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Materials Models and Simulations in Support of Nuclear Fuels Development

Report based on the results of the first three editions of the
Materials Models and Simulations for Nuclear Fuels workshop series
organized by Los Alamos National Laboratory
sponsored by the US Department of Energy, Office of Nuclear Energy
the Advanced Fuel Cycle Initiative program

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with contributions from workshop participants

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Executive Summary

The Materials Models and Simulations for Nuclear Fuels workshop series is organized by Los Alamos National Laboratory, under the auspices of the Advanced Fuel Cycle Initiative program, funded by the Department of Energy of U. S. A. The workshop series aims at stimulating research and discussions on models and simulations of nuclear fuels and coupling the results into fuel performance codes.

The MMSNF workshops started in 2003 with the models and simulations components and over two years attracted many fuel performance people. At present, the two components are better balanced but the integration process is far from being completed.

After 3 editions, the number of scientists, engineers, and managers involved in the MMSNF workshops has reached a relatively stable number of 50. The participants included materials scientists, physicists, chemists, nuclear engineers, computational scientists, software engineers, and managers. There is however a much larger community interested in the workshop subjects and the organizers [M. Stan (LANL), J. Tulenko (Univ. of Florida), and K. Pasamehmetoglu (INL)] need to reach out to them.

Based on the workshop results, a strategy for a combined fundamental and applied research is proposed. The proposed research program targets the development of new, theory based, models of nuclear materials properties and the design of an advanced fuel performance code.

During the last four years of combined theoretical and experimental efforts, models and simulations provided valuable information about materials properties and important phenomena associated with nuclear fuels. However, as of today, models and simulations are still not regarded as critical tools for fuel design and optimization. One of the reasons is the lack of predictability specific to methods based on empirical correlations.

The idea of replacing empirical correlations with theory-based models for the purpose of improving high performance simulation tools was inspired by the DOE sponsored work on alloys and stockpile stewardship. In that program, advanced models and simulations integrate theory, experiment, and computation. In a similar way, advance fuel performance codes can incorporate advanced models and simulations rather than empirical correlations.

During the workshops and follow up discussions, various models and simulation methods have been analyzed and participants made suggestions regarding long and short-term theoretical efforts that can help with improving the models. A large number of materials properties that influence nuclear fuel's behavior in operation have been reviewed. Among them: thermo-mechanical properties, chemical properties, microstructure, and defects.

To address all relevant natural phenomena, models and simulations have been developed for various time and space scales. That includes electronic structure, atomistic and continuum models, and simulations of phase stability and phase transformations, deformation, chemical reactions, and irradiation effects.

The workshop participants have identified the strengths and weaknesses of several commercial fuel performance codes and have proposed critical requirements for a future, improved, fuel performance code. The major drawback of most commercial codes was determined to be the fact that they are too dedicated to a specific fuel form and composition. Another issue was that most commercial codes can not run parallel on large computational networks. The third major difficulty was the lack of compatibility between the commercial fuel performance codes.

The central point of discussion regarding fuel performance codes was the integration of existing codes versus producing a brand new one. Two options have been discussed: A) Integration of existing codes. In this approach, advance models and simulations will be incorporated in existing commercial codes such as FRAPCON/FRAPTAN, TRANSURANUS, TRAC, NITRAF, etc. B): Design of a new fuel performance code. In this approach, workshop participants will engage in developing a new fuel performance code that will address properties and phenomena related to the fabrication, operation, and storage of materials for nuclear fuels.

There was no decision regarding the two options during the workshops. However, extensive discussions led to the conclusion that no matter what path is pursued, there are two software engineering steps that can and must be addressed by the workshop participants: a) defining the scope and b) the requirements of the advance fuel performance code. A preliminary design of an advanced fuel performance code (AFPC) that satisfies these main requirements was proposed by LANL.

The review of fuel performance requirements was accompanied by numerous proposals related to planning, work distribution, and resources. It was determined that there is a need for a comprehensive plan, to allow for both *short-tem and long term* activities. The plan must include adequate resources such as people, high performance computers, and funding. Since modeling of nitride fuels is more advanced in Europe and Japan, US researchers must accelerate their programs to keep up with the results in the rest of the world. Education, as provided at several universities in USA and other parts of the world, was regarded as the main source of new ideas and expertise for the program.

Although current developments in computational science and technology allow for high performance computing, the work on nuclear (ceramics) fuels is behind the work on metals and must catch up as soon as possible. It is unfortunate that current fuel performance codes do not take advantage of this technology and are still running on personal computers. There is a tremendous opportunity for moving to high performance computing for nuclear fuels applications.

Over the last 4 years, the AFCI program allocated an increasing amount of funding to materials models and simulations. AFCI's role in supporting this work and the workshops was extremely important. However, the total funding required for correlating the effort with both the short-term priorities and the long-term objectives must increase to at least $5 mil/year, with support from other programs, such as the DOE Basic Energy Science program and National Science Foundation sponsored programs.

Besides better computers, materials models and simulations require national and international collaborations. Following the MMSNF3 workshop, Nov. 18-19, 2004, Washington DC, USA, the *International Focus Group* (IFG) for Materials Models and Simulations for Nuclear Fuels held its first meeting. The IFG brings together experts in various areas of modeling, simulations, experimental, and technological applications from 10 countries.

Several ideas regarding a better use of resources and more coordinated work converged into proposing the creation of national and international *Centers for Models and Simulations of Nuclear Fuels.* This is a more general concept than models and simulations of materials for nuclear fuels, as defined by the MMSNF workshops. It involves all components of nuclear fuels design and optimization: materials, neutron fluxes, test beds, controls, non-proliferation, safety and security. The mission of such centers would be to provide the scientific environment and resources (people, supercomputers, and funding) for the development of theory-based models, simulations, and computational tools for the design and optimization of nuclear fuels.

1. Introduction

Nuclear fuel materials (alloys and ceramics) are exposed to *complex thermo-mechanical processes* during manufacturing, operation, and storage. The physics, chemistry, and materials science of such materials are tremendously complicated by irradiation effects. That is why many commercial fuel performance codes incorporate empirical correlations to describe materials properties. The applicability of such correlations is limited to a regime where experimental data is available. Past attempts to extrapolate outside this regime have sometimes led to faulty predictions and costly engineering decisions.

To address these issues, several projects have been developed all over the world to assess the properties of multi-component actinide based ceramics. However, most assessments involve *fitting* of known data followed by extrapolations or interpolations into new temperature or pressure regimes. There is an obvious need for a multi-physics approach to develop a fundamental understanding of properties of complex nuclear fuel materials, leading to improved tools for predicting phenomena such as phase stability, heat transfer, species diffusion, and fission products retention.

At Los Alamos National Laboratory, the work on models and simulations of nuclear materials started in 2001. It was supported at a modest funding level, the equivalent of one person's day of work per week (0.2 FTE). The concern was that models and simulations are of little use for solving real problems associated with nuclear fuels fabrication. The concern was justified, at the time. During the last four years of combined theoretical and experimental efforts, models and simulations provided valuable information about materials properties and important phenomena associated with nuclear fuels. As of today, they are still not regarded as critical tools for fuel design and optimization.

The idea of replacing empirical correlations with theory-based models for the purpose of improving high performance simulation tools was inspired by the work on alloys and stockpile stewardship. In USA, the intense focus on computer simulations, generated by the ban on nuclear weapons experiments, did not have a counterpart in the nuclear fuels area. In spite of that, several LANL scientists decided to put some effort into the study of nuclear ceramic fuels, based on two premises:

- Nuclear energy must be part of the USA energy portfolio (new reactors will be built).
- Models and simulations are powerful tools that will eventually be accepted in the nuclear fuel qualification process.

To ensure a coherent framework for the discussions and planning, the following definitions have been adopted:

Model: A logical description of how a system (nuclear fuel material, in our case) performs. Models are based either on theory or empirical knowledge and are validated by experiment or computation.

Simulation: The process of carrying out experiments and/or running computer programs to reproduce, in a simplified way, the behavior of a system.

Fuel performance code: A computer simulation tool able to evaluate and predict the properties and behavior of nuclear fuel materials during manufacturing and operation.

Any simulation requires a tool (computer program, mechanical or electronic device, etc) and is based on a collection of models that describe different features of the system. These definitions are implicitly use in this report.

Fig. 1 shows a much simplified diagram of the integrated program started at LANL. In this representation, advanced models and simulations integrate theory, experiment, and computation. Advance fuel performance codes incorporate advanced models and simulations rather than empirical correlations.

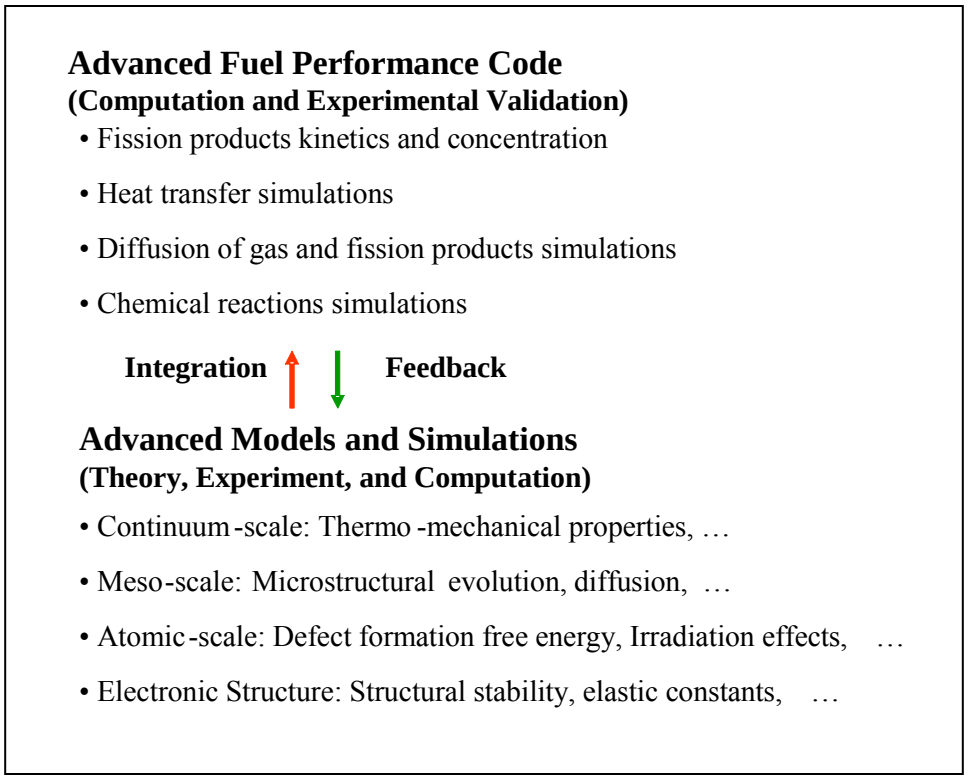

Figure 1. Schematic representation of the relations between models, simulations, and the fuel performance code.

The rational for having two major areas of research originated in the way the scientist can be grouped by expertise. There was a group focused on modeling materials properties at various scales, starting with electronic structure calculations (often wrongly referred to as "first principles") and going all the way to continuum methods, such as Finite Element Analysis (FEA). A very distinct group worked on developing high performance computational tools for simulations of heat and mass transport or hydrodynamic phenomena.

This is not uncommon in materials science and the LANL project simply attempted to bring together the two groups and have them collaborate. To cover the necessary area of expertise, organizing a workshop on models and simulations of nuclear materials appeared as the natural solution. The idea was to start with the models and simulations components to attract as many fuel performance people as possible, for proper integration and feedback. At the date of this report, the two components are better balanced, but the integration process is far from being completed.

2. MMSNF workshops

The "Materials Models and Simulations for Nuclear Fuels" (MMSNF) workshop series was organized as part of the Advanced Fuel Cycle Initiative (AFCI) program, funded by the USA Department of Energy. The workshop series aims at stimulating research and discussions on models and simulations of nuclear fuels and coupling the results into fuel performance codes. The workshops are organized by M. Stan (Los Alamos National Laboratory) and Prof. James Tulenko (Univ. of Florida, president of the American Nuclear Society), with the continuous support of Kemal Pashamehmetoglu (Idaho National Laboratory, AFCI national director for nuclear fuels).

First edition, **MMSNF-1**, June 9-10, 2003, was held in Santa Fe, NM, see: http://www.lanl.gov/mst/nuclearfuels/. It brought together fifty experts in models and simulations from United States, UK, Sweden, and Turkey. There was a good participation from universities (14 people). The workshop was organized over two full days, on 7 sessions: *Programmatic Context* (Chair: K. Chidester), *Modeling and Simulation Scales* (Chair: R. Grimes), *Thermodynamic Properties* (Chair: J. Wallenius), *Phase Stability* (Chair: J. Simmons), *Transport Phenomena* (Chair: M. Baskes), *Irradiation Effects* (Chair: J. Tulenko), *The Impact of Modeling and Simulations on Nuclear Fuels Development* (Chair: E. Arthur). This first edition was focused on Materials Models and Simulations, with less emphasis on fuel performance codes. Presentations detailed results of electronic structure, atomistic, and continuum simulations. There was reference to computational tools such as FRAPCON, Thermo-Calc, and Alchemy. The workshop ended with a plenary discussion of the role of modeling and simulations in designing better materials for nuclear fuels applications. The participants identified critical requirements for each session topic and modeling and simulation issues that must be addressed to meet the requirements.

The second edition, **MMSNF-2**, November 20-21, 2003, was organized in New Orleans, LA, see: http://www.lanl.gov/orgs/mst/mmsnf/. Forty participants attended the meeting, representing Belgium, Germany, Japan, the Netherlands, Sweden, United Kingdom, and the United States of America. Participants from six U.S.A. National Laboratories (Argonne, Idaho, Lawrence Livermore, Los Alamos, Oak Ridge, and Pacific Northwest) were present. University participation decreased, compared to the first edition, but there was a slight increase in industry/private companies' attendance. The presentations were grouped in three Technical Sessions: *Fuel Performance Codes* (Chair: K. Pasamehmetoglu), *Modeling and Simulations* (Chair: M. Stan), and *The Impact of Modeling, Simulations, and Fuel Codes on Nuclear Fuels Development* (Chair: J. Tulenko). The workshop ended with a plenary discussion of the role of modeling and simulations in designing better materials for nuclear fuels applications.

The third edition, **MMSNF-3**, November 18-19, 2004, Washington DC, USA, see: http://www.lanl.gov/orgs/mst/mmsnf/, was scheduled in connection with the winter meeting of the American Nuclear Society. Forty participants attended the third meeting, representing the United States of America, Belgium, Canada, France, Germany, Japan, Sweden, and the United Kingdom. U. S. A. was represented by national laboratories, universities, and private companies. The presentations were grouped into two Technical Sessions: *Models, Simulations, and Fuel Performance.* (Chair J. Tulenko) and *Models, Simulations, and Experimental Validation* (Chair: K. Pasamehmetoglu). The third edition of the workshop shifted the focus of the discussions from materials science to fuel performance predictive codes, design, manufacturing, and operation. The workshop ended with a plenary discussion of the role of the

Materials Models and Simulations in Nuclear Fuels and was followed by a meeting of the International Focus Group.

The fourth edition, **MMSNF-4**, will be scheduled in connection with the winter meeting of the American Nuclear Society, November, 2005.

The organizing committee thanks all workshop participants for their contribution to the success of the workshop. Copies of the presentations, on CD-ROM, are available by contacting Marius Stan (mastan@lanl.gov).

The main ideas resulted from the discussions are presented bellow and accompanied by brief comments. Key concepts and ideas are written using the *italic* font. As with any meeting report, it is impossible to provide a full list of contributors. Numerous problems have been reiterated by several participants and the solutions refined. That is why this report should be regarded as the result of team work. A comprehensive list of all participants is available in APPENDIX A. The author thanks especially Paul Van Uffelen, James Tulenko, Kemal Pasamehmetoglu, Stuart Maloy, Blas Uberuaga, Robin Grimes, and Keneth McClellan, for their comments.

3. Models and simulations

During the workshops and follow up discussions, various models and simulation methods have been analyzed and participants made suggestions regarding long and short-term theoretical efforts that can help with improving the models.

3.1. Fuel types and materials

It was pointed out that there is a need for fuel performance codes that can address *all types of fuels*: oxides, nitrides, carbides, metallic, dispersed (inert matrix), and composite. At the least, a fuel performance code must be able to predict the properties and behavior of a certain fuel type. For example, it should work for all mixed oxide fuels, not for a specific composition only.

The models should address complex, *multi-component materials*. The study of multi-component systems involving U, Pu, Am, Np, Zr, and their oxides, nitrides, and alloys, is a must. The models and simulations should include fission products such as Cs, Sr, He, I, and Tc. Most commercial codes assume homogenous material and average the properties over the computational domain. The specifics of heterogeneous materials must be incorporated and more attention paid to composites.

Most of the results presented at the workshop reflected work on oxides, very little was on nitrides and there was almost nothing on metals. That is a reflection of the overwhelming presence of oxide fuels in existing nuclear reactors. However, the new generation of terrestrial reactors, as well as the reactors for space propulsion, will most likely require *non-oxide fuels*. A well balanced program should include all types of fuels. As of today, the modeling of nitride fuels is more advanced in Europe and Japan and US research must accelerate their programs.

Predicting properties of multi-component materials is a difficult task that involves theoretical, experimental, and computational work. *It is dangerous to empirically extrapolate* properties from elements to binary and ternary systems, not to mention systems of four or more components. That is why a models and simulations program should accompany the fuel performance development effort.

3.2. Material properties

A large number of materials properties that influence nuclear fuel's behavior in operation have been reviewed. Among them, thermo-mechanical properties play an important role.

It was pointed out that *thermodynamic properties* such as enthalpy, heat capacity, thermal conductivity, expansion coefficients, and lattice parameters must be modeled as function of various factors, the most important being temperature, pressure, non-stoichiometry, porosity, and irradiation level. Several of these factors are implicitly included in burn-up. It was estimated that the knowledge of the thermodynamic properties dependence on temperature, pressure, and porosity is satisfactory. However, the influence of non-stoichiometry, irradiation, and burn-up is less understood and more difficult to address. It requires complex, multi-scale modeling.

Several participants pointed out the lack of powerful models and simulations of *mechanical properties.* It was emphasized that both the elastic and plastic behavior of fuel materials must be incorporated in the models. The mechanical properties must be calculated as function of temperature, non-stoichiometry, and the stress/strain relations.

Since temperature and pressure are the control parameters in most processes, the *free energy of all phases* is the most important thermo-mechanical property. Although free energy functions are available for many phases of interest (mostly oxides and alloys) more work is necessary to

cover the nitrides. That requires better coordination between the electronic structure, atomistic and continuum calculations.

Understanding of the *fuel microstructure* (grain size, porosity and chemistry) and the behavior under irradiation and temperature are a priority. The influence of self and external radiation on void and bubble formation, swelling, and creep is also important and must be incorporated in the thermo-mechanical models. One participant said "If we new creep, we new everything". The discussion of creep modeling led to the conclusion that it is very difficult to provide a comprehensive model and that semi-empirical approaches and the only solution, for now.

Real materials are not perfect crystals. In the absence of properties defective structures, many fuel performance codes are using values from databases that have been measured or calculated for perfect crystals. It is important that the new models incorporate point, line, 2-D, and 3-D *defects*. Models of dislocations and fracture should play a central role in improving the Finite

3.3. Phenomena

Modeling and Simulations must address *all time and space scales*, starting with the nucleus, the electronic structure, atomistic and nano-scale, mezzo-scale, all the way to the continuum level phenomena (Fig. 2). The characteristic time step and space length associated with various phenomena can not be strictly defined. For example, diffusion involves the electronic structure properties of the atoms at a microscopic level and nano-second times. Still, the kinetics of bulk diffusion processes can be characterized from a continuum, macroscopic point of view using characteristic times of minutes, hours, and even days.

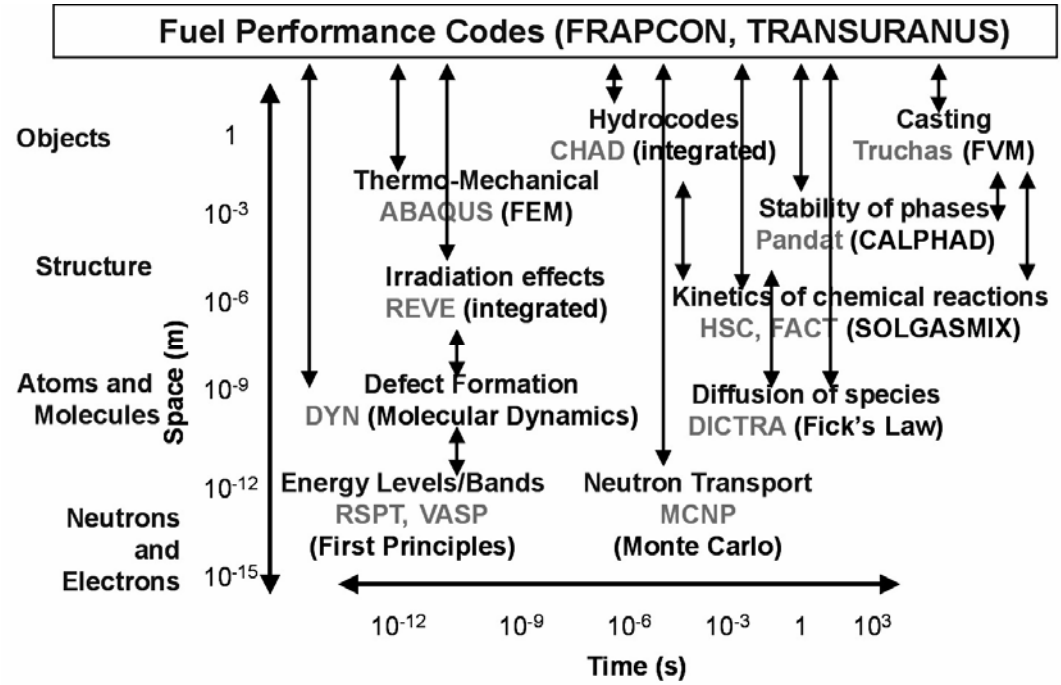

Figure 2. Space and time scales involved in simulating phenomena relevant for nuclear materials (black). The methods are shown in parenthesis. Several software packages (gray) are used to illustrate the type of simulation. [M. Stan, T. Amer. Nucl. Soc, 91 (2004) 131]

All workshop editions were focused on thermo-mechanical properties and phenomena. Still, mechanical phenomena such as pellet fragmentation and *clad-pellet interactions* have been listed as very important and less studied. Commercial codes do not allow for simulations of large changes in gap and clad geometry. That leads to "idealized" results.

It was pointed out that, although *fission processes*, although they were not the main subject, are a critical component of fuel behavior. Phenomena such as fission products release, diffusion, and accumulation have a strong impact on materials properties and influence the heat and mass transport. Up to now, nuclear reactions have been decoupled from the study of material properties. For example, in commercial fuel performance codes, the heat generated during fission is only added as a source term to the finite element calculations. Interaction with the nuclear reaction modeling team is required and it was proposed that future workshops include a "neutronics" session in the agenda.

A lively discussion was centered on the use of irradiation studies on *surrogate materials*. Given the huge resources required to conduct experiments in reactors, it was proposed to develop a set of studies on surrogate ceramic materials, such as cerium oxide or zirconia. The problem with such studies is the transferability of the results. It is not clear if the study of the fission product diffusion mechanism in surrogate material can provide a definitive answer to the questions related to fission products accumulation in a mixed oxide fuel.

Accurate models of *microstructure evolution* (point defects and dislocations along with grain boundary movement) during service lacking in commercial fuel performance codes. There are several "holistic" approached that involve average properties of the grains but complete simulations are missing. The reason is that there are no good simulations of macrostructure evolution in ceramics in general, so there are no models to include in the fuel performance code. Still, several codes account for grain growth (normal and columnar), central void formation (FBR fuel) and some account (empirically) for the high burnup structure. Truchas (LANL casting simulation software) and TRANSURANUS (ITU) were given as examples of codes able to address microstructure information.

Thermo-chemistry of *chemical reactions*, such as oxidation/reduction should be a priority. A good example is the effect of coolant and the radiation-enhanced corrosion. Following the first workshop editions, comments about the absence of presentations and discussion of chemical phenomena led to changes in the structure of the workshop agenda. The third edition dedicated plenty of time to discussions of oxidation, hydration, and corrosion chemistry. The thermo-chemistry of chemical reactions, such as oxidation/reduction must be included. For example, TRANSURANUS accounts for radial redistribution of oxygen in FBR fuel.

Most models and simulation assume equilibrium and calculate steady state properties. Phase stability plays an important role during fabrication and service, when both temperature and pressure change significantly. The modeling work must also address metastability and *non-equilibrium*. Statistical mechanics and thermodynamics treatments of non-equilibrium, irreversible phenomena, such as quenching, must be incorporated in the fuel performance codes. There is recent extensive work in these areas and much progress was made on alloys. Similar studies on ceramics are necessary.

Of critical importance are *heat and mass transport* phenomena. Most fuel performance codes have capabilities for heat transfer and species diffusion simulations. The steady state solution of the heat transfer equations appears to be the standard feature in fuel performance codes. Some codes, such as FRAPTRAN, can address transient regimes and solve for the time dependent

transport equations. An area of improvement is simulation of heat transfer in heterogeneous materials, with porosity and defects distributed in the fuel rod according to experimental data.

Diffusion of fission products is less understood due to the lack of in situ characterization methods. Recent simulations of bulk diffusion of the gas species resulted in good descriptions of fission gas retention in several codes. However, the role of diffusion at the grain boundaries is not elucidated. This phenomenon is strongly related to microstructure evolution and must be further studied using experimental and theoretical tools.

Technological processes are rarely simple; they involve combinations of the above mentioned phenomena. As an example, sintering of ceramic fuel materials involves heat and mass transport, phase transformations, irradiation effects, and changes in mechanical properties. A complex simulation of the sintering process must be developed as soon as possible, to assist with fuel design and fabrication.

3.4. Computational methods

To address all relevant natural phenomena, models and simulations have been developed for various time and space scales. A wealth of results on nuclear fuels materials is captured in journal articles, reports, and databases. It is well understood that *empirical models* are extremely valuable for technological applications. When accurate, they allow for concise descriptions of materials properties and have limited predictions capabilities. However, empirical models are only valid within the confines of parameters and irradiation conditions covered in the database on which they are developed. Interpolation and extrapolation of empirical models is a dangerous practice that can lead to errors. Since the uncertainty associated with empirical models is often large, confidence intervals are difficult to calculate.

There are areas where *theory-based models* can be developed to include the physics, chemistry, and materials science of fuel materials. These models and simulations are often referred to as "mechanistic" descriptions of properties and phenomena. They are expected to provide a deeper understanding of the nature of properties and critical phenomena.

Electronic structure calculations aim at describing properties such as lattice parameters, cohesive energy, and phonon spectra solely based on the electronic structure of the materials. They provide invaluable information about structures for which there is no experimental data. That information feeds into higher scale models and is often used to determine inter-atomic potentials. However, most reliable results from electronic structure calculations are obtained at 0 K temperatures. Unfortunately it is quite common for comparisons of these results with room or high temperature experimental results to be irrelevant. New methods that can provide results at finite temperatures are needed. Another drawback is the difficulty of calculating properties of mixtures and solutions for specific compositions. That is related to the relative small number of atoms involved in the calculation cell.

To retrieve known materials properties and validate the calculations it is often necessary to use corrective parameters. That is why referring to electronic structure calculations as "*first principles"* is an abuse of scientific language. The use of "first principles" should be reserved for calculations that do not involve any fitting or experimentally derived parameters.

Atomistic models and simulations operate at scales of the order of 5 Å, corresponding to inter-atomic distances. Although atomistic approaches are capable of capturing lower-scale properties, they do not incorporate quantum mechanics properties and only operate within the framework of classical mechanics.

Inter-atomic potentials are often used for *Molecular Dynamics* (MD) simulations. Hundreds or even thousands of atoms are placed in the nodes of lattices associated with specific crystal structures and linked using the forces derived from inter-atomic potentials. The atoms are given initial velocities and then the structure is relaxed until minimum free energy is reached. Such simulations can describe times of the order of hundreds of pico-seconds. That is sufficient for calculations of equilibrium energy and for studies of defect formation and dislocation propagation. However, the simulation times are not long enough to address phenomena such as diffusion or cascade effects during irradiation.

To allow for longer simulation times, MD is coupled with *Monte Carlo* (MC) methods. During MC calculations, the solution space is sampled and only points that satisfy certain criteria are accepted. Another option is to use Temperature Accelerated Dynamics (TAD). TAD is based upon molecular dynamics and increases the rate of events by increasing the temperature. The behavior at temperature of interest is determined by a mapping technique.

Atomistic methods rely on good inter-atomic potentials. *Many-body effects*, accounted for in semi-empirical potentials such as the Modified Embedded Atom Method, have been included in potentials for metals and alloys but not for actinide based ceramics. The main reason is the very difficult process of adding charge transfer. As of today, the most reliable models for actinide based ceramics involve pair-potentials.

The *continuum level* simulations make use of *Finite Element Analysis*, Finite Difference, or Finite Volume Methods. Numerous fuel performance codes provide simulation tools for rather idealized geometries, such as planes and cylinders. Since all fuel materials are subject to radiation damage, the models should be able to address real geometries, relevant for the nuclear fuels applications.

There is much progress in modeling phase stability in complex materials. For example, the *CALPHAD method* and the temperature integration of the free energy have been coupled to produce phase boundaries in binary and ternary systems. When taking into account the fission products and the chemical dynamics of the fuel material, it becomes necessary to study systems with 5-10 components to achieve a good description of the thermo-chemical properties of the fuel. Although the results are often requested in an emergency regime, such studies have not been funded yet.

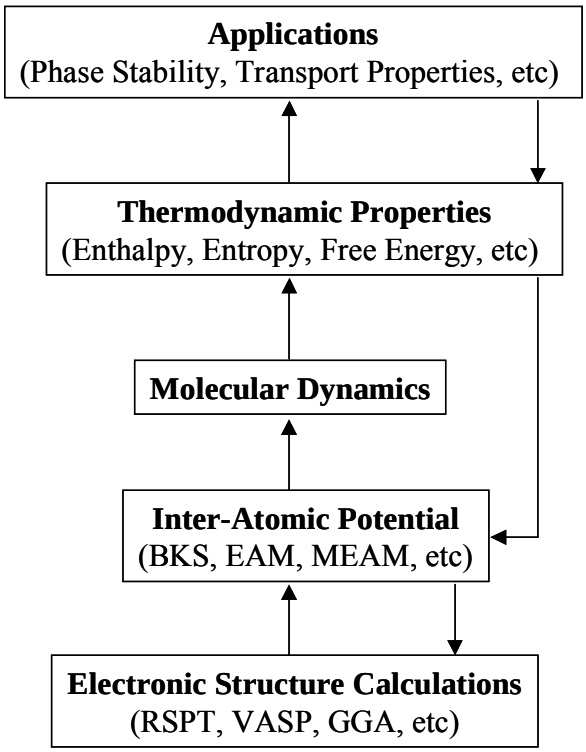

Figure 3. Multi-scale and multi-physics method developed at LANL [M. Stan, T. Amer. Nucl. Soc, 91 (2004) 131]

Fig. 3 shows a schematic description of the multi-scale and multi-physics method used at LANL. Electronic structure results are used to determine inter-atomic potentials for molecular dynamics calculations of thermodynamic properties. Similar approaches have been developed at universities such as PennState (USA), K.T.H. (Sweden), and Imperial College (U. K.).

4. Fuel performance codes

The workshop participants have identified the strengths and weaknesses of several commercial fuel performance codes and have proposed critical requirements for a future, improved fuel performance code.

4.1. Fuel performance codes status

During the first three editions of the MMSNF workshops, the following codes have been either reviewed, discussed, or mentioned as being relevant: **COMETHE** (Belgonucleaire, Belgium), **COPERNIC** (FRAMATOME, Germany), **ENIGMA** (British Energy, BNFL, UK), **FALCON** (EPRI, USA), **FRAPCON** (PNNL, USA), **FRAPTRAN** (PNNL, USA), **LIFE** (ANL, USA), MACROS (SCK-CEN, Belgium), **MCNPX** (LANL, USA), **ORIGEN** (ORNL, USA), **PARFUME** (INEEL, USA), **SPHERE** (PSI, Switzerland), **TRANSURANUS** (ITU, Germany), and **TRUCHAS** (TELLURIDE, LANL, USA).

The major drawback of most commercial codes is the fact that *they are too dedicated to a specific fuel form* and composition. The use of empirical correlations in describing materials properties and the much simplified description of heat and mass transport phenomena make extrapolations and information transfer impossible. There was a general agreement that, in order to make predictions for new fuel types, there is a need to develop more theory based codes. This has become possible with the advances in computation capabilities along with more detailed experimental techniques.

A second major problem is fact that most commercial codes *can not run parallel on large computational networks*. That increases the computation time and infringes upon the use of complex models. It was pointed out that it is difficult to turn serial codes into parallel ones, so it might be easier to design and produce a new code.

The third major difficulty was the *lack of compatibility* between the commercial fuel performance codes. The codes have very useful and complementary features but can not be coupled and executed together. It is also difficult to have them feed information to each other.

4.2. An advanced fuel performance code

The central point of discussion regarding fuel performance codes was the integration of existing codes versus producing a brand new one. There are many advantages in improving upon the available commercial codes, the main being that most of them have been validated and work well within their scope. However, software engineering issues prevent a full coupling of the codes and make very difficult modifying them to run in parallel, as required by large scale simulations of phenomena during fuel manufacturing and operation.

- Option A: *Integration of existing codes.* In this approach, advance models and simulations will be incorporated in existing commercial codes such as FRAPCON/FRAPTAN, TRANSURANUS, TRAC, NITRAF, etc. Workshop participants will team up in developing complex software packages where compatibility and self-consistency play a critical role. The advanced models will replace current empirical correlations and improve predictive capabilities. New models of materials properties will serve as input for the codes and the information will be transferred via a network of input/output files. The advantage of this approach is that the software is already in place and short-term improvements can be obtained. The drawback is that modifying software historically proved to be a counter productive method, often requiring more time and resources than writing a new code.

- Option B: *Design of a new fuel performance code.* In this approach, workshop participants will engage in developing a new fuel performance code that will address properties and phenomena related to the fabrication, operation, and storage of materials for nuclear fuels. The code development will be based on sound software engineering steps and will involve a high level of coordination between the participants. The new code will use all valuable information (models, simulation techniques, and databases) from existing codes and incorporate it in the new computational framework. The main advantage of this approach is that it will produce better code, well structured and capable of running large simulations in parallel (on multiple processors). The drawback is that the approach is time consuming and requires software engineering and computational resources that are outside the scope of the AFCI program.

There was no decision regarding the two options during the workshops. However, extensive discussions led to the conclusion that no matter what path is pursued, there are two *software engineering steps* that can and must be addressed by the workshop participants: defining the scope and the requirements of the advance fuel performance code.

4.3. Scope

During the three editions of the workshop, several versions of the scope of the proposed fuel performance development program have been proposed. Instead of listing all of them, here is a version that captures the essence of the program:

Scope: Develop an advanced computational tool (software and database) able to predict the behavior of nuclear fuel materials during manufacturing, operation, and storage.

The concept "advanced computational tool" allows for a continuation of the debate regarding options A and B, while reinforcing the "advanced" (theory based) feature. The term "predict" was preferred over "describe" for similar reasons. The scope is limited to "materials" and not nuclear fuels in general. So there will be no competition with codes such as TRAC or MCNP.

4.4. Requirements

Several requirements for the advanced fuel performance code development have been defined:

- To address the nuclear fuels material properties and phenomena, the code must include at the minimum the following *modules*:
  - Neutronics (fission and neutrons diffusion)
  - Heat transfer (conduction, convection, and radiation)
  - Mass transport (species diffusion and gas accumulation)
  - Thermo-mechanics (deformation, such as swelling)
  - Fluid flow (to model the coolant, if necessary)
- *Compatibility* with existing programs was emphasized as a major requirement. The advanced fuel performance code must be capable of using as input results form existing codes and, in

turn, to provide information in a format that is accepted by current codes. This goal can be achieved through a careful code design. One solution is to have the code retrieve information from an external database that is kept up to date with the most recent results. That eliminates the need for modifying the code every time new experimental data becomes available.

- Since many workshop participants are fuel performance code users rather than developers, many requirements were related to the *input/output features*. The main request was a friendly graphic user interface (GUI) that allows trained nuclear fuels engineers and managers to use the code in a productive manner, with no need for modifying files or changing software components.
- *Solvers and code design* and are subjects that got less attention. However, based on the experience with current fuel codes, several suggestions have been made:
  - Use the finite element/finite volume method with fixed mesh.
  - Use nested linear + non-linear solvers (Example: Newton-Krylov)
  - Use preconditioning
  - Run parallel using MPI

A preliminary design of an advanced fuel performance code (AFPC) that satisfies these main requirements was proposed by LANL (Fig. 4). It is based on the experience accumulated with developing complex, high performance codes for stockpile stewardship, work funded by the Advanced Simulation and Computing (ASC) program.

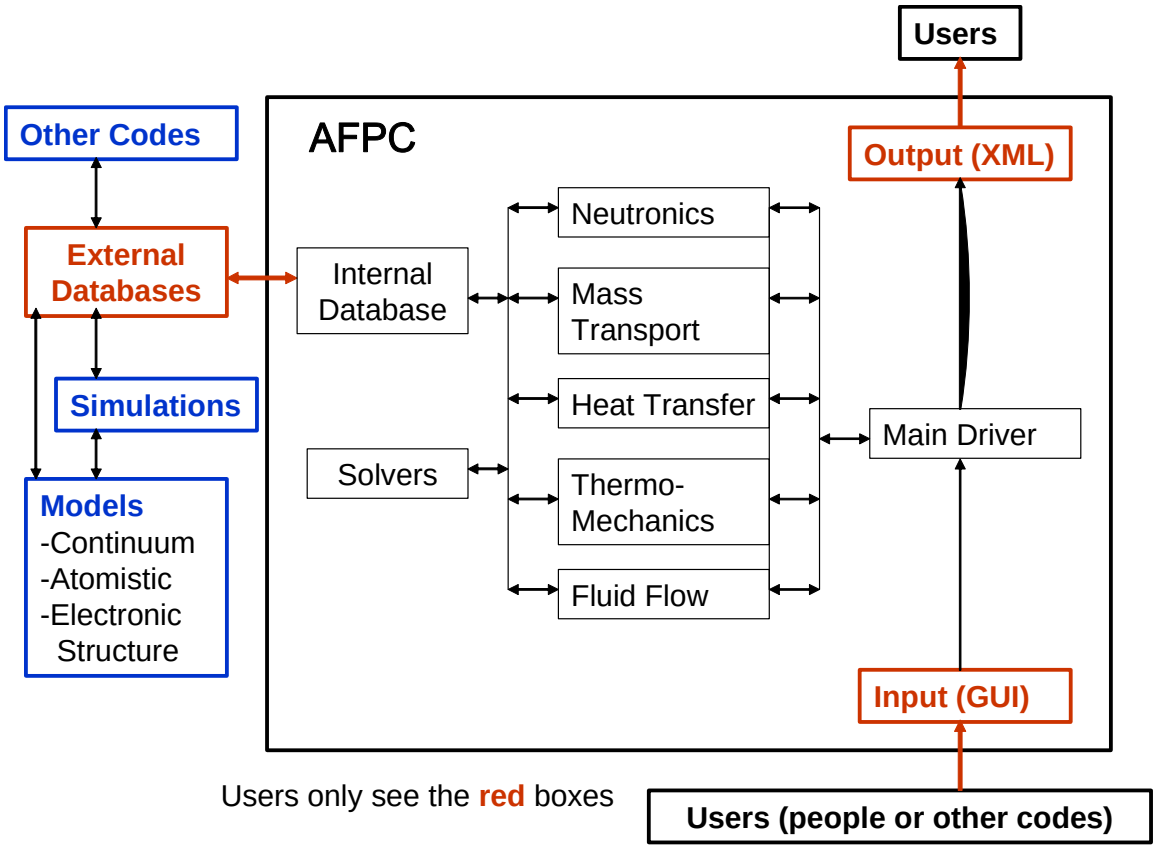

Figure 4. Preliminary design of the advanced fuel performance code [M. Stan, LANL report].

- The models have to be incorporated via *integrated results*, such as mathematical functions or tables. It is unconceivable, at this stage of computational science, to have the atomistic simulations run during each finite element iteration. The question was then: "How is this different form the current empirical approaches?" The difference consists in the fact that there is a validated theory behind the advanced models, as opposite to the current models that are largely based on observation.
- The code must incorporate models that have been first *validated* through experimental or independent computational work and only then used to predict new properties of the materials. This issue led to vigorous discussions about the precedent that experimental work takes over other validation methods. It was pointed out that experimental results have accuracy and precision problems themselves and are sometimes impractical form validation purposes. For example, one does not want to use experiments to validate accident case scenarios. Still, the agreement was that experimental results are the most trusted and powerful validation tools.

Fig. 5 shows an example of integration of models, simulations, and fuel performance code with fabrication and characterization of nuclear fuels.

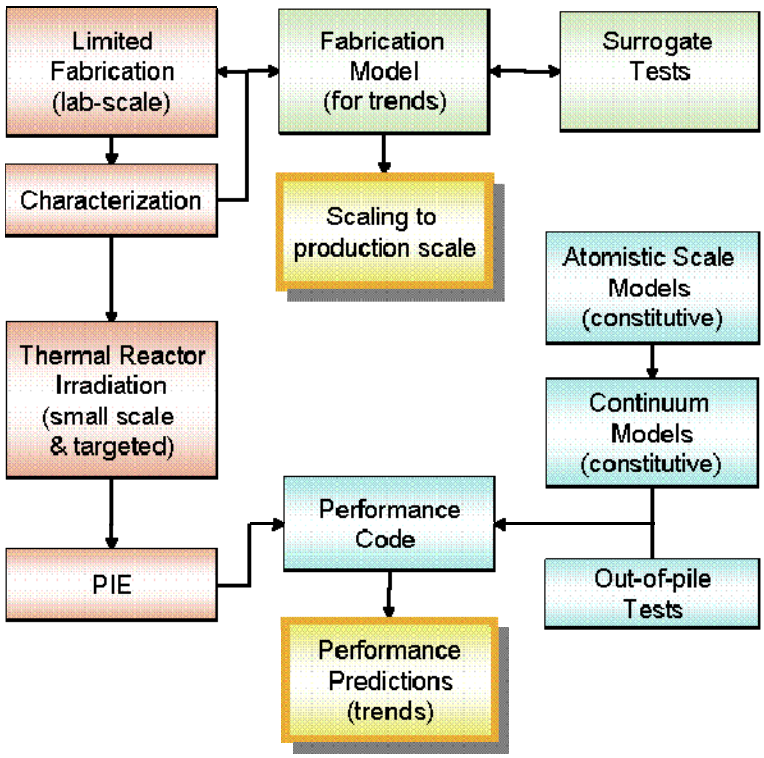

Figure 5. The role of models, simulations and fuel performance codes in the AFCI program (courtesy of K. Pasamehmetoglu)

- Given improvements in accuracy and full validation of the methods, the computer simulations based on sound models of materials properties, as included in the advanced fuel performance code, must be able to assist in the *fuel qualification* process.

5. Planning and Resources

The review of fuel performance requirements was accompanied by numerous proposals related to planning, work distribution, and resources. It was determined that there is a need for a comprehensive plan, to allow for both *short-tem and long term* activities.

It was pointed out that the two main components of the MMSNF approach, model development and fuel performance code development, operate at rather different time scales compared to the fuel design and fabrication. Some models and simulations require years to reach maturity and be validated. The nuclear fuels community often needs immediate results and demands fast calculations that can not be performed at the pace imposed by the fuel development and fabrication. The only solution is to *plan for models and simulations in advance*, such as the results become timely available. That requires tight coordination and discipline as well as appropriate resources to perform the work. This discussion led to the creation of the International Focus Group, described in the section below.

5.1. People.

The number of *scientists, engineers, and managers* involved in the MMSNF workshops reached a relatively stable number of 50. There is however a much larger community interested in the workshop subjects and the workshop organizers have to reach out to them.

As pointed out previously, much modeling and simulation work was dedicated to alloys and there is a wealth of methods developed for metallic systems. With a few remarkable exceptions, the computational materials science community is less interested in ceramics, not to mention actinide based ceramics. The involvement of several prestigious *materials scientists, physicists, and chemists* in the AFCI funded work at national laboratories and universities was viewed as a successful beginning. Their involvement was driven by the interest in solving challenging scientific problems associated with nuclear fuels development, and not by funding.

A number of *materials and nuclear engineers* participated in the workshop and provided the most critical information regarding the requirements for an advanced fuel performance code. Their contribution is essential in ensuring the relevance of the modeling work. Scientists are often tempted to direct their work toward the most interesting and challenging areas, rather then the most relevant ones. The workshop proved that an increasing number of nuclear engineers are familiar with complex simulation tools and use them for optimizing fuel properties. They are the customers of the materials models and simulations work and will benefit the most from the development of an advanced fuel performance code.

No doubt *computational scientists and software engineers* are the key participants in designing and writing the fuel performance code. The question is: should they have the lead in this process? It is known that there is a lot of experience accumulated in developing commercial fuel performance codes. That was generated by the work of materials and nuclear engineers with exceptional computational skills. The programs involve good descriptions of the fuel properties and associated phenomena but the software engineering side is modest. A good example is FRAPCON, one of the few NRC sanctioned codes that proved to be very useful for many nuclear fuels applications and assisted in fuel qualification. Another class of software consists in programs developed for complex simulations in the weapons complex, DOE, DOD, and at NASA. These are much more powerful computational tools but they lack the necessary models to describe nuclear fuels. As an example, TRUCHAS, a LANL developed casting simulation

code, is capable of simulating heat and mass transport in very complex systems and geometries but has no component that can address fission products kinetics and accumulation.

So the question (formulated using the above mentioned codes as generic examples) is: Is it better to attempt to modify FRAPCON to make it structured, run in parallel on a CPU network, and possibly become object oriented, OR modify TRUCHAS to include fission products generation and kinetics, void formation, deformation, and the effect of burnup on materials properties?

To solution of the problem is in the hands of *managers*. The workshop benefited from the continuous support of Kemal Pasamehmetoglu, national director for nuclear fuel, Prof. James Tulenko, president of the American Nuclear Society, and the participation of several DOE representatives. Their active participation in discussions was a success for a meeting originally intended for hard core materials scientists. The management not only became aware of the scientific and computational challenges faced by the models and simulations community, but also provided guidance for future work and priorities.

In spite of the influx of scientist and engineers from other areas, the nuclear fuels community needs to develop their own experts to assist in models and simulations of materials properties. That is achievable through *nuclear materials science and nuclear engineering education,* still provided at several universities in USA and all over the world. There was a natural decline in the enrollment following the ban on building new nuclear reactors in USA, Germany, and other countries. Workshop participants from MIT, PennState, and other universities showed that active programs are in place to reinforce the nuclear materials education in USA, and prepare future experts.

5.2. Computers

The computational resources and the computational time have prevented scientists from running complex simulations on millions of atoms to address bulk properties. Current developments in computational science and technology allow for such calculations and are extensively used for describing metals. Models and simulations of nuclear materials (ceramics) are behind and must catch up with the advancements in metals.

Supercomputers are faster and faster. Each of the top 500 fastest supercomputers in the world can now reach over a teraflop per second. In 2004, the number 1 position in the world was again claimed by the BlueGene/L System, a joint development of IBM and DOE's National Nuclear Security Administration (NNSA) and installed at the Lawrence Livermore National Laboratory in Livermore, California. The European Union and Japan are working on systems that can definitely compete for the first place next year.

Most, if not all, workshop participants have or can gain access to fast computers. It is unfortunate that current fuel performance codes do not take advantage of this technology and are still running on personal computers. There is a tremendous opportunity for moving to *high performance computing for nuclear fuels* applications. Already, neutron diffusion calculations, as well as some safety and security simulations, are performed on such resources. The fuel performance codes can and must become more complex to run on supercomputing networks.

5.3. Funding

Over the last 4 years, the AFCI program allocated an increasing amount of funding to materials models and simulations. AFCI's role in supporting this work and the workshop was extremely important. However, the total funding required for correlating the effort with both the

short-term priorities and the long-term objectives *must increase*. In the area of models developments, AFCI planted the seeds of this work in USA and, after three years, reached the level of 5% of the budget. This is the amount of funding thea most companies and programs allocate for R&D. From now on, the funding for fundamental research can and should grow with support from other programs, such as the DOE Basic Energy Science program and National Science Foundation sponsored programs. Based on the experience with similar programs in materials science, a recommended funding level for the models and simulations components in U. S. A. is $4 mil/year.

The fuel code development work can use a minimum AFCI funding directed toward defining in more detail requirements and for experimental validation work. The core of the funding must be provided by a much larger program. A good example would be the Advanced Simulation and Computing (ASC) program supported by DOE and DOD through NNSA. Within that program, development of computational tools is supported at an adequate level that allows for the participation of large teams of scientists, engineers, and software experts. To achieve the same level of software development, an *AFC program for nuclear fuels* is needed. A typical funding level for such a program in U.S. A. is $3mil/year.

5.4. Collaborations and the International Focus Group (IFG)

As materials science progressed and computers improved, models and simulations of nuclear materials properties became more feasible. USA has a tradition of solid work on oxide fuels combined with experience on nitrides. Still, modeling of nitride fuels is more advanced in Europe and Japan. *US researchers must accelerate the modeling effort* if they want to keep up with the results in the rest of the world. It was proposed that a smaller group of US workshop participants get together and work on prioritizing the research areas.

Besides better computers, materials models and simulations require *national and international collaborations*. We have to team up in developing complex software packages. It was proposed that an international consortium be organized and a program be designed to develop a coherent set of computer programs to simulate fuel behavior under normal operating conditions, with extension to abnormal conditions.

Following the MMSNF3 workshop, November 18-19, 2004, Washington DC, USA, the *International Focus Group* (IFG) for Materials Models and Simulations for Nuclear Fuels held its first meeting. The IFG brings together experts in various areas of modeling, simulations, experimental, and technological applications from 10 countries. The focus group is co-chaired by J. Tulenko (Univ. of Florida) and M. Stan (LANL). A list of the founding members is available in APPENDIX B. Each partner contributes in areas defined based on their national program's priorities. During the first meeting, the co-chairs led discussions regarding the main activities of the group. These activities are:

- Assess the needs of the nuclear fuels technology in the area of materials properties and phenomena.
- Determine the requirements for a science-based, predictive fuel performance code.
- Determine the materials models and simulations that are necessary for the fuel performance code and for directly assisting the development of improved fuel materials.
- Prioritize the needs in both areas and draft of a 10 years plan.

At the next meeting (MMSNF-4), the IFG members will discuss the addition of representatives of South Korea and other countries, as well as a stronger representation of industrial partners.

5.5. The Center for Models and Simulations of Nuclear Fuels

Several ideas regarding a *better use of resources and more coordinated work* converged into proposing the creation of national and international centers for models and simulations of nuclear fuels. This is a more general concept than models and simulations of materials for nuclear fuels, as defined by the MMSNF workshops. It involves all components of nuclear fuels design and optimization: materials, neutron fluxes, test beds, controls, non-proliferation, safety and security.

The *mission* of such centers would be to provide the scientific environment and resources (people, supercomputers, and funding) for the development of theory-based models, simulations, and computational tools for the design and optimization of nuclear fuels.

A brief analysis of the timeline associated with potential developments related to nuclear fuels in USA shows that, in order to produce timely and relevant results, a national center needs to be set up by 2010 (see Fig. 6).

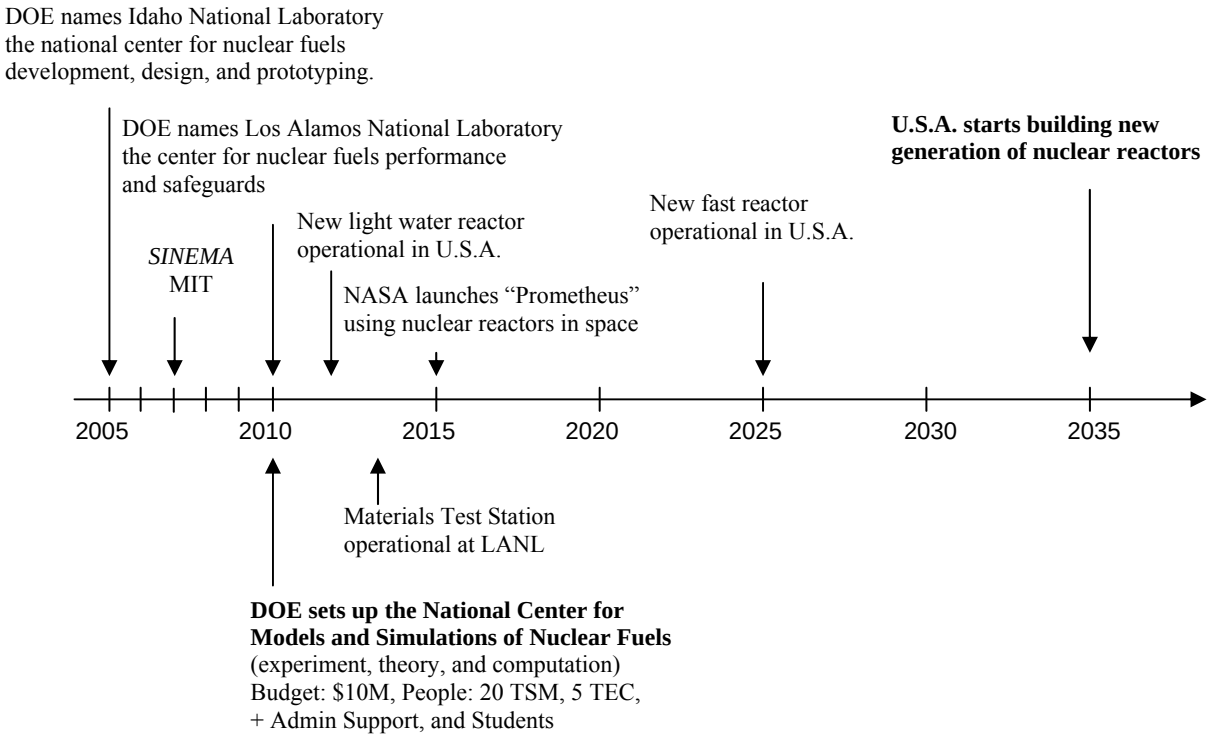

Figure 6. Timeline of potential developments in the area of nuclear fuels [M. Stan, LANL report]

Potential candidates for hosting the USA center are (alphabetically):

- Idaho National Laboratory, has the advantage of being the national center for nuclear fuels development, design, and prototyping, but has little computational capabilities.
- Los Alamos National Laboratory has tremendous scientific and computational capabilities but nuclear fuels are not part of its core mission.
- Massachusetts Institute of Technology (MIT) is already involved in the *SINEMA* project and provides a top nuclear fuels research environment, but may lack the logistics for organizing the center.

Given support from DOE, NNSA, and NSF, and with active participation of the scientific, academic, and industrial communities, the center can become reality.

6. Conclusions and action items

The workshops facilitated a fruitful exchange of ideas and generated numerous proposals for scientific collaboration. Following the third workshops, a strong collaboration between universities and national laboratories started in the USA. Recently, INEERI documents have been signed between USA and European and Japanese research centers on subjects related to models and simulations of nuclear materials properties.

Since this document is in itself a synthesis of extensive discussions, a summary is not necessary. On the contrary, there is a need of identifying specific aspects of fuel behavior and potential reviewers to appraise the current state of understanding in those areas. Almost every paragraph in this report can serve as a starting point for an extensive discussion and various publications. The relevant subjects will be discussed at the upcoming workshop editions and a series of reports and publications co-authored by workshop participants will be published.

The workshop participants proposed the following action items for the period between MMSNF-3 and MMSNF-4 (Nov. 2004-Nov. 2005):

- Organize the fourth edition of the Material Models and Simulations for Nuclear Fuels workshop (MMSNF-4) in conjunction with the 2005 ANS meeting in Washington DC.
- Organize the second meeting of the International Focus Group (IFG) during MMSNF-4.
- Support and participate in the Models and Simulations topical meeting organized by ANS in 2006.
- Support and increase in the models and simulations effort to 5 FTE.
- Support and increase in the code development effort to 2 FTE.
- Setup multi-laboratory collaborations and prepare the software engineering components of the program.
- Support the creation of a National Center for Models and Simulations of Nuclear Fuels by 2010.

APPENDIX A
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APPENDIX B
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