.

V.B Functional Requirements

The application of specialized structural finite element method (FEM) software to reactor systems by researchers has shown reasonable success for characterization of structural response to mechanical and thermal loadings. However, applicability of general purpose structural FEM software for different types of reactor coolants and their respective structural makeup needs further verification.

The basic functions of a new simulation tool should include most standard capabilities of general purpose structural FEM software, including:

- Transient and steady state analysis
- Capability of implicit and explicit time integrations
- Mesh generation which interfaces with common CAD packages
- Adaptive mesh refinement for stress/strain concentrations
- Boundary conditions
- Restart capability
- Parallel computing options
- Vibrations induced by fluid-structure-interactions
- Coupled physics of information with CFD, fuel behavior and neutronics codes
- Seismic Analysis and Base-Isolation
- Reinforced/Prestressed Concrete Modeling

Seismic analysis can be one of the most important inputs into the design of reactor structures and components. Thus the structural analysis capabilities must include seismic considerations. Seismic isolation is very useful to the nuclear industry, since it can reduce design loads, minimize the effects of specific site environments, and contribute to the reduction of materials needed for the major components of the primary system. When properly designed through analysis, seismic isolation greatly reduces the seismic loads transmitted to the structure. This is particularly important in advanced reactor designs where components are designed to be thin-walled structures and with reduced inherent seismic resistance. The advantages of seismic isolation include the ability: (1) to eliminate or significantly reduce the structural and non-structural damage; (2) to enhance the safety of the structures contents and; (3) to reduce seismic design forces.

Typical FEM models produce fairly accurate global strains under general analysis conditions. The local strain concentrations are difficult to obtain with a FEM model due to the level of analysis sophistication, unknown as-built conditions, material conditions and tri-axial stress effects on the failure strain. These global strains produce gross structural distortions or peak plastic strains that do not produce significant distortions. The actual strain can be considerably higher than the calculated strain, which is very important when assessing designs against allowable values. The relationship of the calculated strain and the actual strain value is:

$$\varepsilon_c \leq \frac{\varepsilon_u}{KF_T}$$

Where:

ε_c = Calculated equivalent strain

ε_u = Actual equivalent strain

$K = K_1 K_2 K_3$: Combined knockdown factor

K_1: Knockdown factor for analysis sophistication

K_2: Knockdown factor for as-built configuration

K_3: Knockdown factor for material considerations

F_T: Tri-axial ductility reduction factor

Typical values for the above knockdown factors are as follows for the current state of analysis:

The K_1 knockdown factor was developed to account for the level of sophistication of the finite element model. A finite element model attempts to identify the detail and completeness of the geometry, element refinement, boundary conditions and assumptions made or implied by the model. Any differences between the finite element model and the actual structure are quantified and related to the calculated strain, are used to determine the value of K_1. The range of K_1 varies from 1 to 5; this range is based on the refinement of the finite element model and how well it addresses global strains as well as strain gradients and concentrations due to structural discontinuities. The upper limit of 5 is based on ASME code criteria (Section III and VIII) which states that 5 is the largest concentration factor to be used for any configuration designed and fabricated.

The K_2 knockdown factor was developed to account for as-built configurations and is based on the difference between the structural information available to the analyst and the actual construction configuration. Typical values range from 1 to 1.25, which is based on the parameters of construction materials, weld quality, fabrication tolerances, post weld heat treatment, fabrication residual stresses and details, and plate thickness or bar areas.

The K_3 knockdown factor was developed to account for material degradation and is based upon the effect of material property degradation on the strain at failure and the structural loading of the component. Typical values range from 0.85 to 1.15, which is based on the parameters of corrosion, pitting, cracking, aging, etc. A factor of 1.0 would represent a mean value of material properties.

The F_T reduction factor was developed to account for multi-axial strain effect on the strain level at failure. The ductility reduction in the material, which is a decrease in the failure strain level, due to multi-axial loading effects is addressed by using the tri-axial factor approach. These reductions typically have values from 1 to 2 depending on the overall stress state of the material.

The area of largest uncertainty is typically the model sophistication for analysis. The other factors mentioned are important, as-built configurations, material degradation and the mufti-axial strain effects and need to be addressed. However, the largest area of concern is the model sophistication and how to improve on the accuracy of modeling techniques.

V.C Current Tools and Approach

The information provided in the following paragraphs describes the current and past codes used in the structural mechanics areas for mainly accident analyses and some preliminary design assessments. These are both in-house codes at Argonne and commercial codes. The in-house codes are listed first.

NEPTUNE [64]: A nonlinear elastic-plastic three-dimensional FEM structural analysis code for solid and fluid media. The code is used to analyze transient response of structures and fluid-structure interactions of in-vessel components to off-normal events. Additionally, impact loadings can be analyzed. The code is a three-dimensional finite element code capable of simulating problems that involve: (1) plate and/or shell structures, (2) fluids, (3) continua, (4) fluid-structure interaction, (5) media-structure interaction, (6) contact mechanics (e.g. impact, sliding, contact and release), and (7) silent boundaries. One of the main features of the code is the capability to handle large deformations, and the rate type material relationships can treat large material strains. A large element library provides the user with elements to model bars, plates, shells, solids, fluids, rigid bodies, rigid links, interfaces, and silent boundaries. The solution algorithms can treat short duration transient problems in a very economical manner, and nonlinear static problems are solved using relaxation methods. The purpose of the code has evolved over the years to address the current safety issues in reactor technology. An important feature of the code is its ability to handle nonlinear problems, which often occur during beyond-design-basis loads. The element formulations can properly treat large deformations (geometric nonlinearities), and the rate-type material models can handle large material strains (material nonlinearities). The code has been used to model reinforced concrete structures stressed to their material limits under internal overpressure loading and impact type loading, which arise from accident scenarios.

TEMP-STRESS [65]: A two dimensional axisymmetric finite element code to analyze steel, reinforced and prestressed concrete structures to static and dynamic over-pressurizations. Mechanical as well as thermal loadings can be applied to specialized concrete elements (cracking, beyond elastic compression, etc.)

TEMPOR2: A two-dimensional axisymmetric finite element code used to analyze concrete material for moisture diffusion and heat conduction. The boundary conditions available are those of perfect moisture transfer from the surface to an environment of prescribed, possibly time-variable, relative vapor pressure, perfect sealing of the surface, perfect heat exchange with an environment of prescribed time-dependent temperature, and perfect thermal insulation. The boundary conditions for imperfect moisture or heat transmission at the surface can be also implemented. The finite element program utilizes a quadrilateral four-node element (with variable numerical integration capability), the unknowns being the value of temperature and pore pressure at the nodes. The finite element formulation is based on the Galerkin approach and utilizes a step-by-step algorithm for the integration in time, corresponding to the central difference Crank-Nicholson algorithm for the diffusion equation.

FLUSTR: FLUSTR-ANL (FLuid STRucture Interaction Code at ANL) is a general fluid-structure interaction analysis code. The code is a three-dimensional multipurpose finite element computer program particularly suited for performing seismic analyses of reactor structures and components; and sloshing simulations of vessels or tanks filled or partially filled. It uses a mixed Lagrangian/Eulerian finite element formulation for large displacement fluid-structure interaction problems and employs an implicit-explicit mesh partition algorithm. The software is capable of using a mixed formulation and is therefore very efficient for long-duration calculations.

SISEC: Seismic Isolation System Evaluation Code is a three-dimensional program for calculating the global response of isolated and unisolated structural systems, including the effect of soil-structure interaction.

ICECO: A two-dimensional implicit Eulerian code for calculating fluid transients in reactor containments. This code calculates long-term effects of whole-core accidents and coolant spillage from the primary system.

ALICE: A two-dimensional arbitrary Lagrangian-Eularian, implicit-explicit containment excursion code. It utilizes the hybrid Lagrangian-Eularian mesh for treatment of the coolant motions to minimize the disadvantages for both the Lagrangian and the Eulerian methods (excessive mesh distortions can be handled rather easily).

ICEPEL: The computer code follows the propagation of pressure pulses through the primary piping and calculates the permanent damage and deformation of the piping and its components.

The commercial codes that have been used are listed next.

ANSYS: A system of mechanical/structural codes designed to perform both linear and nonlinear analyses. It contains structural nonlinear analysis capabilities, including complex multi-body contact and thermal stresses.

DYNA-3D: Finite element program which is used for fast, effective resolution of complicated engineering problems such as large deformation, nonlinear material behavior, and multi-body contact typically characterized by transient impact.

SAP 2000: Finite element program for linear and nonlinear analysis for both reinforced concrete and steel structures for general structural analyses of framed type structures.

There are many other commercial codes which are available which have not been described here.

Any of the codes mentioned here typically have the largest uncertainty with model sophistication. Some of the commercial codes have recently incorporated automatic mesh refinements to help reduce the uncertainties from modeling techniques.

V.D Proposed Future Approach

Designing the next-generation nuclear systems which will have improved economics, safety and performance will need an advanced simulation tool. This will be accomplished by integrating highly refined solution modules for the coupled neutronic, fuel behavior, thermal-hydraulic, and thermo-mechanical phenomena. Each solution module will employ methods and models that are formulated faithfully to the first-principles governing the physics, real geometry, and constituents. The aspect of reducing the uncertainties from modeling, as-built configurations, material degradation and the mufti-axial strain effects need to be addressed in future analysis tools. The major item of concern is to improve on the modeling sophistication to reduce the uncertainty which currently could be as much as a factor 5 on strain values. Typically this value may be reduced with proper care in modeling but still is of concern. Future approaches should concentrate on lowering this factor to be no more than 1.5; however this is a difficult task to overcome because of the other uncertainties mentioned.

One of the most important aspects in modeling the structural mechanics is the movement of the core assemblies. This movement comes from the vibrations induced through the fluid-structure-interactions inside the core and bowing mechanisms. The mechanical response for bowing deflection of core assemblies is a function of location in the core, core assembly supporting structures, and type of reactor core. Bowing is typically caused by thermal gradients, swelling gradients and irradiation creep. These mechanical responses can cause significant changes in reactivity during startup, long term operation, transient overpower, and loss-of-flow without scram transients. These effects are generally larger for small cores because the number of assemblies is small, so their individual displacement reactivity worths are large. Bowing of single assembly near the core boundary, where the gradients are most severe, moves substantially greater proportion of the fuel in a small core. The manner in which the core assemblies are supported in the core support plate and within the core barrel is a major design contributor to these transient reactivity effects. The structural support of the core is termed the core restraint system and normally consists of several supports for the fuel

rods. Generally a top nozzle and bottom nozzle support and several (between 2 to 3) grid supports provide the axial and lateral support for the fuel rods.

Currently, the primary analysis tool at ANL to calculate the mechanical response (i.e. bowing) is based on the NUBOW-3D computer code, which was developed at ANL. NUBOW requires as input a structural description of the assemblies and the core restraint system, a description of the thermal and flux fields in the core, and displacement reactivity worths for the individual assemblies.

The specific technique used in the NUBOW computer code, however, does not lend itself to efficient coupling with the thermal-hydraulics/heat transfer and the reactor physics modules. The NUBOW code is based on a finite difference formulation, which in structural analysis applications is an inefficient numerical tool. The main reason being that this computer code is inefficient is because the on the boundary conditions and the structural grid has to be internally coded for each numerical model. NUBOW was originally coded for fast reactors (i.e. LMFBR's) and has been used in the studies of EBR-II, CRBR, FFTF, PRISM, S-PRISM, SAFR and others. A more efficient and problem independent numerical solution is the finite element method (FEM). The proposed approach would be to modify the structural FEM analysis program NEPTUNE. This modified code would be an updated structural mechanics tool which will be modified to incorporate the bowing features of the NUBOW code and the features outlined in the functional requirements above. Additionally, the vibrations from fluid-structure-interactions from coolant flow with the reactor structures would also have to be addressed. A brief description of the coupling of the structural mechanics code and the thermal-hydraulics (CFD), fuel behavior and neutronics codes is discussed below.

Thus, the structural mechanics simulation would interact with the thermal-hydraulics/heat transfer (CFD) via the input of the thermal field and fluid pressure. The structural mechanics code calculations would in turn provide feedback to the thermal-hydraulics/heat transfer modules through movement of the fuel pins and assemblies, which would alter the coolant flow paths. This coupling would also provide the necessary transfer of information to properly capture fluid-structure-interactions.

The structural mechanics simulation would interact with the fuel behavior code through the displacement field to the constitutive modeling of the fuel behavior code. The fuel behavior code would provide the resulting internal forces of the fuel pins into the structural mechanics simulation.

Additionally, the structural mechanics calculations would provide feedback to the neutronics calculations with the changes in neutron leakage and reactivity worths through bowing of the assemblies. The neutronics would provide the effects of the radiation field on the structural materials.

VI Fuel Behavior

VI.A Background

The primary function of a nuclear fuel element is to generate and transfer heat to the reactor coolant. A second major function of the fuel is to contain the fuel and the fission products and provide a barrier against coolant contamination with fission products. This is provided by the outer shell of the fuel element, i.e. cladding, that provides a barrier between the fuel material and the coolant. Thus, the structural integrity of the fuel element must be maintained in compliance with applicable requirements, to prevent such a contact between the fuel heat generating material and the coolant during normal and abnormal conditions.

The modeling and analysis of the thermo-mechanical behavior of a nuclear fuel element is important for predicting and ensuring such structural integrity of the fuel element during reactor operation. This behavior is a complex system of interacting and competing processes as a consequence of the reactor high thermal power densities and neutron flux environment. There are different types of fuel materials, with differences in behavior under reactor operating conditions, which include both ceramic (oxide) and metallic types and are available in different forms. Examples of such materials are UO_2, $(U, Pu)O_2$, U(U,Pu)C, (U,Pu)N in sintered pellet or sphere-pac form or metallic slug such as U-Fs (uranium-fissium), U-Zr, or U-Pu-Zr, with possible additions of minor actinides to some of those forms [66].

Over the life of the nuclear industry, fuel performance models and codes played a role on the advancement of nuclear fuel design and assuring the fuel integrity during both normal and abnormal conditions. It provided tools for understanding the basic phenomena taking place within the fuel and the complex interplay between those phenomena. Expertise from different fields were involved in the developments of such models and codes, including nuclear, thermal, structural, materials, and chemical expertise. Because of the central role of the fuel in the nuclear steam supply system (NSSS), fuel elements of various types and levels of complexity are incorporated in the NSSS codes. [67] Those codes, arranged in ascending order of complexity of the fuel elements models contained in them, include system thermal hydraulics codes, core simulation codes, loss of coolant accident codes, and fuel performance codes. This shows the important role of a fuel behavior code within an advanced simulation initiative as the one considered here, which aims at simulating all aspects of this NSSS.

Advanced fuel behavior codes [68] include both thermal and mechanical modeling, at different levels of coupling between the two types of analysis. Thermal analysis, which determines the temperature distribution within the fuel, is relatively a straightforward analysis due to the general applicability of the Fourier heat conduction law. This analysis is complicated by the changing thermal conductivity of the fuel during irradiation, changes in fuel-cladding gap, and other factors such as phase transformation of the fuel, and constituent redistribution. If those complications are not taken into account (or modeled through empirical correlations), structural analysis of fuel elements represents a

more challenging task. The difficulties encountered when handling the basic equations of structural analysis and material behavior of a fuel element are summarized as follows:

1- Fuel elements are three-dimensional structures and deformation can take place anywhere over its structure.
2- The constitutive laws (stress-strain) are non-linear as a result of creep, plasticity, and other material data. Time occurs as a fourth independent variable. Material behavior may be anisotropic.
3- Materials behavior under irradiation in both fuel and cladding is a complex problem and understanding of the detailed physical phenomena involved remains limited. The inclusion of time as an additional factor complicates the problem even further.
4- Chemical phenomena in the fuel element, such as the fuel cladding chemical interaction and corrosion of cladding by the coolant changes the cladding load bearing properties.

Interconnection of three groups of input parameters into a formal system of equations provides a general representation of the difficult problem of the fuel structural modeling. These groups include materials data, design data, and operational conditions of the fuel. The consequences of the operation are stresses and strains, changes in temperature distribution, changes in materials compositions and properties, and changes in internal and external geometry. These load data are the results of the general solution of the equations system mentioned above. Ultimately, the load data are to be compared to fuel element failure limits. General mathematical representation of this structural analysis system of equations has been attempted in the past [69, 70] and can be described by [71]

$$\boldsymbol{L = f(M, D, O) \leq S} \qquad \text{(VI .1)}$$

where
$\boldsymbol{L}$ = load parameter,
$\boldsymbol{S}$ = failure limit,
$\boldsymbol{M}$ = material quantities,
$\boldsymbol{D}$ = design parameters, and
$\boldsymbol{O}$ = operating conditions

This system of equations is to be solved numerically and represents the core of all mechanistic fuel elements codes. Due to the extreme complexity of solving that system of equations in a complete form, different levels of approximations have to be made to enable the modeling effort. Those approximations range from simple 1-D thermal analysis models to a full thermo-mechanical 2-D finite elements representations [67].

Although there are wide variations in the complexity of the thermo-mechanical fuel codes, the physical models implemented within those codes do not have the same first principle levels of complexity. Most of those models are empirical or semi-empirical models that are based on simplistic phenomenological models which are calibrated to a certain range of operating conditions. The applicability of those models outside this range, i.e. extrapolations outside this range, might not be valid. This lack of

implementation of first principle type models of the physical phenomena into the fuel performance codes combined with simplified thermo-mechanical modeling are some of the motivations for this proposed advanced simulation initiative.

VI.B Functional Requirements

As aforementioned, the fuel behavior codes contain contributions from wide range of modelers including nuclear, thermal, mechanical, and chemical modeling. There are different functional requirements that correspond to each aspect of the modeling activities. The main requirements of the fuel performance codes are to predict the thermal and mechanical response of the fuel elements during normal and abnormal operations of the reactor. Nuclear physics, chemical models, and materials behavior models are interconnected with the thermal and mechanical analysis in those codes. The analysis provides estimates of a number of integral parameters that are observed during the simulations and are usually used by the fuel designer to evaluate the fuel integrity during reactor operations. For a cylindrical type fuel slug enclosed in a steel cladding tube (most common form for fast reactor type fuel) those parameters include:

- Cumulative damage function (CDF) which relates the time under certain stress and temperature conditions to the cladding time-to-rupture
- Stresses on the cladding
- Cladding diametral strain
- Fuel axial growth
- Magnitude of fuel-cladding chemical interaction (FCCI)
- Temperature distribution within the fuel and cladding
- Fission gas pressure and released fraction

For fast reactor licensing activities, there are limits imposed on the values of those parameters that should not be exceeded during reactor operations in order to limit the possibilities of pin failures below licensing agencies requirements.

Some of the above integral parameters can be estimated by post-irradiation examination (PIE) of experimental fuel elements irradiated under reactor conditions. Those parameters include the cladding diametral strain, fuel axial strain, FCCI, and fission gas release. The fuel behavior codes can predict those parameters as long as the operating conditions are within the range of applicability of the validation database. On average (i.e., the average of comparing a number of measurements to the corresponding calculations), comparison of the measured parameters to the calculated parameters can yield small errors. Those uncertainties can be as low as 5% or less for each of those parameters. However, if one looks at an individual measured parameter that corresponds to a certain pin and possibly a certain location over the pin, substantial uncertainties can be found. Those uncertainties can be as high as 50% for most of those parameters. Thus, statistical uncertainties in the fuel behavior codes can be low; however local uncertainties can be very high. Those high uncertainties are attributed to a number of factors including uncertainties in basic materials properties and changes on those properties during irradiation, in addition to uncertainties in the correlations that approximate the physical

models. Other uncertainties can be attributed to the type of thermal and mechanical analysis performed. For example, the use of a fuel performance code that divides a fuel pin into a number of axial segments that are not mechanically connected (through finite element modeling) can lead to errors in the predictions of axial fuel growth. In addition to errors in material properties and thermo-mechanical model approximations, errors in the operating conditions of the reactor can lead to further uncertainties in calculated integral parameters. Uncertainties in the pin power densities, magnitude and shape of the neutron flux (accumulation of fission products and actinides within the fuel) and flow temperature, can increase the uncertainties of calculated parameters. Notice here that most cladding failure take place at a certain location over the pin geometry and unlikely to happen uniformly over one axial location.

Uncertainties in other calculated parameters such as peak fuel temperature and cladding stresses can be as low as 10% during the initial stages of irradiation. However, those uncertainties increase with irradiation. Uncertainty in fuel thermal conductivity can be as high as 25% for unirradiated fuel of certain alloys; however the uncertainty increases with irradiation as the fuel porosity changes, possible sodium logging (sodium cooled FRs), changes in fuel density, fuel restructuring, cracks growth, and change in grain size and possible phase transformations. All of those phenomena that cannot be measured in most situations contribute to further uncertainties in fuel thermal conductivity and further uncertainties in fuel temperature predictions. As for the stress on the cladding, those stresses are mostly attributed to fission gas pressure during the early stages of irradiation, and can be estimated with high accuracy during those stages. However, as the solid fission products accumulate within the fuel and fuel start to load the cladding, fuel cladding mechanical interaction (FCMI) takes place, and the stresses on the cladding becomes less predictable.

VI.C Current Tools and Approach

Large numbers of computer codes that simulate fuel behavior are available. Generally, those codes can be divided into three major categories which include simple correlation fuel performance codes, fuel model codes, and mechanistic fuel performance codes [67, 72]. The latest category is of interest here, since the former categories provide simplistic representation of the fuel behavior that are limited to certain applications and cannot be used to extrapolate the fuel behavior. Among the mechanistic fuel codes there are codes that simulate the fuel in thermal reactors and there are fast reactors fuel performance codes. Of interest to the current report are the codes related to fast reactors applications. In general, mechanistic codes contain both thermal and mechanical analysis of the fuel elements. Table VI.I shows a summary of the mechanistic fast reactors fuel performance codes.

Table 1. Summary of mechanistic fast reactors fuel performance codes [67].

Code	Country	SMiRT No.	Ref.	SS, T, SST [a]	Dimen. [b]
ACTIVE	Japan	4	MMM	SS	1.5
BEHAVE-2	USA	4	D/0	SS	1.5
		5	D7/1	SST	1.5
COMETHE-III	Belgium	1	C2/1	SS	1.5
		4	MMM	SST	1.5
CYGRO-F	USA	4	D/0	SS	1
FMODEL	USA	1	C3/4	SS	1.5
FPIN	USA	4	MMM	T	1.5
		5	D7/1	T	1.5
		9	Vol. C, p. 3	T	1.5
FRUMP	UK	2	D1/8, D2/2	SS	1
		3	D1/12	SST	1
		4	MMM	SST	1.5
		5	D7/1, MMM	SST	1.5
IAFETIN	FRG	6	D4/6	SST	2
		7	C5/3	SST	2
IAMBUS	FRG	4	C4/12	SS	1.5
ISUNE-5	USA	7	C4/7	SS	1
JANE/KRASS	USA	5	D6/4	SST	1.5
LIFE-II	USA	1	C4/1	SS	1.5
-II		2	D2/5	SS	1.5
-III		4	D/0, D1/4	SS	1.5
-UNCLE		4	D/0, MMM	SST	1.5
-4		5	D1/1	SST	1.5
-4CN		5	MMM	SST	1.5
-GCFR		6	D4/4	SS	1.5
-4CN		6	D4/1	SST	1.5
-METAL		9	Vol. C, p. 11	SST	1.5
NERFS	UK	2	D2/2	SS	1
NUFROD	USA	5	D7/3	T	1.5
SATURN-1	FRG	1	C4/2	SS	1
		4	D1/6	SS	1
		6	C1/2	SS	1
SLEUTH	UK	4	MMM	SS	1.5
TEXDIF-P	FRG	6	C1/2	SS	2
URANUS	FRG	4	C1/2, D1/2	SS	1.5
		5	D3/1	SS	1.5
		6	D4/2	SST	1.5
		7	C4/3, C4/4	SST	1.5
		8	C2/8	SST	1.5

[a]Steady state (SS), transient (T), or steady-state-and-transient (SST)
[b]One-dimensional codes include a radial analysis model only. 1.5-D codes also include provisions for dividing the fuel into axial segments with different operating conditions. Coupling among axial segments varies from code-to-code.

As shown in the table, the codes are 1-2 D codes, and each code has its own approximations of the structural analysis. Most of the codes use structural analysis approximations to avoid the use of finite element analysis, such as the LIFE series of codes [73] (however, the LIFE code remains the main fast reactors steady state code, and the FPIN code [73, 74] is the code for transient behavior in the U.S., especially for metallic fuel) . Other codes that use finite element analysis limit the analysis to 2-D analysis with assumptions regarding constitutive laws. The Japanese ALFUS code (not listed in the table) [75] is an example of such a code (2 ½ D, as it does not account for the azimuthal variations around the periphery of the pin).

In addition to the structural analysis limitations of the existing codes, there are also limitations on the implementation of the physical models within the codes. For example,

most of the existing codes use correlations for the representations of the fission gas release within the fuel, instead of implementing a physical model that predicts the release as a function of the neutronics parameters, the microstructure of the fuel, temperature, and other factors. This highlights the need for implementation of more detailed physical models that predicts the phenomena of interest based on first principle. Those limitations of the existing codes limit the ability of the codes to extrapolate the designs beyond certain boundaries which are determined by the validation database. For example, lack of axial coupling between the different axial sections can lead to errors in the estimation of fuel axial growth during irradiation as discussed before.

VI.D Proposed Future Approach

In order to go beyond the existing state of fuel behavior simulation codes a number of requirements will be needed in the new code as follows:

1. General 3-D elastic-plastic deformation finite elements framework for structural analysis.

2. Detailed physical (materials and chemical) models for the different phenomena that take place within the fuel slug and the cladding material.

3. Detailed materials properties estimated at each time step as a function of operating conditions and fuel structure through data tables within the code or through communications with external databases that are based on first principles estimation of materials properties; or perform the detailed calculation of those parameters if possible.

4. The computer programming to implement the basics of object orientation paradigm to allow for modular programming that can be easily maintained and modified. In addition, the programming should allow for easy communications with external programs and exchange of data between those programs (e.g., input data from thermal-hydraulics calculations or detailed first principles material properties models).

Figure VI.1 shows the transition from the current fuel performance code methodology to the new paradigm that includes the above requirements. Notice the feedback effects between the physical models and the materials database and the other reactor simulation codes. The code's physical models both receive material properties from the properties database and/or first principle modeling and provide input parameters to those models. For example, at the start of irradiation, the database will provide unirradiated fuel thermal conductivity to the performance code. The code's physical models will estimate the evolution of phenomena that can affect the thermal conductivity, such as porosity and phase transformation, and feed that information back to the first principle models to update the fuel thermal conductivity. Similarly, models that account for irradiation hardening of the cladding material will feed information into the cladding detailed tensile properties model that follow the dislocation and grain growth in the cladding, and reside

outside the fuel performance code. In addition, the figure shows feedback to and from the other codes simulating the NSSS such as the thermal hydraulics and neutronics codes providing the operating conditions of the fuel pin.

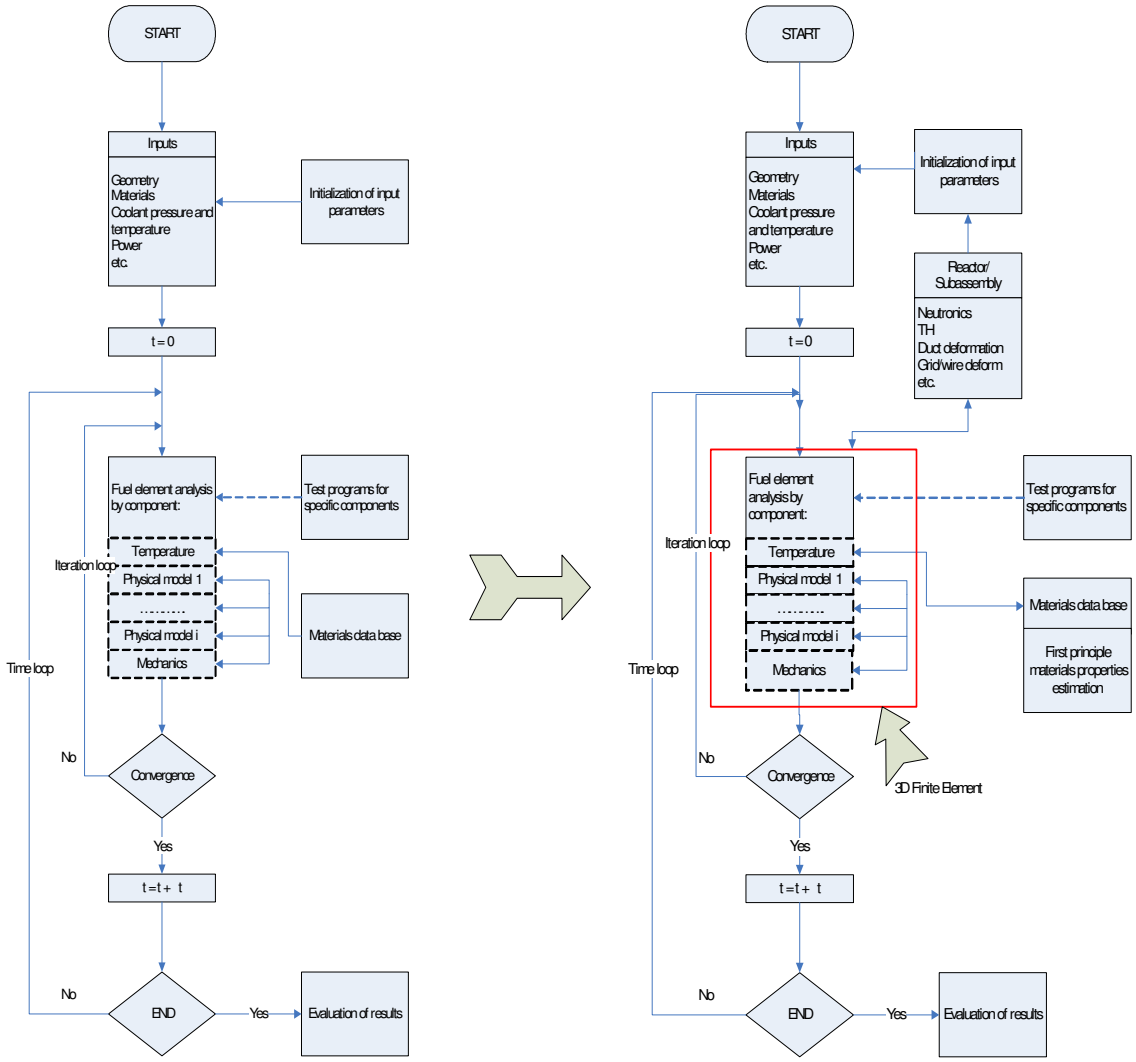


Figure VI.1. Basic Structure of a General Computer Code for Fuel Element Behavior and Proposed Approach

The construction of a fuel behavior code with the above criteria is faced with different types of challenges. Figure VI.2 shows the computational challenge caused by the use of a 3-D finite element framework [76]. The figure shows the number of operations required for the simulation of one fuel rod over one year of irradiation. As shown in the figure, a tera-flops scale computer level is required for such calculations. This computational burden is a result of the detailed structural analysis requirement only, with physical models mostly represented by empirical correlations. The use of detailed physical models will further increase the computational burden. Another level of computational complexity can be expected if more than one element in a subassembly is

to be simulated, especially if details of the effects of neighboring elements are thought to be important. In additional to the increased computational effort needed, the development of detailed physical models is a very complicated and challenging task by itself. Those models are inter-dependent and some of the parameters involved cannot be measured experimentally, requiring the development of first principles detailed models.

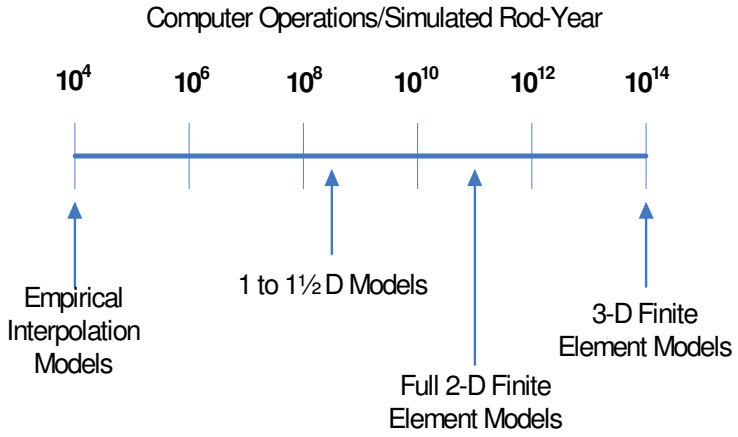


Figure VI.2 Spectrum of Fuel Performance Model Complexities

The ultimate rewards achieved through the implementation of such a complicated simulation tool are numerous. As aforementioned, large uncertainties, as high as 50%, are associated with the fuel performance codes' predictions of some of the integral performance parameters at the local level. Those uncertainties can be reduced with the proposed simulation tool. For example, experimental observations of FCCI show large variations in the magnitude of this interaction at the same axial location over the fuel and different locations around the periphery. The proposed tool can account for variations, over the periphery of the fuel, in FCCI related parameters such as fuel and cladding temperatures, migration of fuel constituents, and duration of fuel-cladding contact. Estimates of these detailed 3-D calculations, combined with high fidelity estimates of the operating parameters are expected to reduce the uncertainties in the estimates of the FCCI. An optimistic goal of the reduction in calculations uncertainties in the local parameters can be within the uncertainties of the average parameter discussed earlier of about 5% or less. However, given the uncertainties in the operating parameters, and the possible lack of experimental measurements to validate some of the detailed models, a 10% uncertainty will be more realistic for some of the parameters. Ultimately, this reduction in uncertainties will have significant impact in improving safety margins for fuel such as the fuel power to melt and the hot channel factors and ultimately improve the economics of future nuclear power plants.

In addition to the goal of reducing calculations uncertainties compared to measurements, such a high fidelity tool will be useful to both core designers and experimentalists. The core designers will be able to use the code to perform parametric studies and the study of new fuel types with little or no irradiation database available, and extrapolate existing

designs beyond the validation database. Also, the new fuel performance code, with its detailed complex physical models, can help planning costly irradiation experiments and limiting its scope to certain space of parameters based on the code's predictions. This can ultimately lead to significant reductions in the R&D cost of new fuel designs and enhancing the operating parameters of existing designs.

VII Balance of Plant

VII.A Background

There are on-going efforts to expand the range of application of nuclear power plants to cogeneration functions, in particular high temperature production of hydrogen for transportation fuels, with nuclear heat. However the current application of nuclear power plants, in the current fleets of industrial utilities world-wide, to electricity generation is a very important and significant one, borne out by decades of optimized and well-balanced operations of the Gen-II light water reactor ((LWR) units. These units have operated well in the industrially developed nations over the past decade. They have contributed to diversification of energy supply, reduced the carbon demand on the environment and conserved hydrocarbons, particularly oil, for future generations. But improvements in performance will be ever-more important as the globalization of the demand-curve and the ever-tightening supply curve make their effects felt. The energy conversion part of the nuclear power plant, which is responsible for the generation of the electrical power supply to the grid from the nuclear heat is currently a large footprint both in number of systems and building area of the plant. Technical improvements in this part of the plant which can lead to higher thermodynamic efficiency, reduction in capital cost, higher reliability coupled with less downtime and lower maintenance requirements in terms of cost and manpower could have a significant impact on the performance of the plant as a whole. Improvements in energy conversion efficiency affect the total mils/kwh while capital reduction on the nuclear island would only affect part of the cost.

Proposals have been made that future generations of reactors be coupled to direct energy conversion systems such as thermoelectric based or thermionics- -based systems to reduce the current number of thermal-hydraulic systems. In the specific case of LMRs, MHD coupling has been proposed. For the purposes of this report, the discussion will be limited to the classical rotating turbo-machine and the related auxiliary thermal-fluid systems coupled to the electrical generator. Phenomena which then are to be simulated are (1) fluid, (2) mechanical/materials and (3) electrical. Fluid flow expanding through the turbine, heat transfer and two phase generation in the heat exchangers, mechanical stresses and high-temperature materials integrity of the turbo-machinery blades and wheels, and the coupling of the stator and rotor magnetic fields in the electrical generation are all phenomena, more advanced simulation of which could lead to the technical improvements that could result in enhanced performance parameters such as higher energy conversion efficiency. Improved simulation of these phenomena would have to cover not only the static range but also the dynamic range inherent in the plant duty cycle. The plant duty cycle has inherent to it, conditions from normal operation to off-normal transients and beyond to the design basis and the beyond design basis accidents. The transient performance would therefore be continuous from the mild dynamic effects of operational load change to turbine deblading accidents at full power and pressure. In addition to the inherent range of the various phenomena imposed by the dynamics, the computational performance of the simulation codes also have requirements. The two basic applications of the simulation tools would be (1)

Component Computer Aided Design (2) Plant Operation Diagnostics and Control Aid (on-line and off-line). This would then cover the whole range of the plant duty cycle.

VII.B Functional Requirements

For (1) Component Computer Aided Design, the major need would be in accuracy in design of component tolerances such as turbine blade gap clearances, less than fractions of mils to compute bypass leakage losses. Computation time for ultimate usefulness to the component designer would be turnaround in terms of minutes. Component design would not only be aimed at thermodynamic and mechanical efficiency, but would also include issues regarding component reliability and lifetime. Vibration questions, fluid-structure coupling and thermal stress would need to be addressed. These would then lead to the simulation of materials response. Models of materials wear fatigue and failure would also be required to be coupled in.

For (2) Plant Operation Diagnostics and Control Aid, there would be both static and dynamic applications. Off-line application would aid in the management of maintenance schedules. Corrosion, fatigue, and wear and tear on bearings, seals and other subcomponents, if accurately simulated could allow plant management to avoid coolant leaks which could lead to fires. Simulation tools for this function would not need instantaneous turnaround but would require accuracy on the computing of parameters such as crud deposition on rotating shafts leading to pump binding. On-line applications would be operator aids in the computer control of plant integrated systems and require prompt turnaround. Control decisions may have to be made in fraction of seconds with simulation of many potential diagnostic scenarios combined with mitigative actions. This would definitely be a dynamic application and accuracy would also be needed. In both types of applications, interaction and feedback from the plant sensors would be required. This would call for a series of AI based diagnostic and control algorithms interacting with the simulation of the plant BOP. Given that this report restricts itself to conventional turbo-machinery, details of the simulation requirements would be focusing on two major lines of turbo-machine and associated thermodynamic cycle equipment. (1) Single Phase Gas Turbines (2) Two Phase Vapor Turbines

VII.C Current Tools and Approach

In the case of (1) single phase gas turbines, the future focus may be on helium (inert gas) and supercritical carbon dioxide (around the critical point) working fluids [Pino: Need to focus to GNEP systems]. But there are other possibilities such as nitrogen. The thermodynamic cycle utilized would be the single phase Brayton cycle and variations thereof [77]. The usage of and the number of stages for recuperation, inter-cooling and recompression are all variations which need to be treated. In the case of (2) two phase vapor turbines, the future focus may be on supercritical water but there are other possibilities, in particular a mixture of fluids with different boiling points. The thermodynamic cycle utilized would be the Rankine cycle and variations thereof 78]. As with the Brayton cycle, there are potential variations in regenerative heating, pre- and re-heating and superheating features. The discussion at this point will be illustrative using

each of the two cycles with its associated equipment to present issues where advanced simulation capabilities would be of utility. Table VII.I addresses the single phase cycle, while Table VII.II addresses the two-phase cycle. Currently the state-of-the-art to aid in the design of the turbomachinery and the associated component systems, are CFD tools utilized in the simulation of the fluid flow. For the gas turbine cycle, there are a number of specialty codes specifically for the design of turbines, circulators and compressors. Specific gases are treated on a case-by-case basis, allowing for unique features in the cycle such as supercritical fluids operating in a stability range around the critical point. There are also a number of general purpose CFD codes which are being applied to these design problems but the application is more towards the associated heat transfer equipment. One of the key pieces of equipment in this category would the intermediate sodium to gas heat exchanger. This heat exchanger would form part of the primary system boundary and the design for thermal stresses and general boundary integrity would have an influence on the reliability and availability of the plant. Improvements in the computation time of days through improved stability of numerical schemes would be an advance. For the steam turbine cycle, the available CFD codes with two phase capability are limited. A complete steam turbine design without accompanying experiments at this stage is still to be achieved. Not only are there limitations on the turbo-machinery side but also the CFD tools for the design of the two phase heat transfer equipment such as the steam generator are limited. Not only are these two-phase flow equations numerically and computationally challenging but the phenomena modeling equations themselves are the subject of research. The interfacial transfer terms require experimental work and at this point cannot be resolved by simulation alone. Fluid flow asides there are issues regarding fluid structure interaction and associated materials behavior/design questions. There is some existing capability with CFD tools being coupled to structural analysis tools, but the vast potential is still to be explored. The coupling is essentially explicit. So there are possibilities for other numerical schemes.

Table VII.I. Gas Cycle Major Components

(1) Rotating Turbomachinery
1.1 Turbine
1.2 Compressor/circulator
(2) Heat Transfer Equipment
2.1 Recuperator
2.2 Precooler
2.3 Intercooler
2.4 Intermediate Heat Exchanger

Table VII.II Steam Cycle Major Components

(1) Rotating Turbomachinery
1.1 Turbine
1.2 Feedwater Pump
(2) Heat Transfer Equipment
2.1 Steam Generator
2.2 Condenser
2.3 Feedwater Train
2.4 Reheater
2.5 Moisture Separator

In the case of aids for plant operation diagnostics and control there are real-time operator training simulators for two-phase systems and single phase systems but those are for prescribed scenarios where the solution are known a priori. Not only are there these limitations but in addition the phenomenological models are zeroth order. One-dimensional integrated plant system codes used for accident analyses are more detailed in

modeling but as a consequence are not capable currently of real-time and faster-than real time response. Sodium reactor systems simulation codes such as SASSYS [79] and Light Water reactor codes such as CATHARE [80] and RELAP5 [81] are examples of such one dimensional integrated plant system codes. These codes have stand alone models for specialized components such as turbines, circulators and pumps and much more generic thermal–hydraulic components such as pipes, heat slabs ,volumes and junctions which can be connected together to form a general thermo-fluid network. There is considerable flexibility, but for a plant operator aid, a number of scenarios would have to be run faster than real time, for the current AI diagnostic decision making systems to discriminate and filter down the scenarios based on feedback from the real-time measurements. Not only are there opportunities for improvements in the plant simulations but also in the algorithms of the AI diagnostics and control. Current event-based decision making should eventually be replaced by first-principles function-based decision making. There is a need for R&D in this particular area in parallel with the R&D on the plant simulation models. Coupling in the materials behavior simulation models would help in establishing decision criteria. For the ABTR and eventually the ABR, this class of operational aids would significantly improve the availability and reduce the down time of sodium plant systems. Maintenance, inspectability and surveillance of under-sodium components could benefit significantly. A core basis for these operational aids could be the simulation code SASSYS which has been verified and validated for sodium systems and the IGENPRO [82] suite of diagnostic/monitoring tools (MSET/PRODIAG [83, 84]) which have been developed for generic thermal-hydraulic systems.

VII.C Proposed Future Approach

Computer hardware has made major advances in the past and will in all likelihood continue to make significant advances in the future both in terms of speed and capacity. In this approach, message passing may be the choke point which needs resolution for both the component design aid and the operation diagnostics and control aid. Parallel computing and modularity would appear to be optimum approach to take; modules for fluid flow physics interfacing with those for structural mechanics and those for materials behavior. Then the diagnostic/control A-I module could play an overall supervisory role. This calls for a focus on interfacing and in particular on coupling the different physics and the identification and characterization of the key variables. Implicit coupling would have its own special requirements in this approach. There may be some very large property changes which need to be addressed in the stability of the coupling. Fluid flow would have to be coupled to structural behavior and then with the other phenomenological physics and eventually to AI diagnostic and control algorithms. Stability will be a key feature. To determine whether or not progress has been achieved in the R&D areas for this approach, it is recommended that a sequence of target tests be specified in order of difficulty. These tests and their results would form the milestones in this program. The comprehensiveness of the results would indicate what the status of technology is at each stage of the R&D phases. The key in the evaluation of the progress in the milestone for tests would be in the reduction of the need to perform experiments, both developmental and confirmatory.

For the component design aid, certain illustrative future 5 year milestones for the gas turbine cycle [85] are suggested here for initial discussion. Corresponding milestones can be proposed for the steam turbine cycle. For the turbo-machine development, the following specific data needs are to be obtained by simulation alone. These data form the following deliverables and the acceptance criteria would include the target computation time.

- Determine flow velocity and temperature profile at the turbine inlet to quantify potential flow misdistribution.
- Validate analytical performance maps by obtaining the precise configuration of compressor blades and turbine blades derived from simulation.
- Demonstrate journal and thrust catcher bearing performance, electric control system performance, and rotor dynamic stability with prototypical bearings.
- Determine electrical properties of generator windings in a gas environment and obtain insulation data under simulated blow-down conditions to confirm structural integrity.
- Demonstrate the ability of the turbo-compressor casing to contain missiles as a result of turbine deblading.
- Determine turbine rotor vibration characteristics, including rotor natural frequencies and deflection magnitudes.
- Determine static seal system (e.g., seal between the turbocompressor and inlet ducts) performance and determine materials data for segmented piston seal rings and the mating surfaces, with which the seals are in contact. Obtain data on seal coating materials, life expectancy of materials as a function of wear, and the coefficient of friction in gas to be used for resistance to sliding motion.

For the pre-cooler (PC) and intercooler (IC), the following specific data needs are to be obtained by simulation alone.

- Determine the flow distribution and magnitude of hot/cold streaks at various cross sections, including the inlet to the PC/IC tube bundles.
- Determine leak rates for PC/IC high pressure seal arrangement to assess coolant bypass.
- Determine presence of PC/IC flow induced vibration characteristics, such as flow-induced turbulent buffeting, vortex shredding, or fluid-elastic instability, which can cause dynamic instability and tube damage.
- Confirm inspection capability and inspection equipment sensitivity for the specific PC/IC tube circuit geometry.
- Confirm PC/IC shell- and tube-side heat transfer characteristics and shell-side flow resistance and determine the effective flow resistance of the finned tube bundle.
- Quantify the tube side erosion/corrosion rates as a function of the operating parameters, water chemistry ranges, and tube geometry.

The benefits in being able to design without the need for testing and experimental facilities proved very attractive to aircraft companies. Large-scale test facilities and

thermo-fluid experiments can require tens of millions of dollars and can take years to construct and perform. Improvements in generation efficiencies of a few percent for a large reactor plant would be a significant contribution to the capital cost amortization over the plant lifetime. For a fleet of plants it would be even larger.

For the plant operation diagnostics and control aid, the milestone test goal would be to, in five years, implement the operator on-line aid on the plant computer of a test facility and put the system through a limited number of duty cycle events. This would be a real-time test. For the management of maintenance, past data from past power plant system failure events could be used. Determination of status in the R&D progress towards this goal for this part of the program would include:

(1) Portability – can handle different T-H systems and
(2) Accommodation of unanticipated events – can handle events that were not used in the development

with diagnostics (identification of malfunctioning component) of "good" accuracy and transient management (recommendation of sequences of operator action) which are "reasonably" optimal. Criteria for "good" accuracy diagnostics could be (a) no misdiagnosis, (b) 95% of the cases with less than two to three potential candidates identified within a minute of transient time. Criteria for "reasonably" optimal control could be (a) no component damage within the DBA envelope, (b) number of recommended operator steps "fewer" than existing procedures generated by vendor/utility system engineers for existing facilities. To demonstrate this, proof-of-concept testing will be performed for a wide range of transients but only three types will be required (a) mass imbalance, (b) momentum imbalance, (c) energy imbalance. Testing transients will vary in extent/severity and duration from mild/slow (0.01%/hr) to severe/short (10%/minute). The tests will be performed in two stages (i) off-line, (ii) on-line.

(i) Off-line: The test plan for the diagnostics combines the use of synthesized/simulator signal data and post plant instrument data. There are databases of full-scope operator training simulator system transient data for commercial plants. For the transient control, the plan is to test by comparing recommended sequences of operator actions produced by the modules against existing alignment procedures, AOPs, and alarm actions for the same event produced by vendor/utility system engineers for the current fleet of power plants.

(ii) On-line: Accommodation of variations in signals during day-to-day, hour-to-hour operations can be best tested out on-line. In a staged approach, the milestone in five years could be to select an auxiliary system to implement and test the operational aid.

At current rates for electric energy costs, a downtime of days would be worth a few million dollars to a utility for a single large reactor plant. The benefits of a plant operation aid which could make a significant contribution to improvements in plant availability of days over an operating year would be considerable. System-wide, the cost-benefit ratio would be even more significant.

VIII Safety Analysis

VIII.A Background

The functional requirements for safety analysis of advanced liquid-sodium-cooled nuclear reactors are discussed in this section. However, at the highest level, the topics, concepts, and approaches discussed here also relate to other advanced nuclear reactor concepts.

This discussion relates to developmental needs for new computational techniques applied to research, development, and licensing of future generation nuclear power reactors, with special emphasis on liquid sodium-cooled fast reactors.

For research and development, computational analyses tend to be of an exploratory and scoping nature, with a need for flexibility, generality, reliability, and a level of accuracy commensurate with resolution of the technical issues under investigation. Simulations are conducted to produce scoping estimates for planning of experiments and tests, to provide understanding of experiment and test results, and to extrapolate testing results to full-scale design applications.

For licensing analyses, reactor and plant simulation requirements are specifically targeted to quantify performance of structures, systems, and components in the design. The level of accuracy required must be sufficient to assure compliance with design guidelines and standards for design performance, as specified by the designers and verified by the regulators.

In a commercial nuclear reactor, the performance objective is generation of energy as heat, and energy transfer to a power cycle for generation of electricity. Heat created in the nuclear fuel is transferred by conduction and convection to a circulating liquid coolant that carries the heat to the power cycle. Safety analyses are performed to provide confidence that radioactive elements, charged particles, and energy rays created by fission are contained to protect the public and plant employees. Furthermore, the safety analyses must show that power operations proceed while maintaining mandatory safety margins to accommodate equipment failures and operator errors.

The traditional safety philosophy employed in the design of commercial nuclear power reactors is based on the concept of defense in depth. In design, the defense-in-depth concept is manifested by the use of multiple barriers or design features (structures, systems, and components) to provide protection of the health and safety of the public and the plant employees. In addition, the defense-in-depth barriers or systems must be independent and with sufficient diversity to prevent the possibility of a single failure that breaches all the barriers or fails all the systems. For example, the barriers for containment of radioactivity are the fuel cladding, the primary coolant system, and the reactor containment building. The reactor protection system consists of two independent and diverse reactor shutdown systems. The reactor shutdown cooling system provides two (or more) paths for removal of residual decay heat.

Safety analysis simulations for nuclear reactors address the physical phenomena and conditions during at-power plant operation and following shutdown. Heat generation in the fuel is quantified by models of decay heat generation, fission rate, and heat release. The fission rate can be simulated with reactor point kinetics or reactor spatial kinetics, depending on the assumed operating conditions and accuracy requirements. Heat release from the fuel is limited by the heat conductivity of the fuel material, and the thermal resistance presented by the fuel/cladding interface, the cladding conductivity, and the convective heat transfer limits at the cladding/coolant interface. The fuel thermal conductivity may depend on fuel structural and chemical changes caused by irradiation, and the fuel/cladding thermal resistance may depend on geometrical and chemical changes caused by irradiation. Consequently, basic heat generation and transfer models for nuclear fuel are usually augmented by coupled chemical and structural/mechanical models for fuel and cladding irradiation behavior. At the cladding/coolant interface, the heat transfer capability is determined by the coolant properties and flow rate.

In a reactor sized for commercial power generation, there will typically be tens of thousands of cylindrical fuel elements. Safety analyses usually consider only a subset of this number, and the limiting element, called the hot pin or hot channel, is normally identified and analyzed with conservatisms to compensate for phenomenological, manufacturing, and operational uncertainties. The technique of using the hot pin to establish safety margins evolved during an earlier era when consideration of analysis details was limited by computer hardware capabilities.

VIII.B Functional Requirements

The complexities associated with functional requirements for advanced nuclear reactor safety analysis simulations may be categorized according to the objectives of the analysis. For research and development, the objective is to gain understanding of physical phenomena and their interactions relevant to materials and equipment performance in proposed reactor arrangements and operating conditions. In licensing analyses, the objective is to provide a very high-confidence measure of the safety margins, quantified in terms of material temperatures and strengths relative to failure limits.

The essence of research and development is to understand the physical phenomena that govern the performance of materials in engineered applications. The scientific method of gaining such understanding usually consists of observation, model proposal, and validation by testing. Computational analyses are employed to provide numerical solutions of phenomenological models, producing quantitative predictions of material behavior that may be compared to observations from testing. Once validated, scientific models may be applied to investigate the impacts of various initial and boundary conditions and input assumptions, within the validation range of the model. Therefore, the overall functional requirement for the analysis method is to provide a reliable, “best estimate” numerical solution of the proposed model. This function is most often fulfilled in today’s research environment by computational software executing on computer

hardware. Such computational software usually provides not only a numerical solution of the equations representing the phenomenological model, but also graphical displays of solution results and condensed summaries of solution metrics for purposes of reporting. Hence, the functional requirements for simulation are to provide a reliable model solution with efficiency and clarity.

In the nuclear reactor licensing arena, modeling and analysis provides predictions of the performance of reactor systems, components, and structures in relation to safety limits established by regulatory requirements. The models and data employed in the analyses are subject to regulatory review, and hence must present a consensus view by applicant and regulator technical experts for reactor behavior. Uncertainties in the analysis must be quantified to a degree that satisfies a level of confidence set by the regulator. Analyses submitted by the applicant must be reproducible by independent reviewers representing the regulator. The analyses must produce quantified metrics that measure margins to safety limits according to formats and standards established by law, interpreted by the regulator, and documented in published guidelines. The functional requirements for safety analyses in the licensing process may therefore be strictly specified by regulations. However, in every licensing application, there arise situations that require negotiations between the applicant and the regulator because the particular analysis may not be covered by a previous ruling or judgment.

According to format specifications issued by the U.S. Nuclear Regulatory Commission for safety documentation [86], the license applicant is required to define and perform a number of design basis analyses that demonstrate the compliance of the reactor and plant design with the safety design requirements. The analyses must be carried out with a degree of conservatism that envelopes relevant uncertainties. The uncertainties include manufacturing tolerances, material property measurement uncertainties, operational conditions, and computational procedure uncertainties, among others. While the specific design basis simulations depend on the nature of the design, the scenarios must demonstrate that safety systems for reactivity control, cooling, and containment are capable of protecting the public and the plant personnel from excessive radiation exposure in all anticipated, unlikely, and extremely unlikely accident occurrences. (Accident scenarios are classed according to their frequency and consequences). These accident scenarios are normally initiated by an assumed equipment failure (single fault), followed by activation of safety systems to limit accident consequences and prevent releases of radioactivity in excess of regulatory requirements for the class of accident under consideration. The analyses of these design basis accidents (DBA) become part of the license application, and are reported in Chapter 15 of the submitted Safety Analysis Report (SAR).

Although they are not formally part of the licensing requirements, simulations of beyond-design-basis accident scenarios have traditionally been performed to demonstrate the margin of additional protection provided by the design beyond that required by the normal regulations [4]. These sequences are initiated by assumption of an equipment failure and failure of the safety system (double fault) designed to protect against the consequences of the initial failure. By design, the probability of such double fault

accidents is less than one in a million years of reactor operation. Analyses of beyond design basis accidents (BDBA) are usually performed with "best estimate" modeling assumptions, that is, without consideration of uncertainties. For liquid metal fast reactors, the three most notable BDBA scenarios are 1) the unprotected transient overpower (UTOP) accident, in which it is assumed that one or more control rods withdraw and the reactor scram system fails, 2) the unprotected loss-of-flow (ULOF) accident, in which it is assumed that the coolant pumps cease operation and the reactor scram system fails, and 3) the unprotected loss-of-heat-sink (ULOHS) accident, in which normal heat rejection to the power cycle is lost and the reactor scram system fails. Analyses and reactor testing in U.S. and internationally have shown that liquid sodium cooled fast reactors have sufficient inherent safety margins to mitigate the consequences of low-probability, beyond-design-basis accidents, and to prevent the development of conditions (coolant boiling, cladding failure, fuel melting) that could release harmful radiation.

VIII.C Current Tools and Approaches

The limitations associated with existing models used in nuclear reactor safety analysis simulations may be categorized into two areas: geometric and phenomenological.

Traditionally, safety analysis simulations have been limited in the number of fuel elements that could be analyzed, and in the dimensionality of coolant flow directions. There are typically tens of thousands of fuel elements in a commercial-sized nuclear power reactor, and computer hardware limitations have limited the number of fuel elements that could be analyzed in detail to one or a few or several dozen, at most. The principal computer hardware limitations have been processor speed and size of memory. Modern computer hardware development has now progressed to make available relatively fast processors at low cost, and large capacity memories. Further, multiple processors and memories have been coupled to create parallel computer systems that are many orders of magnitude more capable than the batch computers that served as the developmental platforms for much of the existing safety analysis software. The modern expansion of computer hardware capability now makes possible the reformulation of safety analysis software to utilize the greatly expanded hardware capabilities. With this reformulation, the level of geometric detail, in terms of the number of fuel elements considered and the dimensionality of coolant flow directions, can be increased by many orders of magnitude. The consequence of this greater geometric detail will be the reduction of conservatism associated with the averaging inherent in "hot channel" and "hot spot" modeling techniques. By eliminating unnecessary conservatisms, advanced analysis techniques will produce a reduction in uncertainties and a real increase in permitted operational upper limits.

The physical models in existing safety analysis simulation software have also been limited in the phenomenological scope of the representational models by computer hardware limitations. These models include descriptions of reactor kinetics, heat conduction and convection, fluid dynamics, chemical interactions, and structural mechanics. Within each of these areas, individual modeling aspects of physical behavior

has been simplified to meet computational limitations. In addition, the coupling of individual models, representing the effects of non-linear dependencies, has been simplified. For example, dependencies exist among the 1) reactor power and reactivity, 2) fuel, coolant, and structural temperatures, and 3) reactor heat removal capacity. Simplifications of complex phenomenological models and dependencies have been made in past safety analyses to accommodate computer hardware limitations. With the advent of modern computer hardware, these limitations may be removed to permit greater accuracy in representation of physical behavior of materials in design basis and beyond design basis conditions, and hence more accurate assessment of the true safety margins.

The SAS4A/SASSYS-1 computer code system [87] is an example of the current state-of-the-art in liquid sodium-cooled fast reactor safety analysis software. The SASSYS-1 computational path is optimized for analysis of design basis accidents (DBA) and anticipated transients without scram (ATWS), and the SAS4A path is employed to assess the consequences of severe accidents involving coolant boiling, cladding failure, and fuel melting. Both computational paths provide single-pin thermal and hydraulic subassembly models that can be used to represent as many reactor subassemblies as needed. In addition, the SASSYS-1 code has a multiple-pin subassembly model in which every fuel element and coolant sub-channel in a subassembly can be modeled explicitly. The level of geometric detail in the reactor thermal-hydraulic model is limited only by the computer hardware capability (speed and memory size). SAS4A has models for single and two-phase coolant dynamics, fuel element transient behavior, and fuel/cladding melting and relocation. SASSYS-1 adds models for primary and intermediate coolant systems heat transfer and hydraulics, plant control systems, and balance-of-plant components and hydraulic systems. Both SAS4A and SASSYS-1 are coupled to point and spatial reactor kinetics models for prediction of reactor power in transient simulations.

VIII.D Proposed Future Approach

The best approach for future safety analysis simulation capabilities is a dual-path program for research and development analysis on the one hand, and licensing analysis on the other. The research and development path requires highly flexible and robust computational software that can serve as a framework for integration of diverse phenomenological models and databases, capable of simulating proposed and actual experiments and tests. The licensing path requires a significant extension of the phenomenological and geometric capabilities of existing reactor safety analysis software, capable of detailed simulations that reduce the uncertainties inherent in current capabilities and provide a basis for optimal reactor operating conditions. Both paths must implement techniques that take advantage of modern parallel computing architectures.

The objective of the research and development path is to provide a tool that frees the researcher from the burden of model integration and numerical solution, and thus speeds the research and development process. Experience in nuclear reactor research and development has shown that the majority (greater than 50%) of a researcher's time is spent not in creating models and interpreting results, but in obtaining reliable numerical

solutions. Development of dedicated software to reduce the effort needed to obtain model solutions will make researchers more efficient, and shorten the research and development time frame. The new software will integrate user-supplied models with available heat transfer, fluid dynamics, structural mechanics, and chemical analysis software. The integration function of the software will include a user interface that combines maximum flexibility with ease of use. If it were possible to halve the research time needed for analysis, the overall research and development time frame could be reduced by up to 25%.

The objective of the licensing path is to reduce unnecessary conservatism in licensing analyses by providing more detailed geometric and phenomenological modeling capability for use by the safety analyst. From the view of the regulator, the new capability must be seen as an evolutionary development of existing software, providing continuity with current practice. The new approach will replace certain components of the current "hot channel" technique with deterministic modeling, and take advantage of modern computer hardware performance to permit more extensive analysis of reactor operating conditions and situations now bounded by imposition of overly conservative uncertainty factors. The net impact of the new approach will be enhancement of reactor performance. For example, typical coolant enthalpy increase hot channel factors range from 1.04 to 1.08. Assuming that these translate directly to allowable temperatures (and power generation rates), a gain of 2% might be possible by more detailed analysis that eliminates only the geometric uncertainties. For the current U.S. installed nuclear capacity of 102 GWe, this would represent the equivalent of two 1000 MWe nuclear plants.

IX Chemical Separation and Processing

IX. A. Aqueous Processing

IX.A.1 Background

The Global Nuclear Energy Partnership (GNEP) is developing technologies to greatly expand repository capacity, improve proliferation resistance, and recover valuable energy that would otherwise be discarded; thus assuring a stable energy supply for the future. An important element of this initiative is the separation of key radionuclides followed by either superior waste-disposal forms and/or transmutation of long-lived isotopes. To that end, GNEP is developing advanced fuel reprocessing systems that separate key radionuclides from spent fuel using solvent extraction. [88]

In solvent extraction, an organic phase, the "solvent," containing an extractant is contacted with an aqueous solution containing a mixture of metals with which it is immiscible. The two liquids are mixed and then separated. Any of the metals that bind to the extractant are transferred to the organic phase, leaving unbound and thus inextractable metals in the aqueous phase. By repeatedly contacting the initial aqueous solution with new solvent, essentially all of the extractable metal originally present in the aqueous phase can be removed with a very high purity. The extracted metals are then recovered by repeatedly contacting the solvent with an aqueous stream in which extraction of the metals is reversed, i.e. the metals are stripped from the solvent. By this process elements can be separated and purified from a complex mixture such as that which comprises spent fuel. There are several different types of solvent extractors, but the most compact and efficient unit is the centrifugal contactor.

UREX+1a is the baseline solvent extraction process under development to achieve the separations and product purities required for GNEP. The spent nuclear fuel is first dissolved in nitric acid. The dissolved fuel is then contacted with a series of solvents that sequentially extract key components, isolating them from the remaining mixture. The UREX+1a process consists of a series of four solvent-extraction flowsheets that perform the following operations: (1) recovery of U and Tc (UREX), (2) recovery of Cs and Sr (CCD-PEG), and (3) recovery of TRU and rare earth elements (TRUEX), and (4) separation of TRU elements from the rare earths (TALSPEAK). By adjusting process feed compositions and flow rates and the number of contact stages the effectiveness of the extraction can be maximized.

The UREX+1a process is the central operation of an engineering-scale demonstration of an advanced spent fuel reprocessing facility. However, there are many operations within the facility that must be integrated with UREX+1a and with other unit operations in the design of an actual operating plant.[89] The spent fuel must be transferred to the plant, chopped and dissolved. The cold feeds to all processes must be stored. The effluents must be collected and recycled or processed further to generate solid products. Acids, water

and off-gases must be captured and treated for recycle or release. Solidified products must be packaged for storage, transport, or disposal. Plant operations must be scaled based on process stream volumes, processing times, and space requirements for specific equipment.

IX.A.2 Functional Requirements

The design of a chemical reprocessing plant requires the integration of a number of individual unit operations. The design must incorporate detailed models of individual operations which in turn require chemical property data and the manipulation of very complex chemical compositions. Thermodynamic properties must be obtained from databases or calculated from the molecular structures if not available. The lack of detailed chemical properties for many components in spent fuel or used in solvent extraction is a major factor limiting realization of chemically rigorous process models. For many operations where extensive process data does exist, such as distillation, the lack of chemical and thermodynamic properties for a few key component will be limiting.

The modeling of transient operations for both single units and plant-wide is a goal in developing a detailed model of a reprocessing plant. Upstream deviations from steady-state will permeate through the plant, and therefore it is critical to understand the cause of any observed transients and the appropriate real-time responses. The time dependent response of the entire plant is important for process design, equipment design, defining the plant layout, and for safeguards and security. Transient models will be implemented in the development of process control software and in any software that is used to train operators.

In terms of safeguards and security, it is critical to model the expected movement of material both at steady-state and under transients. While existing safeguards technology is well-developed for PUREX, the UREX+1a process has never been implemented at the plant-scale and will required implementation of novel safeguards methods. Detailed models would determine for optimal use of state-of-the-art instrumentation and materials tracking systems. Current analytical methods are limited by measurement uncertainties that can be mitigated significantly by a detailed understanding of process transients--transients that can lead to long-term deviations from the expected process behaviors or stream compositions.

Exiting models simulate ideal systems functioning properly very well. As a result, experimental data tend to diverge from model data where chemical systems begin to diverge from the ideal. This divergence is generally at the margins where concentrations are low or a multiple species contribute to the chemistry associated with a single element. To some extent this divergence is associated with limitations in chemical analysis techniques; however, increasing chemical complexity, particularly for dilute species, where minor bulk species begin to affect the behavior also contributes. Therefore, greater accuracy in these models, particularly as they apply to real systems can be gained in modeling the divergence from ideal systems as the number of species increases from one to two, three or many more.

IX.A.3 Current Tools and Approach

The Argonne Model for Universal Solvent Extraction (AMUSE) [90, 91] is used to calculate flowsheets that achieve the product recoveries and purities required for UREX+1a. The code consists of two sections, SASPE and SASSE. SASPE contains all of the chemical property data and the algorithms that are used to calculate the chemical speciation in a solvent extraction process for a given feed composition. SASSE performs a mass balance for a unit operation given the process flow rates and the number of stages. AMUSE iterates between SASPE and SASSE until the program converges to a solution. AMUSE calculates steady state processes. The capability to model the transient approach to steady state can be built into the model, and it can be modified to track transients derived from process upsets.

Currently AMUSE is a stand-alone application, developed in Microsoft Excel, that is capable of modeling steady-state solvent extraction processes. In the reprocessing plant design, AMUSE must be viewed as a unit operation that can be incorporated at any point in the plant. This requires AMUSE to run efficiently and to interface effectively with other unit operations that are designed using commercial process simulators. Conversion of the AMUSE code to a higher level language is essential since the overhead associated with inter-process communication and the speed at which AMUSE executes in its current form will be a bottleneck in running simulations. After conversion, AMUSE should retain its current functionality plus provide a framework that can easily handle the incorporation of additional solvent extraction methods and chemical components. This will allow for modular additional of other solvent extraction processes where specification of component properties and the chemical speciation is done by user input rather than by recoding. It also should have coding hooks that can communicate easily with external process simulation programs such as Aspen Plus.

A similar solvent extraction simulator, the PAREX code, has been developed by the CEA for design of solvent extraction flowsheets based on PUREX, DIAMEX, SANEX, and other processes. This flowsheet simulator is not commercially available, though modeling results are similar to those obtained using AMUSE.

Several commercial chemical process simulators exist, though the number of suppliers is severely limited. These programs are used to design the chemical processes that are the core of typical chemical plants, though many of these programs are geared to the petrochemical industries. Aspen Plus [92] from Aspen Tech is probably the most global process simulator in terms of range of applicability. Rapid prototyping is available because Aspen Plus has built-in unit operations that can model many processes in a reprocessing plant. As the plant design is fine-tuned, built-in unit operations that do not accurately model an operation can be replaced by customized models. However, Aspen Plus is limited to steady-state models and therefore cannot be applied much beyond the initial plant design. Other commercial products from Aspen Tech, such as Aspen Dynamics and Aspen Custom Modeler will model transient systems. Aspen Custom Modeler provides the most flexibility, but has no built-in models; rather, it is a tool to

solve simultaneous equations. The equations that define specific plant operations are written into the program, and the solution algorithms built into ACM solve these equations. Coupling unit operations within the code allows an entire plant to be modeled.

There are disadvantages to using these commercial packages for designing the plant. Firstly, without a costly license from Aspen Tech, the simulations cannot be run. Secondly, the solution methods are black boxes, and there is no way to examine the underlying source code when convergence problems do occur. Thirdly, the Aspen Tech packages are designed for the wide range of unit operations that are encountered in the chemical process industries and so are not optimized for a unique application like a reprocessing plant. It would be very beneficial to develop advanced solution algorithms to solve this plant design to improve efficiency in attaining a solution, particularly as the plant grows in complexity.

Generally, the accuracy of the chemical process simulators is limited by the quality of the chemical properties database. Therefore a key facet of process design is developing accurate chemical models and the algorithms that can model compounds for which good data do not currently exist. These models must be developed through a combination of experimentation and computation.

Experimental data tend to diverge from model data where chemical systems begin to diverge from the ideal. This divergence is generally at the margins where concentrations are low or a multiplicity of species contributes to the chemistry associated with a single element. As an example, for species that are strongly extracted AMUSE will predict concentrations of 10^{-12} M or lower. These values do demonstrate the major observed behavior of the element. However, in experimental systems the actual measured values may be 10^{-6} M; the difference may be due to analytical limitations, or to contributions from species that are not modeled, or simply to the limits of the model reached. Therefore, greater accuracy in models, particularly as they apply to real systems can help explain the divergence from ideal systems as the number of species increases from one to two, three or many more or where concentrations are low.

In modeling a complex plant, such small deviations over time and across several processes, may contribute to accumulation of significant quantities of a material in streams where these species are not desired. For example the Cs content in the CCD-PEG raffinate may be calculated as 10^{-10} g/L; at a flow of 10 L/min, 1.44×10^{-4} g/day is accumulated in the raffinate tank. If the actual values is 10^{-7} g/L, 0.144 g/day accumulates in the tank, which may result in an off-spec product. To compensate, the raffinate would require additional processing. If this behavior is expected adding additional extraction stages may result in the required decontamination. Improved models of chemical behavior at these margins, would allow these additional process steps to be built into the plant design or to alter processes to account for this behavior in the design stage.

IX.A.4 Proposed Future Approach

Development of a detailed transient model of a chemical reprocessing plant process will contribute to development of: 1) an improved plant design, 2) process control systems, 3) safeguards methods, 4) operator training tools, and 5) tools for post-process analysis. The integration of AMUSE and Aspen Plus will provide a steady-state model in the near-term. However, in the future, a transient model is required to accurately predict the composition of any stream at any point in the process, as would be required for development of accurate safeguards and to ensure that the stringent requirements for the myriad products can be met. Aspen Custom Modeler (ACM) provides the tools to develop a transient model, but requires conversion from built-in Aspen Plus unit operations models to custom-designed models. However, more advanced solution methods may provide significant benefits in plant applications where very complex mixtures occur.

An efficient plant model can be used to aid in the development of, or perhaps implemented in, process control or safeguards systems at the plant. For example, the process control system and its responses to off-normal conditions will be developed from simulations of the expected off-normal conditions. The deviations from normal modes of operation must be discerned as soon as possible, with the magnitude, accuracy, and effect of the appropriate response pre-determined. A highly efficient model may be directly implemented into the process control system if the computational requirements are reasonable. In this case, the mechanical response to an off-normal signal will be derived directly from the simulated process response rather than the process control algorithm.

Advanced safeguards and instrumentation will rely on accurate determination of process behavior. Chemical reprocessing plants based on the UREX+1a process recover high purity uranium and mixed tranuranium oxides for reuse as LWR and fast reactor fuel, respectively. However, there may be off-optimal conditions where components may accumulate in an incorrect stream. It is difficult to detect small-scale deviations because the quantities involved may be within the degree of uncertainty of the analytical methods used to verify the quantities of material throughout the plant. A process model that provides a detailed picture of the global effects of specific small deviations in process plant flowsheets would allow detection of small-scale diviations that may not be detected readily, thus greatly improving safeguards. Operators and “intelligent instrumentation” will be trained to recognize the process-related signatures of a small-scale deviations, and determine where in a plant to optimally locate detection and analysis systems. Because the simulation follows transient operation, the outcome of any change in the plant process flows will be visible immediately, and detection can focus on those segments of the plant.

In terms of chemical accuracy, implementation of detailed chemical properties calculations developed from a more fundamental basis can be tailored for the specific needs of the chemical processing plant. This approach greatly increases the flexibility of such codes to modeling of systems where experimental data are limited. In an experimental plant, efficient and flexible process control and process development models are critical to optimization of operations for eventual implementation at a larger-

scale facility. On a more fundamental level, changes to the chemical structure of extractant molecules can be computationally tailored to achieve higher selectivities for specific elements. Such calculated structures can then be synthesized and tested in the laboratory to achieve the desired improvement in selectivity and product quality and incorporated into novel extraction processes.

IX. B. Pyrochemical Processing

IX.B.1 Background

GNEP is developing pyrochemical processing technologies for treating fuel discharged from advanced burner reactors. Pyrochemical processes or pyroprocesses separate the actinides, for recycle, from the fission products contained in spent fuel by electrochemical or selective oxidation – reduction processes. They typically use chloride-based molten salts as the process medium but may also utilize liquid metals as solvents for the actinides. Pyroprocesses have been studied since the 1950s for treating spent fast reactor fuel and were used to recycle fuel in the Experimental Breeder Reactor I and II. More recently they were developed to close the fuel cycle for the Integral Fast Reactor. They are ideally suited for treating short-cooled fuels as they are radiation resistant, tolerant of the high decay heat generated by the short-cooled fuel, and the molten salt solvent has a high solubility for actinides as actinide chlorides. The compact nature of pyroprocesses favors co-locating a fuel recycle facility with a group of advanced burner reactors. For example, an on-site 10 MTHM pyroprocessing facility could treat fuel discharged from four advanced burner reactor systems. Two types of fuel are currently being considered for use in the advanced burner reactors, metallic and oxide.

A typical metallic fuel treatment process consists of chopping the spent fuel and placing it into anode baskets for use in the electrorefiner. In the electrorefiner, uranium anodically dissolves to form uranium chloride in the LiCl – KCl eutectic molten salt. The uranium chloride serves as a transport mechanism to transfer the uranium ion to the cell cathode where it is reduced and deposited as metallic uranium. Uranium collected on the cathode is reused to fabricate fresh fuel after residual salt is removed from its surface by a vaporization process. The transuranic and active fission product elements (e.g., Cs, Sr, lanthanides) also anodically dissolve in the electrorefiner to form soluble chloride species in the eutectic salt. Noble metals fission products (e.g., Zr, Mo, Tc, Ru) remain in the anode baskets. These fission products are converted to a durable metallic waste form designed for geologic storage. The transuranic elements are recovered from the molten salt solution by electrolysis. During the electrolysis process, the transuranic elements present as ions in the molten salt are reduced and deposited as metals at the cathode of the electrolytic cell while chlorine gas or a salt soluble chloride is produced at the anode. The transuranic metals are used to fabricate fresh fuel after the residual salt is removed.

Spent salt that contains the fission product chlorides is occluded in a zeolite, which is blended with glass frit to produce a durable, leach resistant ceramic waste form.

Treatment of spent oxide fuel requires one additional unit operation that converts the metal oxides to their base metals. In this electrolytic process, the spent fuel oxide is placed in the cathode of the cell and as current is applied to the cell, the metal ions of the metal oxide are reduced to form the base metal and oxide ions are liberated to the molten salt, $LiCl - Li_2O$. The oxide ions transport to the cell anode and are oxidized to produce oxygen gas, which is released from the cell. The cathode containing the base metals is transferred from the oxide reduction cell to the electrorefiner where it serves as the anode of the electrochemical cell. The rest of the oxide fuel treatment process is identical to that described for metallic fuel.

Numerous opportunities exist for the application of advanced simulation tools to the pyrochemical treatment of spent advanced burner reactor fuel. These opportunities range from fundamental electrochemical cell design and performance studies based on first principles calculations to pyroprocessing facility design optimized for low cost fuel treatment. Application of advanced simulation tools will result in decreased development time and lead to enhanced resource utilization.

IX.B.2 Functional Requirements

Many of the pyrochemical processes proposed for implementation in GNEP rely on electrochemical methods for recovering the actinides from spent nuclear fuel. Electrochemical cell design and simulation is needed to advance the state of the art of pyroprocessing. The simulation system should combine thermodynamic, transport and electrodynamic phenomena within the cell to calculate the potential and current distribution within the cell, the concentration profile of the ionic species in the anode, electrolyte and cathode, the extent of reaction or reaction kinetics for the process, etc. The simulation system should be capable of treating gas evolution at the anode of the cell as well as define the constitution of the cathode as a function of time. Ideally the simulation system will allow for cell design, virtual evaluation and optimization prior to experimental validation so that the number of required experiments is reduced.

Beyond electrochemical cell design and evaluation, there exists a need for pyroprocess flowsheet and plant design simulation tools. Flowsheet design tools should have the capability to describe the thermodynamic, kinetic, and transport properties of each unit operation. They should predict product yields, decontamination factors for the process, and provide material balance data. They should be easily configured for evaluating different and competing process options. Additionally, a design and simulation package is needed to construct and evaluate a virtual reprocessing facility. An operational model of the facility should be developed and used to verify the design with respect to throughput requirements, identify process or plant shortcomings, determine bottlenecks, test proposed changes to facility processes for effectiveness, and provide equipment utilization data.

IX.B.3 Current Tools and Approach

Pyrochemical processes have been primarily developed by traditional experimentation methods coupled with limited simulation tools. Previous electrochemical cell models were based on solving special forms of the Maxwell equations for ionic mass transfer in conjunction with Navier-Stokes equations for fluid flow. The modeling was carried out in stages to calculate concentration effects near electrode surfaces as well electric field and current density distributions within the cell. The results of the model were verified against experimental data. However, the system was not used for cell design but rather to elucidate cell operational behavior. With the exception of one recent design study, pyroprocessing plant design has followed a similar pathway. Both activities would greatly benefit from the development of modern simulation tools. Since simulation has played a limited role in pyroprocess development to date, several areas have been identified for development – electrochemical cell design from fundamental principles, process flowsheet simulation for a pyrochemical plant, and an operational model to aid in plant design and optimization.

IX.B.4 Future Tools and Approach

Most of the modern pyrochemical processes proposed for treatment of fuel discharged from ABRs are based on electrochemical cells. In some cases such as electrorefining, the cells are based on design data collected over the past decade but two important technological areas, transuranic element recovery and conversion of UREX+ product from oxide to metal, would benefit greatly from the development of simulation tools. These areas are technically less mature than electrorefining and represent key technology needs for the GNEP. Traditionally electrochemical cells are designed by an experimenter or group of experimenters, they are then fabricated, and their operation evaluated over a range of conditions. This experiment-driven approach can be expensive and can become quite time consuming. A simulation tool will be developed to aid in the design and preliminary evaluation of electrochemical cells. The model will describe the thermodynamic, transport, and electrodynamic phenomena of the electrochemical system evaluating Navier-Stokes and Maxwell equations to determine the reaction kinetics, ion concentration in the electrolyte, and current / potential distribution within the electrochemical system. It will allow the performance of the cell to be evaluated prior to experimental validation. Note that this approach requires an extensive knowledge of the physical chemical properties of the system, which may require additional fundamental studies to acquire the needed data. Parallel computing architecture will be used in place of the more common multi-stage approach to arrive at a solution.

Commercial software exists for modeling process flowsheets but these packages focus almost exclusively on the petroleum industry. Building from these commercial packages, a module will be developed to simulate ABR spent fuel processing by pyrochemical methods. The module will comprise thermodynamic, kinetic, and transport data for each

of the processes as well as data describing unique unit operations such as electrochemical systems. This simulation tool will allow for design of advanced fuel treatment flowsheets, provide guidance for completion of experimental flowsheet demonstration activities, and ultimately lead to the development of optimized flowsheets for pilot-scale evaluation.

In close coordination with process flowsheet simulation, a tool will be developed for a virtual spent nuclear fuel treatment facility (e.g., AFCF) based on pyrochemical processes. The plant design will developed from data for each unit operation in the flowsheet. Plant requirements will be derived from a comprehensive analysis of the interfaces among individual unit operations, between the equipment and the facility, and between the facility and the outside. Process, facility, mechanical and electrical equipment design, operations, maintenance, and safeguarding considerations must be incorporated in the requirements. An operational model will be developed and used to verify the design with respect to throughput requirements, identify design shortcomings, determine bottlenecks, test proposed changes to facility processes for effectiveness, and provide equipment utilization data.

Implementation of these new tools will lead to shorter process development time requiring fewer experiments to validate optimum process parameters and process efficiency, and lead to the design of more efficient and economical plant layouts, which optimize resource utilization.

X Sensitivity and Uncertainty Analysis

X.A Background

Sensitivity and uncertainty analyses are the main instruments for dealing with the sometimes scarce knowledge of the input parameters used in simulation tools. For sensitivity analysis, sensitivity coefficients are the key quantities that have to be evaluated. They are determined and assembled, using different methodologies, in a way that when multiplied by the variation of the corresponding input parameter they will quantify the impact on the targeted quantities whose sensitivity is referred to. Sensitivity coefficients can be used for different objectives like uncertainty estimates, design optimization, determination of target accuracy requirements, adjustment of input parameters, and evaluations of the representativity of an experiment with respect to a reference design configuration.

In uncertainty assessment [93], the sensitivity coefficients are multiplied by the uncertainties of the input parameters in order to obtain the uncertainty of the targeted parameter of interest. The origin and quality of the uncertainties of the input parameters can be different and vary quite a lot. In some cases, they are provided by the expert judgment of qualified designer. In some other cases more useful information is available, for instance from experimental values, and they are cast in more rigorous formalism. This is the case, for instance, of covariance matrix for neutron cross sections, where correlations in energy and among the different input parameters (reactions, isotopes) are also provided.

Design optimization [94] can take advantage of sensitivity coefficients by using them in optimization algorithms. The main problem in this case is related to the fact that in most cases the sensitivity coefficients are calculated with linear approximation. Thus they need to be determined repeatedly to take into account the nonlinear effects. Related to this subject is also the problem of taking into account multi-physics effects. In general, sensitivity coefficients have been evaluated only relative to one field (e.g. neutronics or thermal-hydraulics).

Target accuracy assessments [95] are the inverse problem of the uncertainty evaluation. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data. In fact, the unknown uncertainty data requirements can be obtained by solving a minimization problem where the sensitivity coefficients in conjunction with the existing constraints provide the needed quantities to find the solutions.

Sensitivity coefficients are also used in input parameter adjustments [96]. In this case, the coefficients are used within a fitting methodology (e.g. least square fit, Lagrange multipliers with most likelihood function, etc.) in order to reduce the discrepancies between measured and calculational results. The resulting adjusted input parameters can

be subsequently used, sometimes in conjunction with bias factors, to obtain calculational results to which a reduced uncertainty will be associated.

A further use of sensitivity coefficients is, in conjunction with a dispersion matrix [97], a representativity analysis of proposed or existing experiments [98]. In this case the calculation of correlations among the design and experiments allow to determine how representative is the latter of the former, and consequently, to optimize the experiments and to reduce their numbers. Formally one can reduce the estimated uncertainty on a design parameter by a quantity that represents the knowledge gained by performing the experiment.

Uncertainty analysis can be performed also without the help of sensitivity coefficients. In general, uncertainties on input parameters can be propagated either using a stochastic approach (Monte Carlo methods type) or by some regression techniques. In the case of the Monte Carlo methodology [99], several runs of the same problems are performed with different random input values, taken within the range of the specified uncertainty and associated distribution law, and then at the end the final results are statistically combined in order to determine the average value and the associated standard deviation. Smarter sampling techniques (e.g. Latin Hypercube [99]) for Monte Carlo simulations are developed in order to minimize the total number of direct calculations.

X.B Functional Requirements

An essential attribute of the advanced simulation tool should be the capability to conduct comprehensive sensitivity analyses and uncertainty evaluation. This sensitivity capability has to be based on sound theoretical ground using deterministic and/or probabilistic methodologies. This capability would achieve several goals, including identifying trends and issues, designing a focused set of validation experiments, quantifying uncertainties, and assessing the quality of data used in the design process.

Sensitivity analysis allows true system optimization. The proper use of sensitivity analysis as an integral part of the simulation can lead to more robust systems that can better withstand transients and off-normal conditions.

The sensitivity analysis capability has to be incorporated from the beginning, in the case of writing of new codes, or added for existing ones that are selected and adopted for the design of new plants as an integral feature of the tool.

The following domains have to be equipped with sensitivity analysis capability:

- Neutronics, Fuel Cycle, Decay Heat
- Thermal-Hydraulics
- Structural Mechanics
- Fuel Behavior
- Balance of Plant

- Chemical Processing

In addition, when needed (e. g. safety analysis), coupling among the different fields has to be covered by the sensitivity analysis capability. This implies that nonlinear behaviors due to feedback effects need to be taken into account. Moreover, not only static problems but also time-dependent transient ones have to be treated.

Because of the nature of the sensitivity evaluation (performed in general at first order approximation), the sensitivity coefficients can be calculated at a level of accuracy that is not the same as that of the high fidelity calculation. However, some degree of sophistication will be required in specific cases. For instance, it is very likely that for certain configurations a three-dimensional description would be needed, even if in conjunction with a low level of discretization.

Finally, particular care has to be devoted to assembling the uncertainty data of input values. Quality, consistency, and interrelationship have to be insured. Correlations should be provided whenever available and significant for the impact on the problem under study. This implies a rigorous approach and a scientific based methodology in their evaluation.

X.C Current Tools and Approach

There are two main methodologies developed for sensitivity and uncertainty analysis. One is the forward (direct) calculation method based on the numerical differentiation, and the other is the adjoint method based on the perturbation theory and employs adjoint importance functions. In general, the forward approach is preferable when there are few input parameters that can vary and many output parameters of interest. The contrary is true for the adjoint methodology.

For the forward method, there are several different approaches that can be used. The first one is stochastic (probabilistic with Monte Carlo method) and it has been briefly described in the background section in the uncertainty analysis paragraph. The main drawback of this approach, besides the large number of direct calculations, is the fact that only uncertainty can be evaluated and sensitivity coefficient cannot be directly obtained. The method has been widely used in other fields than nuclear, and it is very popular for waste repository assessments, for instance with the GOLDSIM code [99].

Another forward method is the automatic differentiation. In his case, codes are directly modified in order to evaluate derivatives, through direct calculations, for all input parameters that are deemed to vary. This translates in one direct calculation for each input parameter of interest, and it can be very computational intensive. Moreover, as it was said, it requires direct intervention within the code. Argonne has developed software that directly modifies a code to add automatic differentiation if the used language of programming is FORTRAN or C [100]. Several other universities and lab sites have

software with similar capabilities, though Argonne is the unique US site with both FORTRAN and C code transformation capabilities.

Recently, P. Turinsky has proposed a new forward method based on random perturbation of input parameters. It is claimed that the proposed Efficient Subspace Method (ESM) [101, 102] can efficiently approximate the huge sensitivity (Jacobian) matrix, resulting from a large number of input and output parameters, with a limited number of direct calculations. This method relies on the singular value decomposition technique in identifying the important subspaces of the domain and range spaces of the Jacobian matrix. A major advantage of this method is that no modifications to existing codes are necessary, but only pre- and post-processing of the input and output quantities are needed.

The adjoint methodologies are based on the perturbation theory originally developed in the quantum mechanics field. Classical perturbation theory that makes use of the adjoint function (also called importance), has been widely used in neutronics to calculate the variation of the fundamental eigenvalue. Subsequently, the general perturbation theory was proposed by Usatchev [103], extended by Gandini [104], and implemented in several neutronics codes around the world (e. g. [105, 106]). In this case, a generalized importance is calculated for each output parameter of interest by solving an inhomogeneous adjoint neutron transport equation that contains a source term depending on a specific output parameter.

This type of approach has been extended to other fields including nuclide depletion calculations where the adjoint solution of the Bateman equation is employed [107]. Depletion Perturbation Theory (DPT) [113] calculates the importance functions for the coupled neutron and nuclide field. Oblow [109] and others have extended the adjoint methodology to the thermal-hydraulics field. Cacuci [110], Park, [111] and Gandini [112] have developed adjoint methodologies for time-dependent transient problems for application to safety analysis or reactor operation optimization. Automatic differentiation tools employing the so-called reverse mode are able to compute a discrete adjoint; in practice, the reverse mode requires more user intervention than forward sensitivity computations.

The main drawback of the adjoint methodology is related, as pointed out before, to the number of adjoint functions that have to be calculated if there is a large number of objective parameters. In many cases, the memory requirements for the adjoint method are significant, as many intermediate states must be recorded. Also inconvenient is the fact that the adjoint solution has to be coded directly inside of the code.

Among the existing codes that are widely used, mostly in neutronics, we can mention VARI3D [113] and its DPT version [114] at ANL, the sensitivity capability of FORMOSA [94] system (mainly for thermal reactor applications) at the North Carolina State University, the TSUNAMI [115] (limited only to K_{eff}) and FORSS [116] system at ORNL, the sensitivity and uncertainty modules that are part of the French fast reactor code system ERANOS [45].

In the field of thermal-hydraulics, the only code that has adjoint capability with uncertainty analysis is the balance of plant code CATHARE [80, 117], where also regression is used for uncertainty evaluation [118].

X.D Proposed Future Approach

Integrated uncertainty assessment of leadership class nuclear reactor codes will be achieved by a combination of techniques that leverage very recent advances in computational differentiation and novel mathematical techniques. The challenges posed by the large number of dependent and independent variables and parameters could be met by a combination of stochastic and deterministic techniques.

In the case where the uncertainty assessment involves average quantities, advanced sampling techniques will be developed. Randomized Quasi Monte Carlo (RQMC) [119] techniques will be implemented for assessing the uncertainty in cases where there is a large number of uncertain parameters (such as the cross sections) but the effective dimension is low, as was indeed demonstrated in work by Turinsky [120]. The advantage of RQMC methods is that they need only forward calculations, they are non-intrusive with respect to the various software modules and they exhibit a rate of convergence that is far superior to the classical Monte Carlo method.

To provide effective uncertainty assessment beyond the linearization calculations provided by sensitivity analysis, one can use the derivatives of the objectives with respect to the uncertain parameters, provided by the sensitivity analysis, to generate an importance sampling approach. The latter will be used for the estimation of both the averages and the confidence intervals and probability ranges with far lower variance, and thus it will allow fewer samples compared to brute force Monte Carlo approaches.

The coupling of sensitivity models from the multiple physics models offers a broad spectrum of challenges, not the least of which is a substantial increase in the number of intermediate sensitivity objectives and variables. This would result in huge sensitivity matrices which are generally fully dense and for which even the storage could be difficult on the most advanced architectures. Nonetheless, sensitivity matrices that involve pointwise quantities (such as pointwise temperatures versus pointwise heat generation rates) tend to exhibit an exponential decay with respect to the distance between them, making them effectively sparse. The Bayesian approach currently in use for the detection of sparsity patterns could be extended to the detection of the effective sparsity patterns. In turn, this will result in sensitivity computations that can be carried out and stored on current architectures. The resulting information can be used as the primary information in design of experiments and numerical optimization. For uncertainty assessment, to correct for the error made in the dropping down of small entries in the sensitivity matrices, one can use the resulting approximate sensitivity for importance sampling approaches.

The proposed effort will benefit from the latest advances in computational technologies, including high levels of abstraction that will make the addition of forward and adjoint sensitivity calculations much easier to implement compared to previous efforts. Nonetheless, the adaptation procedures in sophisticated modern simulations such as adaptive mesh refinement and finite tolerance iterative linear algebra make sensitivity calculations far less accurate. To address this one can use a modified PDE technique [121] that gives the same sensitivity results in the limit but that does not differentiate through the adaptation procedures and results in much more robust sensitivity estimates.

XI High Performance Computing Enabling Technologies

XI.A Background

The majority of the simulation projects proposed in this document involve huge ranges of temporal and spatial scales whose full resolution typically leads to systems of equations with upwards of billions of unknowns and beyond. In many cases (e.g. thermal hydraulics and neutronics), even this level of accuracy is not enough to resolve the full range of scales of dynamical importance. One typically makes compromises in grid resolution, physics modeled, number of particles, etc. by first considering the reality of available computing resources (in terms of disk space, RAM, and billions of floating point operations per second (GFlop/s)). These values then both set limits on the largest computation that can be performed (in terms of scales resolved, number of particles, length of integration, etc.) as well as determine what physics must be further simplified and modeled in order to make a computation feasible.

Over the past thirty years, CPU peak performance and memory have roughly followed the so-called "Moore's law", which predicts a doubling of capability every eighteen months. Current state-of-the-art peak single processor speeds and RAM are in the range of 4 GFlop/s and 8Gb, respectively. Fifteen to twenty years ago, when most of the standard simulation tools in nuclear engineering were developed, typical values were hundreds of times less than this. While one might expect that legacy codes could automatically adapt to single processor improvements, this is often not the case -- often the physics has already been greatly homogenized, or physical effects are excluded, promising techniques not explored, and data limits at least implicitly hardwired, precluding the tools efficient use on more advanced architectures.

Single processor performance is only a small piece of the story, though. Far more significant is the trajectory of leading edge, exotic computing platforms that enable orders of magnitude increases in computing speed and memory over conventional desktop tools. Traditionally these machines have been built around a huge range of architectural and design concepts -- the history is too involved to discuss here, but it is worth mentioning two broad categories -- the Cray vector architectures dominant in the eighties and early nineties and the currently dominant massively parallel architectures built typically with cache-based non-vector chips. Massively parallel itself includes dozens of distinctions, from shared to distributed memory, constellation architectures, clusters, vector-parallel hybrids, etc. From the perspective of the (naive) application programmer, though, we can lump together all distributed memory machines, and for them a single programming model has emerged as dominant and become the current de facto standard for accessing these architectures -- the Message Passing Interface (MPI). The emergence of MPI/Fortran and MPI/C as the standard programming model has made general HPC much easier and more accessible to application programmers.

While MPI gives a standard for carrying out interprocessor communication, a major advance of the past decade has been the emergence of a sophisticated layer of HPC "middleware" that abstracts and shields from the application programmer much of the

complexity of designing efficient parallel algorithms, i/o strategies, mesh generation, etc. Popular examples of such tools/stardards are PetsC, HYPRE, Visit, Cubit, Aztec, HDF5 etc. While the ultimate motivation and most of the headlines are reserved for scientific and engineering results, some of the most complex problems and the greatest overall gains in efficiency come from sophisticated implementations of these underlying enabling technologies. Certainly, designing a class of codes that efficiently leverages state-of-the-art computing resources (viz. 100,000+ processors) for first-principles physics simulation requires a substantial investment in supporting HPC tools.

XI.B Functional Requirements

For development and deployment efforts in the multiscale fuel and materials properties modeling, thermal hydraulics, and neutronics components, as outlined in the respective sections, access to tens of millions of cpu-hours on a BG/P or Cray XT3 type leadership-class system will be absolutely required to meet the scientific targets. Petaflop archival and temporary storage systems, high throughput i/o, advanced parallel visualization, and fast data transfer will all be critical requirements of the computing system to achieve scientific discovery. Detailed needs are outlined in the respective sections.

Additionally, the development projects here absolutely must have access to and continue to push the forefronts of research in the following HPC tools/technologies:

- Scalable highly parallel solvers for sparse linear and non-linear systems
- Scalable performance analysis tools for both communication and single node components
- Scalable parallel file systems and higher-level structured i/o libraries
- Efficient architecture-aware compilers (e.g. to achieve double-hummer performance on BG/P)
- Efficient memory and scalable load balancing and data redistributions tools
- a wide range of parallel preconditioner and solver strategies (CG, SuperLU, multigrid, etc.)
- Parallel grid generation for complex geometries
- Tools for language interoperability and component defintion (e.g. Babel)
- Scalable debugging tools
- Assimilation/fusion of experimental data with simulation
- Standardized interface definitions
- Parallel multiphyiscs coupling
- Process workflow technologies/legacy code integration

The above list is not exhaustive but identifies many of the key areas that need to continue to mature in order to meet the eventual goals of the current project. In most areas substantial progress has been made to date (see next section), but the tools will need to continue to evolve to meet the demands of new (petascale) platforms and to continue to improve to meet the increasing application demands. More details are given below.

XI.C Current Tools and Approach

We consider current tools/approaches both from the side of the application and the side of the enabling technologies. From the application side, it is clear that current approaches in the field of nuclear-related simulation have lagged behind state-of-the-art in related disciplines (e.g. weapons simulation, aircraft design, etc.). Many of the examples of such limitations have been provided in the individual sections above. From the perspective of HPC tools and technologies the current limitations can generally be identified:

- lack of use of parallel computing (and thus much less physics or less fidelity in modeled physics)
- lack of use of modern software design principles (and thus code brittleness)
- lack of use of modern software development supporting tools/practices, such as testing suites, repository management, bug tracking, coding standards, auto-documentation, etc.
- failure to leverage existing efficient open source solver libraries
- weak and ad-hoc coupling techniques for inefficient workflow

Form the side of HPC enabling technologies and what is actually available, the state of the art has matured considerably over the past ten years (in large part as a result of the ASC program) both in the commercial but especially the DOE-funded space. Highly flexible parallel linear and non-linear solver libraries (e.g. PetsC, Hypre, ESSL), parallel mesh management frameworks (e.g. SAMRAI, Chombo, Paramesh), efficient mesh generation toolkits (e.g. Cubit), parallel i/o (MPI-IO, HDF5, PNetCFD), performance evaluation tools (e.g. PAPI, Kojak, Tau), advanced visualization (e.g. Visit), and full integrated application codes (e.g. Flash, NWChem) have all demonstrated good scalability (at least for certain problems) and are designed and distributed in a robust and well documented way. The state of maturity of these and other similar tools not mentioned above has enabled a tremendous amount of research and is a major advance in the use of advanced simulation as a tool for discovery. Many of the projects listed above are continuing under SciDAC and similar DOE programs.

XI.D Proposed Future Approach

We articulate the proposed future approach both from the perspective of application needs as well as the enabling technologies themselves. The first-principles physics approach advocated here almost without exception implies the need for leadership class computing resources – that is, as identified in the individual sections, the main physics modules will need to run efficiently on single processor machines (for quick parameter studies) and small to moderate clusters as well as leadership class platforms. To do this, higher-level libraries, such as those mentioned above, should be leveraged whenever possible. This has the effect of increasing the productivity of the application developers and users by offloading much of the burden of scalability, portability, etc. as well as the solver technology to the enabling technology teams. This strategy is particularly

important for the cutting-edge machines that can target more exotic architectures and require a relatively high degree of sophistication to both port and optimize existing codes.

Furthermore, it is absolutely critical that modern software engineering be brought to bear on the group development process. This must be done with great responsibility and sensitivity to some past failures in this area. On the one hand, producing integrated software, particularly in the HPC arena, is an extremely complicated task that quickly becomes an unmanageable disaster if not done in a modern and responsible way. This is particularly true for HPC for two reasons: 1) The physics/numerics results in tight coupling between different physics components and 2) rapid prototyping and evolving architectures are important since the requirements cannot always be fully specified a priori. This does not mean that superior modeling and analysis should take a back seat to fancy software engineering concepts. Rather, improved modeling and usability must drive the process, but it is a process that can only succeed with a dedicated software architect and a clear and modern set of rules/guidelines for the development process (see above). This will need to be an integral part of the current project.

From the HPC tools perspective, significant ongoing work is required to both enhance the existing tools and demonstrate their scalability on the newest class of ultra-parallel machines (as well as maintain and add superior functionality). Furthermore, existing areas of CS engineering/research that impact this area directly and need to mature more rapidly are in the open source arena are:

- General parallel coupling tools (what exists is very specific or not mature)
- Parallel mesh generation tools for finite element meshes
- Advanced parallel visualization for complicated geometries
- Data reduction techniques
- Fast data transfer

Tools to close the peak/realized performance gap (e.g. better compiler technology)

XII Conclusions

This report has presented requirements for advanced simulation of reactor and chemical processing plants that are of interest of the GNEP initiative. Justification for advanced simulation and some examples of grand challenges that will benefit from it have been provided.

In order to effectively deal with the complexity of the problem an integrated software tool that has its main components, whenever possible, based on first principle methodology is proposed. The main benefits that are associated with a better integrated simulation have been identified as: a reduction of design margins, a decrease of the number of experiments in support of the design process, and a shortening of the developmental design cycle. This type of benefits translates in economical savings, but enhanced simulation will also bring, as added value, a better understanding of the physical phenomena and the related underlying fundamental processes, which, in turn, will enable to pinpoint potential, and often unexpected, innovations.

For each component of the integrated proposed software tool background information, functional requirements, current tools and approach, and proposed future approaches have been provided. Whenever possible, current uncertainties have been quoted and existing limitations have been presented. Desired target accuracies with associated benefits to the different aspects of the reactor and chemical processing plant design were also given. In many cases the possible gains associated with a better simulation have been identified, quantified, and translated in economical benefits. For example, a reduction of 2% in power distribution uncertainty it would represent the equivalent of two 1000 MWe nuclear plants when applied to a fleet of 100 reactor plants.

Finally, it should be mentioned that to any advanced simulation software tool development a validation action has to be associated in order to insure the validity, quality, and usefulness of the tools that are developed. The validation would consist of two main components: numerical, and experimental. The numerical validation has to prove that the methodology used is delivering the expected results. The experimental one, where calculational results are compared against those measured, makes sure that also the data that are used are in the simulation are of good quality provided that the employed methodology is accurate enough.

While in the past, the preferred approach has been to use integral (global) experiments for a general validation of both simulation tools and evaluated parameters, a clever innovative validation methodology has to be developed. A set of analytical (differential) experiments has to be devised in order to provide a better physical validation of the fundamental processes that govern the macroscopic behavior. An advanced simulation can surely provide the tools and insights to this purpose, but this novel validation constitutes per se a new big challenge that will require ingenuity as well imagination for its development.

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