

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

## White Paper on Integrated Performance and Safety Codes

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This white paper discusses some key requirements for integrated performance and safety codes (IPSC) for nuclear energy systems. By IPSC we envision a suite of modern, integrated simulation tools that model the key physics relevant to both design optimization and licensing for the different stages of the nuclear fuel cycle – the separations plant, the reactor, fuel design, waste forms, repository, etc. The discussion is not intended to be exhaustive or encompassing; rather, it focuses on the challenges in modeling key physical phenomena common to many of the domain areas. The reader should be left with an appreciation of the complexity and unique requirements of some of the models, in particular as they relate to the need for extreme computing.

All of the IPSCs envisioned here share certain important features. Foremost is the goal of pursuing a “science-based” approach – solving the governing equations of motions on detailed three-dimensional geometries with minimal empirical calibration. That is, the goal focuses on modeling the basic physics rather than strictly the behavior of a specific device. By the term science-based we do not mean to imply that all scales of motion are explicitly accounted for. The IPSCs ultimately must include whole device models, and to carry out these simulations in many cases sub-grid models will be required. The goal is to formulate these models using a combination of basic theory and localized, highly detailed numerical experiments.

Our basic tenet here is that the science-based approach is inexorably linked to the availability and exploitation of high-end computing hardware together with robust and efficient solver technology. The new paradigm is to use numerical simulation much more as a predictive tool, carried out in advance of physical experiments, and with the goal of minimizing, targeting, and better instrumenting the corresponding experiments. This process obviously requires an extremely thorough and exhaustive analysis of the predictive capability of codes, both vis-à-vis their numerical formulations (verification) and their demonstrated ability to mimic measured physical phenomena (validation). A comprehensive validation and verification strategy a priori is thus critical to the success of the IPSC project. This strategy is discussed in a companion V&V white paper.

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Additionally, the incorporation of highly predictive simulation tools has the potential to reduce the regulatory timeline greatly, currently a major component of the overall economics of the design of nuclear facilities. Through the use of advanced simulation, the probability and/or consequences of complicated accident scenarios can be explored with minimal reliance on full-scale testing. Component and small-scale tests can potentially be more easily extrapolated to full device behavior by per-component validation together with integrated device simulations. An important aspect of the ISPCs is that such a deviation from traditional practices will require a close connection between the regulatory agency and the code development teams early in the process.

All of the ISPCs require highly detailed simulations that couple various physics across a wide range of length and time scales. This includes carefully developing framework strategies that facilitate integration among various subsets of the available physical models according to the needs of specific calculations. Highly detailed simulations might be used, e.g. for late stage design studies, or to develop parameterizations for full-device models for a particular geometric configuration. Coarser models might be employed on mid-range computing clusters to carry out broad parametric studies. Even for a single IPSC, the range of physical effects to be modeled is far too large to be covered in this brief document. Instead, we focus on exascale computing needs for some of the relevant physics common to most domains -- including neutron transport, fluid flow, fuel behavior and a range of structural mechanical issues.

### Neutron Transport

Two general classes of methods, **Deterministic and Stochastic**, are currently used for simulating and modeling nuclear reactor problems, particularly neutron interactions. **Deterministic** methods have always played a fundamental role in reactor modeling and simulation. A first principles treatment requires solution of the linear Boltzmann transport equation which for practical applications demands enormous computational resources because the problem has seven dimensions: three in space, two in direction, and one each in energy and time. For several years the resource requirements of neutron transport calculations have dominated those of all other physics components in multiphysics simulations. The advent of high performance computing has helped reduce the computational burden, however the scalability of parallel algorithms for solving the transport problem have been limited in part because of the basic source iteration technique used to solve the equations.

One of the important current research efforts in advanced Boltzmann solvers for reactor applications has been the effort at ANL as part of the **DOE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program**. The UNIC code is being developed at ANL to solve large-scale nuclear reactor core problems governed by the seven dimensional (three in space, two in angle, one in energy, and one in time) Boltzmann equation. The goal of this simulation effort is to reduce the uncertainties and biases in

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reactor design calculations by progressively replacing existing multi-level averaging (homogenization) techniques with more direct solution methods. Currently UNIC has two solvers for the neutron transport equation which are based upon the second-order even-parity transport equation and utilize a spherical harmonics and a discrete ordinates approximation for the angular approximation. A third solver based on a first-order method of characteristics has also been implemented in order to provide a more efficient capability of explicit geometry modeling. UNIC uses an unstructured mesh and to represent the complex geometry of a reactor core, billions of spatial elements, hundreds of angles, and thousands of energy groups are necessary, which leads to problem sizes with petascale degrees of freedom. These calculations can exhaust memory resources on current and even next-generation architectures. ANL has evaluated the performance of UNIC and the potential impact of higher-fidelity methods for two representative fast reactor problems (PHENIX and ZPR-6) by using the leadership computing platforms at Argonne and ORNL. In each case, UNIC showed a weak scalability of over 80% on up to 163,840 cores of BlueGene/P (Argonne) and 131,072 cores of XT5 (ORNL). One focus of continuing research efforts will be to improve the per-processor performance while maintaining the high parallel efficiency which can be achieved with better algorithms (such as spatial p-refinement, multilevel preconditioners, and weighted partitioning for load balancing). Because the dominant computational phase in UNIC is the conjugate gradient method which exhibits memory bandwidth limited performance, it is not anticipated that near peak performance can be achieved on leadership class computers. However, ANL appears to have set a new standard for achievable parallel performance with UNIC for the solution of the deterministic neutron transport equation.

The second class of methods for reactor analysis is **Monte Carlo** methods which model the nuclear system almost exactly and then solve the exact model stochastically anywhere in the modeled system. Monte Carlo methods are based on first principles nuclear reactions and therefore provide greater accuracy and efficient parallel algorithms for particle tracking at the extreme computing level but also face many significant challenges. For reactor applications, Monte Carlo codes have long been used to calculate integral parameters such as the effective multiplication factor or **a reactivity coefficient** of a reactor, even when all geometrical detail of each individual fuel pin of each fuel assembly is modeled. However, when more detailed information is required such as the local power density, possibly for small regions of a fuel pin in the axial and/or radial directions, it is much more difficult to achieve acceptable results with respect to the standard deviation within a reasonable computation time. This becomes even more difficult if results for a large number of tallies are required, for instance the local power densities in all fuel pins, subdivided in a number of axial and possibly radial regions. Nonetheless, this is the requirement for current design calculations of a nuclear reactor core.

In an invited lecture at the M&C 2003 conference, Kord Smith [1] formulated the challenge for future Monte Carlo simulation as the calculation of the local power of each of the fuel pins in a fuel assembly when subdivided in 100 axial and 10 radial zones for burnup calculations. The number of fuel pins in a fuel assembly of a PWR core is about 300 while the number of fuel assemblies in a reactor core is around 200. This results in

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total of about 60 million tallies. For an acceptable result, Smith specified the standard deviation in each local power region should be 1 % or less. In addition, Smith considered 100 different nuclides for which the reaction rate is needed, bringing the total number of tallies to 6 billion. These huge numbers of tallies not only pose a problem in CPU time but also in computer memory. Smith estimated on the basis of Moore's law that it will be 2030 before such a full core Monte Carlo calculation could be done in less than one hour on a single CPU. Bill Martin [2] analyzed the situation in some detail in his invited lecture at the M&C 2007 conference. Assuming that Moore's law manifests itself as only more cores in a desktop computer, Martin estimated that it would be 2019 before a full reactor core calculation with 40,000 fuel pins and 100 axial regions and 1 % statistical accuracy for local power estimates could be accomplished. There are several reasons why the advances in efficiency of full core Monte Carlo reactor calculations may be better or worse than estimated above. However, it appears certain that Monte Carlo codes will not be able to calculate the power density distribution in a full size nuclear reactor core with sufficient statistical accuracy within the next 10 years, especially when considering the additional complexities such as thermal feedback and error propagation for practical core applications such as fuel depletion.

It therefore appears that for practical reactor core modeling and simulation, deterministic methods will be used principally in the short term (3–5 years) with Monte Carlo as a benchmarking tool. In the intermediate term (5–10 years) Monte Carlo methods could be used as a hybrid tool with multiphysics coupling to deterministic neutronics and thermal hydraulics codes. One of the promising research efforts in hybrid Deterministic / Monte Carlo methods has been the work at ORNL in the development of the SCALE-6 nuclear analysis suite. The MAVRIC sequence in SCALE-6 incorporates a new, three-dimensional, discrete ordinates (SN) transport code, Denovo, with a modern Monte Carlo transport solver, Monaco. The released version of MAVRIC is designed for nuclear shielding and radiation dose assessments, but on-going development includes the extension of Denovo for reactor simulation applications. For somewhat simplified problems, Denovo has been demonstrated to scale to 40,000 processors of XT5 (ORNL) in a simulation of an entire PWR facility that completed in just over an hour (with setup and I/O) and included over 1 billion spatial elements, 27 energy groups, and 624 directions ( $1.7 \times 10^{13}$  dof).

It is evident that both deterministic and stochastic methods will play an important role in the near and long-term applicability for high-fidelity nuclear reactor physics simulations and. However, significant research must be performed if these methods are to fully benefit from extreme computing. Fundamentally new solution algorithms should be developed for **deterministic methods** in order to achieve maximum parallel performance. A key feature of these methods would be adaptability in all seven dimensions. Current adaptive methods generally relate only to spatial adaptivity and the extension of such capability to angle and improved energy discretization techniques are necessary to achieve the highest efficiency for the Leadership-Class Computational Platforms and to make presently intractable problems possible. With regard to **Monte Carlo methods**, further extension of **hybrid deterministic/Monte Carlo** algorithms are important to more efficiently compute the spatial distribution of neutrons throughout a

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reactor geometry on a non-orthogonal grid of cells, particularly in support of multiphysics coupling. The use of Monte Carlo methods for practical reactor applications will also require research on methods to achieve a tighter integration of reactor depletion and kinetics, as well as methods to propagate the uncertainties in the nuclear data along with statistical uncertainties throughout the reactor depletion/kinetics process.

Science-Based approaches for the design and analysis of nuclear reactors are clearly an achievable goal with extreme computing. While the research challenges are substantial, the long term benefits of reducing the reactor innovation cycle and the need for time consuming and expensive experimentation provide more than an acceptable return on the near term investment.

### Thermal Hydraulics

Thermal hydraulic (TH) analyses are a critical aspect of both the design optimization and safety analyses of reactors. This includes very detailed understanding of heat transfer and mixing processes to predict hot spots, detailed temperature distributions, a wide range of whole plant analyses related to safety, as well as localized phenomena such as thermal striping, fretting, and flow induced vibration.

Even for non-boiling flows (such as in normal operating conditions in a Liquid Metal Fast Breeder Reactor (LMFBR) or Pressurized Water Reactor (PWR)) generally speaking a first-principles direct numerical simulation (DNS) of the Navier-Stokes equation across the entire domain of interest is not possible even on existing high-end computational resources. This is true for a range of fluid phenomena – mixing in the upper plenum, stratified pipe flow, heat exchanger analysis, etc. Probably the most canonical and important example though is heat transfer in a rod bundle. A typical *per-channel* Reynolds Number is in the range 10,000-100,000, rendering DNS of even a single channel at the far reaches of existing high-end computational capability.

To focus on a specific example, typically fast reactor designs call for sodium-cooled rod bundles, arrayed in a triangular pitch within hexagonal subassemblies comprising 217 pins. Each subassembly is hydrodynamically isolated by subassembly walls and fuel pins are separated using either wire wrap spacers or spacer grids. The choice and design of the spacers has a direct impact on pressure drop through the core and on coolant mixing, which influences peak fuel pin temperatures. Understanding of these flows is thus important for estimating pumping power and realizable power output. Because of its central importance to reactor performance, rod bundle flow has been chosen as the initial test problem to drive the advanced thermal-hydraulic simulation development within the DOE/NE NEAMS Program.

During normal operation, coolant is forced through the channels between pins and between the pins and the walls. The wire-wrap spacers serve to direct flow between adjacent channels and thus enhance cooling of isolated hot pins. There are three channel types—interior, edge, and corner (respectively, 384, 48, and 6 of each in the case of 217

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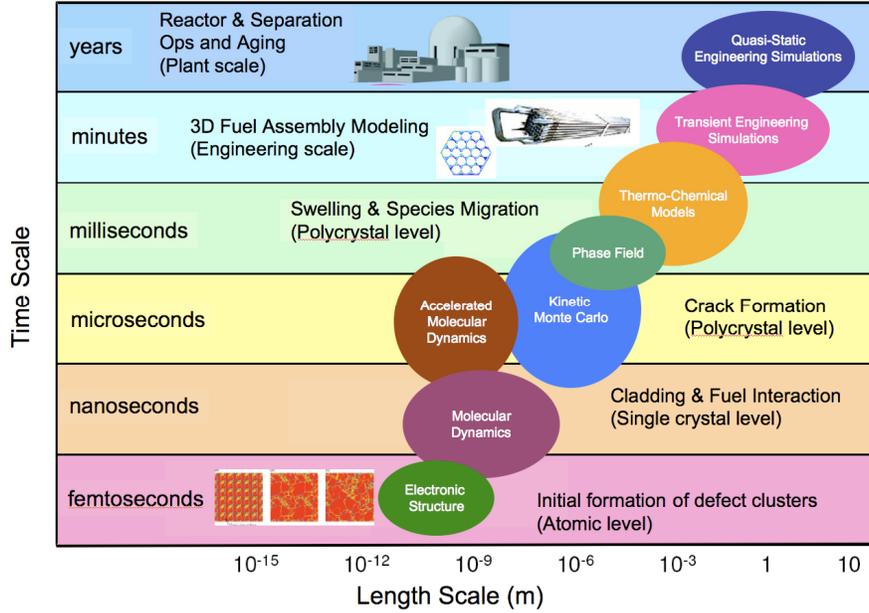
pins). While the bulk of the flow passes through interior channels, bypass and perimeter swirl flow through the edge channels can significantly impact the overall cooling; alternative channel configurations are thus of interest. Moreover, the influence of the edge channels inhibits direct extrapolation of low pin-count tests (numerical or experimental) to higher pin counts. Typical Reynolds numbers are  $Re_h \sim 50,000$ , based on channel hydraulic diameter  $D_h$ , which implies fully turbulent flow. The corresponding Peclet number is only  $Pe_h \sim 350$  because of the high conductivity of liquid Sodium.

Unfortunately, the geometric- and scale-complexity of turbulent flow through  $> 400$  channels, each of length  $L > 500 D_h$ , precludes the use of first-principles-based direct numerical simulation (DNS) or even large-eddy simulation (LES) for a full 217-pin subassembly. Consequently, the advanced TH simulation program is built on a hierarchy of simulation capabilities, each operating at differing scales. DNS and LES are used to compute fine scale turbulence in relatively simple geometries with a minimum of turbulence modeling assumptions (none, in the case of DNS). With significantly less computational effort, Reynolds-averaged Navier-Stokes (RANS) simulations are used to compute the mean flow effects in more complex domains. RANS simulations rely on turbulence closure models that are often case-specific. The RANS models are thus validated against corresponding LES simulations in small domains that are tractable with LES. Finally, at the design scale, “subchannel” codes are used to rapidly predict heat transfer without accounting for the geometric complexity of the spacers. Subchannel codes rely on empirical velocity field data, which in the past was provided solely through experiments. Advanced simulation will supplement the experimental database in new design regimes.

## Nuclear Fuel Modeling

The challenge of simulating nuclear fuels is to develop analysis capabilities that span widely disparate length and time scales, as shown in Fig. 1. This figure relates the fuel physical phenomenon occurring at each scale along with the modelling methods applicable to that scale. Figure 2 shows typical inputs and outputs and phenomena that need to be modelled in a fuel performance code (taken from D. Olander with some additions) and given particularly for a metal fuel.

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**Figure 1. Multi-scale challenge.**

First principles lower-length-scale (smaller than engineering scale) modeling of fuel behavior under irradiation has been pursued in the past. However, limited computer power prevented comprehensive mechanistic modeling informed by atomistic, molecular and meso-scale insights. Indeed, many atomic scale fundamental issues related to fuel performance remain unanswered. The IPSC project is poised to make significant advances by necessarily bridging time and length scales, thus informing higher length-scale models with lower length-scale insights. Such multi-scale simulations will be based upon accurate atomic scale physics not currently present in fuel performance codes. Furthermore, basing IPSC on an accurate representation of the fundamental phenomena allows for it to be predictive across a wide range of fuel compositions, reactor conditions, etc. The development of first principles informed mechanistic models will be significantly aided by HPC capabilities. Our increasing computational capabilities allow micro-scale representations of the materials and physics to inform the system-level simulation.



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in simulations where conditions are too harsh for direct observation. More importantly, the application of the capabilities to model the fuel behavior under normal and accident conditions will be possible for licensing process.

As the modeling and simulation progresses towards more fundamental modeling and away from a heavily empirical approach, considerable efforts will be needed to couple the phenomenology at different length- and time-scales (hereafter referred to as “scale-bridging”). The scale-bridging concept is also a key for the successful management of the program towards a common objective. Figure 3 shows a recently developed hierarchical multi-scale modeling and simulation (M&S) concept for clad materials (developed by Arsenlis, Tome, Lebenso, Maloy, and Unal). The green boxes in this figure represent codes/tools we need in each scale. The yellow boxes represent the information required as input and output coming from each tool. The fuels performance code at the engineering scale is at top level. This code communicates with Visco Plastic Self Consistent (VPSC) code developed for poly crystal scale. VPSC takes strength and creep laws generated by the single crystal level simulations and produces homogenizations for the development of poly crystal strength and creep laws to be used in the engineering scale. The engineering scale code inputs temperature, dose and strain (or stress) of a finite element volume and VPSC code returns stress (or strain) at input conditions.

Figure 4 includes all other modeling and experimental needs. In this paper, we don’t discuss the details of each box because of page limitations. Each scale is extended as shown in Figure 5 for poly crystal scale simulations. Necessary input coming from lower length scale simulations are identified. The experimental and validation requirements are given with the risks involved in the proposed approach. The rough schedule is also included to give an idea the expected time requirements of the research and development needed. Simulation maps for each scale are developed but not included. A similar simulation map is being developed for fuels modeling that will be more complex than clad modeling. It is likely that a different simulation maps for oxide and metal fuels.

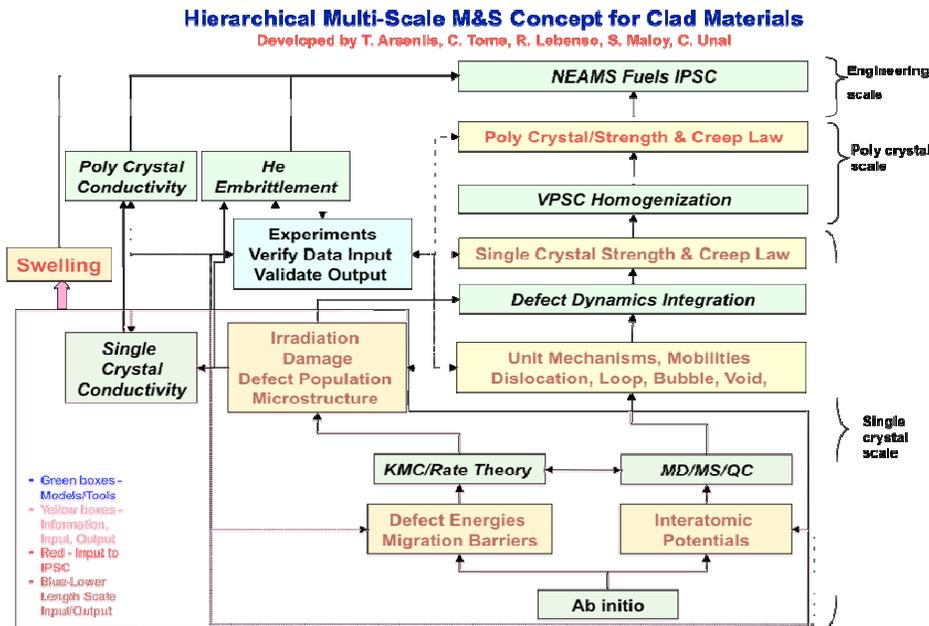


Fig. 4. A hierarchical multi-scale M&S concept for clad materials.

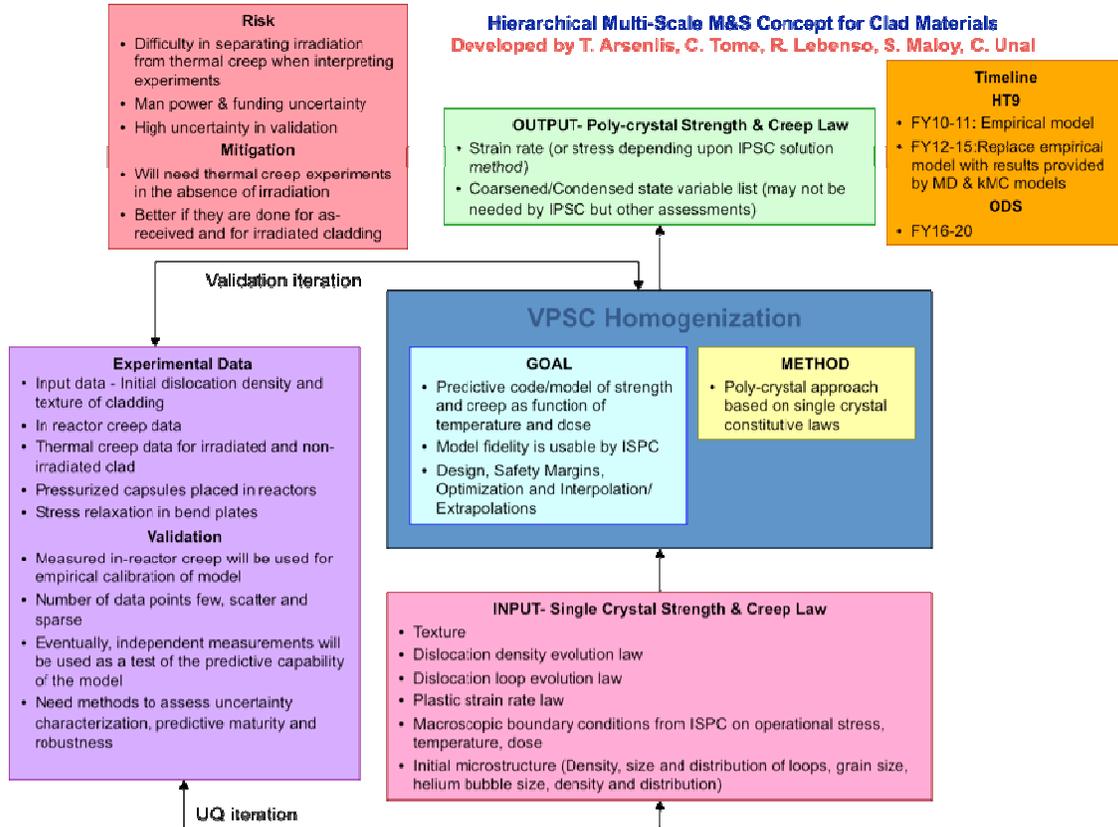


Fig. 5 Poly crystal scale simulations with input/output, experimental and validation requirements.

## NEAMS FUELS IPSC TECHNICAL CHALLENGES

### Radiation induced micro-structural evolution

The nature of radiation induced micro-structural evolution and the associated property changes require a multi-scale approach to their understanding and mitigation. Primary damage formation occurs on a time scale of femto-seconds to picoseconds in a volume of a few cubic nanometers. This involves very high local energy transfer events (both electronic and nucleonic), creating both point defect and fission product formation. The primary deficiencies in this multi-scale modeling scheme are the lack of well-defined methods for directly linking models operating at different scales and strategies for determining when tight linking is appropriate (as opposed to simple information passing).

### Electronic structure methods for actinides

The need to develop robust electronic structure methods for actinides in which the behavior of 5f electrons is strongly correlated and requires the consideration of

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relativistic effects is a major scientific challenge. A new underlying theory is needed to compute fundamental properties such as defect formation and migration energies in both the pure metals and compounds (oxides, nitrides, carbides) involving these metals.

### **Thermodynamic quantities in UO<sub>2</sub>, PuO<sub>2</sub>, and mixed-oxide fuels**

A fundamental understanding of thermodynamic quantities in UO<sub>2</sub>, PuO<sub>2</sub>, and mixed oxide fuels is needed. This problem is strongly related to the electronic structure issue described above. The presence of the actinides makes the chemistry of nuclear reactor fuel initially complex, and continuous loss of U and Pu and formation of a broad range of new species due to fission introduce a challenging time dependence to this chemistry. The fuel ultimately contains multiple f electron elements: U, Pu, Am, Np, and Cm as well as many lighter elements. This situation leads to the potential formation of many phases that can influence critical physical properties such as thermal conductivity.

### **Meso-scale modeling**

Model development is required at the meso-scale for simulation of micro-structural evolution of fuel and the effects on thermo mechanical response of fuel. The challenges are both computational and conceptual. Defect generation information obtained from atomistic simulations indicates the need for simulating the interaction of irradiation induced point defects with the microstructure (grain boundaries, dislocations, second phase precipitates, gas bubbles, and voids) and its evolution. Such simulations must incorporate all relevant grain boundary and dislocation processes, gross deformation processes such as crack nucleation and propagation, and transport phenomena to account for fission product migration and precipitation. Approaches for combining methods such as front tracking and phase field models into an integrated meso-scale model may offer the opportunity to advance the state of the art.

### **Modeling of fuel cladding and core structure**

The modeling and simulation needs for fuel cladding and core structural materials have certain similarities. However, the radiation induced phenomena are quite different (creep is most critical for the brittle ceramic fuels while visco-plastic deformation is responsible for cladding deformation). Current *ab initio* theories need much improvement, with the primary needs being the ability to scale up with temperature and to evolve from pure metals to complex, multi-component alloys. Eventually, the theory should include magnetism in ferritic alloys.

### **Integral fuel performance code**

The development of a next generation integral fuel performance code that is based on state of the art physics models is a major engineering need for the fuels IPSC project. The development and use of this code have direct safety and licensing implications. For example, the chemical form and location of fission products and fuel cladding integrity largely dictate the source term in many accident scenarios. This challenge requires that

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many other challenges be solved first: e.g. fission gas retention and release, thermal conductivity variations with composition, burnup, etc.

The integral fuel performance code is supported by the lower-length scale simulations those themselves may require high performance computing capabilities. Thus, the interfacing between integral fuel performance code and the lower-length scale simulations are not defined clearly yet. Ideally, the strategy would be the development of an integrating modeling and simulation data management framework that can interface between multi-scale modeling capabilities and data for a desired fuel safety and licensing calculations.

### **Integrating NEAMS VU Program into the IPSC Project and Experimental Needs**

The NEAMS program supports a separate VU program element that is responsible for developing necessary tools and frameworks for verification, validation, uncertainty quantification of modeling and simulations. The development activities are done at different organizations. The collaborations and cooperation between these organizations is necessary in order to develop useful and practical tools. The validated as borne concept is also necessary to provide validated IPSC's.

The development of lower length scale models may require different types of experiments than what AFCI TFC plans to conduct. These experiments are not clearly defined yet and may depend upon the fuel types. The experimental requirements by all scale model and simulation activities are going to be developed in the first several years of the program as we understand the needs better.

## **FUELS IPSC M&S CAPABILITY REQUIREMENTS**

The modeling and simulation requirements for fuel performance (given fuel and cladding type, fuel element design, and reactor environments) are as follows:

- The ability to predict the fuel element safety margin during normal reactor operation and design-basis accidents. A safety margin is defined as the margin between the nominal thermo-mechanical state of the fuel element and its acceptance threshold.
- The ability to predict when a fuel-element-cladding breach will occur.
- The ability to design fuel (including cladding) for optimal performance

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**Table 1. Key Fuel Performance Modeling Capabilities**

<b>M&amp;S Capability</b>	<b>Why Capability is Needed</b>
Temperature distribution throughout the fuel element	Maximum fuel and cladding temperatures are set by the design limits of the fuel element. To predict the margin, the code must constantly check the nominal temperatures against the design limits.
Stress-strain state, dimensions of the fuel and cladding, and the fuel-cladding mechanical interaction	Maximum cladding strain is set by the design limits of the fuel element. To predict the safety margin, the code must constantly check the nominal cladding strain against the design limit. Fuel dimensions affect core criticality, which influences reactor control. Cladding dimensions affect coolant flow in the subassemblies.
Irradiation effects in fuel, such as change in actinide and fission product inventory, fission gas release, constituent redistribution, oxygen redistribution, restructuring, solid and gaseous fission product swelling, cracking, densification, and creep	Irradiation alters fuel material properties impeding heat transfer in the fuel element and causing the fuel to operate at a higher temperature to generate the same amount of energy. Maintaining the fuel temperature within the design limit while coping with irradiation-induced degradation of the fuel and cladding is the main fuel safety challenge. Irradiation effects cause the decrease of the fuel melting temperature.
Irradiation effects in cladding such as material degradation, irradiation-induced creep and thermal creep, swelling, hardening, and embrittlement	The degradation of properties of core materials determines the service life of fuels in a reactor. The core (cladding and duct) materials in a fast reactor are exposed to an extremely challenging environment including neutron irradiation, liquid metal corrosion, and fuel interaction combined with significant stresses depending on the location. Irradiation effects in cladding reduce cladding load bearing capacity. Thermal creep is a primary failure mechanism of some cladding types Creep and swelling contribute to the cladding strain.
Cladding wastage due to fuel-cladding chemical interaction and coolant-cladding chemical interaction	Cladding wastage reduces cladding thickness, thus reducing cladding load bearing capacity. Fuel-cladding chemical interaction results in low-melting products, thus reducing maximum allowed fuel operating temperature.
Cladding failure criteria	Cladding failure criteria must be determined in order to predict cladding breach and service time limit to breach.
Heat transport from the clad into the coolant across the span of steady-state operation and design-base accident environments	To provide proper characterization of fuel and cladding behavior to provide other M&S capabilities.

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[2] William Martin, Invited Keynote Address, Joint International Topical Meeting on Mathematics and Computation and Supercomputing in Nuclear, April, 2007, Monterrey, CA.