Workshop on 'High End Computing for Nuclear Fission Science and Engineering'.

Held in Salt Lake City, UT, February 23-24, 2006.

Summary Report

Introduction

The workshop addressed access to Department of Energy high end computing facilities for basic research and engineering research in support of the renaissance of nuclear energy in the United States. At the beginning of the workshop, access to Department of Energy (DOE) high end computers was discussed by Doug Kothe (representing the National Leadership Computing Facility - NLCF) and Francesca Verdier (representing the National Energy Research Scientific Computing Center - NERSC). Then scientists and engineers from DOE National Laboratories, academia and the nuclear power industry delivered technical presentations. The presentations on basic research applications were initially divided into three sessions. Two presentations on nuclear reaction cross section modeling were added to form a short fourth session. These sessions focused on four research domains:

1. Computational Fluid Dynamics and Transport.
2. Computational Materials Science.
3. Computational Chemistry.
4. Nuclear Reaction Cross-sections.

In addition to these "science" groups, two sessions were devoted to Nuclear Engineering and Reactor Physics. These two sessions were:

E1. Nuclear Engineering Applications
E2. Scientific and Computational Requirements

The contents of the meeting presentations and the outcome of discussions for each of the above five categories are identified and discussed in turn in the remainder of this report. They are followed by a presentation of the agreed-to path forward.

Presentations from the workshop can be found a
http://www.inl.gov/cams/workshops/highendcomputing/

Science Group Reports (Groups 1-4)

Of the first three groups, only the computational chemists possess ready to run code that has been developed to run efficiently on high end parallel supercomputers (NWchem [1] developed primarily at the Pacific Northwest National Laboratory[1]). Code has been developed to run on parallel computers by individuals or small groups in the other research domains. However, scalability to a large number of processors has not been demonstrated for all codes and many, if not most, of the existing codes are expected to perform poorly on systems with thousands, tens of thousands or hundreds of thousands of processors.

The computational materials science community has used a very wide range of numerical methods, based on a multitude of theoretical approaches. For this reason, and the 'small science' tradition in this area, the large teams consisting of domain experts, applied mathematicians and computer scientists needed to develop code that can run well on high end computers have not been put into place. An important product of the workshop was the recognition by the computational materials group that computational chemistry packages such as NWchem could be used to address a variety of materials problems of relevance to the development of advanced nuclear power systems. This will provide the computational materials community with an opportunity to bring high performance computing to bear on materials science and enhance their familiarity and experience with high performance computing. This also provides an opportunity for the computational materials and chemistry communities to collaborate to mutual benefit.

The computational fluid dynamics community is also faced with extreme computational challenges. Direct numerical simulation (DNS) is restricted to flows with Reynolds numbers that are significantly smaller than those found in boiling water reactors and potential high temperature gas cooled reactors. Phenomena such as nucleate boiling and bubbly flow with bubble coalescence and fragmentation are also extreme computational challenges. There may be an opportunity for collaboration between the computational fluids dynamics and the computational chemistry/computational physics practitioners to address problems such as nucleate boiling.

Accurate information on difficult to measure nuclear reaction cross-sections is needed to support the design of advanced nuclear fission reactors. At present, first principles methods can be used only for very light nuclei. The calculation of cross sections for heavy element nuclei, such as the heavier plutonium nuclei will require the development of new theoretical methods. In the future, the first principles calculation of cross sections may require high end computing. At present, the calculation of cross sections is based on semi-empirical models that are calibrated using experimental data.

[1] A variety of *ab initio* quantum mechanics, molecular dynamics and mixed quantum mechanical/molecular dynamics capabilities are available within NWchem. NWchem can be implemented on a wide range of parallel and sequential computers, and its performance has been benchmarked as a function of the number of processors employed on a variety of systems.

Computational Fluid Dynamics Group report (section 1)

The Computational Fluid Dynamics and Transport Group presented for general discussions a number of topics on multiscale modeling and simulation methods for high-order Computational Fluid Dynamics (CFD) with uncertainty quantification as well as specific industrial applications and limitations in the use of CFD in fuel assembly design and licensing. The group participants and the primary topics addressed were:

George Karniadakis, Brown University -- Parallel high order CFD with uncertainty quantification
Thomas Kehely, AREVA, NP -- Use of CFD in fuel assembly design and licensing
Simon Lo, CD-adapco, UK -- High end computing for nuclear reactor simulation with STAR-CD
Gretar Tryggvason, Worcester Polytechnic Institute -- Direct numerical simulation (DNS) of multiphase bubbly flows
Eric Volpenheim, CD-adapco
Yassin Hassan, Texas A&M

Much of the presentations and following discussions centered on methods development and problem applications. With the anticipated rapid advances in computing power, both hardware and software, more complex fluid dynamics simulations could be carried out. The development of a multilevel parallelization strategy to exploit the hierarchy of structures in physical problems and in computation architectures was addressed. Examples of fluid flow past a cylinder and fluid /structure interaction were presented. A study of direct numerical simulation (DNS) as a promising tool for understanding the complex physical phenomena associated with turbulence in bubbly flows was presented. An example of a bubbly flow at relatively modest Reynolds number, where the channel flow is laminar in the absence of bubbles, was shown. In spite of the small size of the simulated system and the assumption of spherical bubbles, important physical features are revealed. However, DNS is restricted to flows with relatively low Reynolds numbers that are significantly smaller than those found in some nuclear applications, and the challenge of simulating subcooled and nucleate boiling phenomena, characterized by a wide range of physically important time and length scales, has not been met. The limitations of existing CFD codes were also discussed in the context of the real industrial applications of fuel assembly design and licensing. The opportunity of using high-end computation to address the coupling of CFD with other codes, such as neutronics and structure codes, was discussed. Such coupled codes will be needed for full reactor simulations. Several urgent industrial issues utilizing high end computing for nuclear science and engineering were identified. These include ‘crud’ deposition, fluid flow induced vibration, subcooled and nucleate boiling and critical heat flux.

Collaboration between the computational fluid dynamics group and the nuclear engineering/reactor physics group was identified as a critical need in the development of full plant simulation through the coupling of neutronics and thermal hydraulics codes for high-performance computing. The two groups are planning to develop a proposal for the simulation of nuclear reactors on high-end computers and the development of a “Virtual

Nuclear Reactor Center". The discussions also paved the path for interactions between the CFD and computational science groups to address the multiscale multiphysics modeling and simulation of fluid-structure interaction phenomena.

Computational Materials Science Group report (section 2)

The Computational Materials Group presented for general discussions a number of topics on multiscale modeling and simulation methods as well specific research problems in radiation effects on materials. The speakers and the primary topics addressed were:

R. Averback (University of Illinois) -- A generic radiation damage code
V. Bulatov (Lawrence Livermore National Laboratory - LLNL) -- Phase-field method
D. Wolf (Argonne National Laboratory - ANL) -- Mesoscale method linking atomistics with finite element
W. Weber (Pacific Northwest National Laboratory - PNNL) -- Materials/Radiation effects challenges (PNNL Perspective)
B. Uberuage (Los Alamos National Laboratory - LANL) -- Accurate defect energy calculations (LANL perspective)
B. Wirth (University of California at Berkeley) -- Radiation effects in fuels and structural materials
S. Yip (Massachusetts Institute of Technology - MIT) -- Reaction pathway sampling: water-silica interactions

Much of the presentation and following discussions centered on methods development and problem applications. This is not surprising since radiation effects on materials entail a very wide range of scientific issues and challenges. While practically all the participants acknowledge the importance of a multiscale approach, there does not yet exist a single simulation code with sufficient capabilities to address all the relevant problems. Averback and Bulatov initiated a step in this direction, with emphasis on the role that a new form of phase-field modeling can play. The Vienna *ab-initio* simulation package (VASP), a quantum mechanical molecular dynamics code developed for materials applications scales well on parallel systems and has relatively modest memory requirements. VASP is based on pseudopotentials and a plane wave basis set. However, from the standpoint of having codes that are sufficiently developed and benchmarked for high-end computing, much organization and work still lies ahead for the computational materials community.

A very significant outcome of the discussions on the second day, after presentation by the Computational Chemistry Group, is that a collaboration between the Chemistry and Materials groups would be extremely beneficial. The former can provide quantum chemical calculations on actinide materials in nuclear fuels and waste forms to enable the development of interatomic potentials that the latter can use to investigate various physical behavior of radiation damage. This synergy is most timely since the Chemistry group is much further ahead in terms of developing and benchmarking their codes for high-performance computing.

The two groups are planning to work together to prepare an End Station proposal, focused initially on studying uranium fuel. The expectation is that once the two sides are engaged, there will be no shortage of other highly relevant problems to attack.

Computational Chemistry Group Report (section 3)

The computational chemistry needs for Nuclear Fission Science and Engineering were discussed by the following:

Bert DeJong (Environmental Molecular Science Laboratory -EMSL, PNNL) – Quantum chemistry applications for actinide science with a focus on structures, vibrational spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy
Aurora Clark (Chemistry, Washington State University) - Quantum chemistry applications for actinide science with a focus on environmental applications (silicate actinyl interactions)
Rich Martin (LANL) - Quantum chemistry applications for actinyl oxides in the solid state and ultraviolet-visible (UV-Vis) spectroscopy
Ben Hay (PNNL) – Molecular mechanics and quantum chemistry applications to the design of separation systems as well as structure building approaches
Dave Dixon (Chemistry, The University of Alabama) – Quantum chemistry applications to electron driven chemistry in solution and to actinide structures and spectroscopy

The group presented results on how quantum and other aspects of computational chemistry can be used to address real problems in actinide science such as those summarized above. Because of the difficulty and expense involved in conducting experiments with radioactive materials, it is important to employ computational chemical methodologies which include relativistic effects for accurate calculations on molecular systems containing the actinides and lanthanides in order to guide the choice of experiments, to reliably extend the available experimental data into all of the regimes of interest, and to optimize the experimental work on radioactive materials. Calculations are needed to provide insights into molecular structures and speciation and to help interpret experimental data, for example, X-ray adsorption fine structure (EXAFS) data generated from light sources, or UV-vis, NMR, and vibrational spectroscopy. Accurate calculations of heavy elements can be very difficult and require the use of large basis sets. There are issues with the treatment of relativistic effects such as spin orbit and scalar relativistic contributions and potentially a large number of states. To interpret experimental data, it is important to be able to study a range of structures and to be able to study such structures in different environments such as solutions, the solid state and at interfaces. Such a computational capability in terms of methods, software, expertise, and access to high performance computers is needed to help mitigate the Nation’s loss of expertise and experimental capability in the area of actinide chemistry that is so critical to the multiple missions of the DOE, especially in the area of next generation nuclear reactors. Advances in theory are required notably in the areas of basis sets, solutions, solid state, and density functionals although progress in all of these areas is occurring with large impacts. The

question of the kinetics of the reactions of actinide containing compounds has rarely been addressed computationally and needs to be.

The design of new separation systems is critical to the success of the Advanced Fuel Cycle Initiative (AFCI) program. Weak interactions, such as hydrogen bonds and van der Waals interactions, and stronger interactions, such as ion-ion interactions and bonds between ligands and metal atoms, play crucial roles in the area of separations science. These types of host-guest interactions are responsible for the formation of molecular complexes without creating a 'chemical' bond, e.g., the amount of electron sharing between the interacting species is small compared to covalent bonds. Because these interactions are relatively weak except in the case of cation/anion interactions, the processes of making and breaking these bonds are usually more facile and reversible than for chemical bonds. Processes regulated by host-guest interactions generally involve multiple interactions between the guest (e.g., a metal ion) and the host (e.g., an interaction site on a macromolecule). Therefore, the dynamics of the process involves collective effects and more complicated reaction coordinates than simple bond breaking or formation. Host-guest interactions are central to separations systems, in which the competition between ion-solvent, ion-ligand, and ligand-solvent interactions controls the selectivity and efficiency of separations systems used to extract specific species from mixed wastes. Separation systems design is based on designing organic molecules that form strong complexes with discrete chemical species, in general cations and anions. Concepts embodied in *de novo* structure-based drug design are currently being adapted to the design of separation systems for cations and anions. The adaptation requires the development of methods for generating candidate structures and the use of molecular models for evaluation and prioritization of these structures with respect to their binding affinity for a specific guest. The computational approaches need to be developed and applied in close collaboration with experimental efforts to understand how the structure of host molecules governs guest recognition, and to identify candidate host architectures for synthesis and testing. Computer-aided host design has been shown to lead to dramatic increases in metal cation binding affinity (e.g., UO_2^{2+} or Cs^+) and recent efforts seek to extend such computational approaches to the design of hosts for anionic species (e.g., TcO_4^-, I^-, or NO_3^-). Computational tools allow accurate characterization of host-guest interactions, including an understanding of how the interaction energy changes with structure of the molecular complex and how molecular environment affects the interaction. Computational approaches that account for dynamics and fluctuations of the molecular complexes are essential to understand the thermodynamically stable conformations and to unravel the dynamical mechanism of complex formation. The ultimate goal is to generalize a computational approach to allow the deliberate design of efficient and selective host molecules for use in sensors and chemical separations for the advanced fuel cycle initiative.

Because of the complexity inherent in treating electron-driven processes in water, important questions regarding the primary chemical events remain after decades of inquiry. The excitation, relaxation, and reaction processes driven by electrons in aqueous systems span a wide range of energies and time scales: from thermal energies up to tens of eV and from femtoseconds to microseconds or longer. These processes include

scattering of electrons from molecules with relative translational energies up to 10s of eV, the dynamics of highly excited (electronic, vibrational, and rotational) states, the relaxation of energy in the condensed-phase environment, chemical reactions under highly nonequilibrium conditions, and the reactions of thermalized, but highly reactive, radical species. In all of these processes the role of water is poorly understood, if at all. Until very recently, one would have been tempted to conclude that the sheer complexity of the problem would preclude any attempts to establish realistic reaction pathways. A fundamental understanding of the complex collection of processes driven by low-energy electrons will enable progress in addressing longstanding issues in understanding radiation effects in aqueous environments including those related to energy production and waste processing. Computational chemistry will be critical in unraveling all of the interactions.

The above short summaries point out the need to develop methods that provide accurate results for use in engineering simulations and databases that contain the best computational and experimental results for use in benchmarking and in engineering simulations. Thus there needs to be close collaborations with experimental groups and the computational groups as well as among the different computational groups who use different approaches. We see that the first set of strong interactions will be with the Computational Materials Group as the methods used by both groups at the atomic level have substantial overlap and by the blurring of boundaries between the different disciplines from chemistry, physics, and materials engineering. A specific area of overlap is the development of new potentials for use in coarser grained simulations, especially for treating larger spatial systems at longer time scales.

Nuclear Reaction Cross-section Group report (section 4)

Accurate information on difficult-to-measure nuclear reaction cross-sections is needed to support the design of advanced nuclear fission reactors. At present, first principles methods can be used only for very light nuclei. *Ab initio* nuclear structure calculations can accurately be performed for light nuclei starting from protons and neutrons and realistic interactions. For heavier systems, nuclear density functional theory is employed and provides us with masses, deformations and scattering-vector (Q)-values across the nuclear chart. The RMS error on theoretical masses is about 700 keV. The calculation of cross sections for heavy nuclei is based on semi-empirical models that are calibrated using experimental data. More fundamental models for the prediction of these cross sections are being developed and implemented in reaction codes, and require much larger computing resources than those used at present, as detailed below. These developments will significantly improve the reliability of the predictions and reduce the uncertainties (quantified) on the nuclear data needed for the design and development of the next generation of nuclear reactors.

A first principles calculation of cross sections requires us to determine a more accurate nuclear density functional than presently employed. This will be possible by extending microscopic nuclear structure calculations to medium mass nuclei and neutron rich

isotopes, as this could be used to constrain and validate the nuclear density functional where no experimental data is available. The microscopic nuclear structure calculations (Green's function Monte Carlo, No-core shell model, coupled cluster theory) and complete mass table calculations via nuclear density functional theory are computationally expensive. They are presently performed on high-end computing facilities at Argonne, Livermore, NERSC, and Oak Ridge. Presently employed codes scale well to hundreds of processors. Progress in first principles calculations of nuclear cross sections will require us to develop new techniques (e.g. time-dependent nuclear density functional theory, time dependent coupled-cluster theory, fission dynamics), and will depend on access to peta-scale computing facilities.

Part of the low-energy nuclear structure theory community has submitted a SciDAC proposal titled 'Nuclear structure and low-energy reactions', and the Oak Ridge National Laboratory theory group submitted a successful proposal titled 'Ab-initio nuclear structure computations' to NLCF.

Engineering Group Report (Section E)

Survey of presentations

The nuclear engineering group presentations were split and presented over two sessions. On the first day, with input from Professors Turinsky and Anistratov, Dr. Ougouag presented a Computational Grand Challenge for nuclear engineering. This Grand Challenge entails the systematic, detailed, and extremely high-fidelity modeling of a nuclear reactor starting from first principles. Using a proposed hierarchical architecture of computers, computational and physical models, it is becoming increasingly plausible to devise a computational framework that produces useful information in a reasonable wall-clock time, while providing as high a level of fidelity as required. The hierarchy of models and computing processors would allow high level models to produce extremely high fidelity results by relying on multiple layers of lower level models that increase in sophistication and get closer to a full fledged first principles treatment as the level depth increases. When such a "virtual reactor" model is available, it could be used for design and optimization, as well as for playing what-if scenarios and for assessing data variances impact. It could also be used for exploration of phenomena at the edge or beyond the edge of experimental exploration.

The second presentation in the nuclear engineering series, given by Dr. Gehin of the Oak Ridge National Laboratory (ORNL), focused on providing a complete snapshot of the state of the art of reactor physics computations and identified current directions of research. Whereas the presentation was specific to existing methods and on-going developments at ORNL, its conclusions apply to the entire field of computational neutronics. This presentation complemented the first one by providing a comprehensive survey of the methods that need to be developed and/or adapted for the development of a virtual reactor, while it also identified current topics of active research. The main conclusion is similar to that of the first presentation, in that methods from a variety of

complementary fields will be needed, covering neutronics, thermal-hydraulics, and multiphysics in general.

The following two presentations of the nuclear engineering group were more specific to the development of methods for solving the neutron (and photon) transport equations on parallel platforms and for applying them with a high degree of detail and fidelity both in space and in the energy variable. The two presentations, by Professors Rahnema and Haghighat, respectively, addressed two distinct, independent, and different approaches to splitting the neutron transport problem in order to make massively parallel treatment possible. Both presented results from the implementation of their methods in parallel computing environments, up to hundreds of processors, with possible scaling up to thousands or higher.

The method presented by Prof. Rahnema relies on the decomposition of the transport problem into a very large number of local problems coupled at interfaces using a completely new technique for representing the angular dependence of the interface angular fluxes. The new method, embodied in the COMET code, is based on a hybrid approach. In this approach ultra-accurate transport theory response functions are pre-computed (normally using a Monte Carlo code) and then are used in a global transport theory solution for the entire reactor core. The method was shown to have an efficiency similar to that of diffusion theory applications, while allowing the accurate transport theory treatment of very large domains, even entire reactor cores.

Prof. Haghighat discussed efforts by the University of Florida Transport Theory Group to develop new parallel deterministic algorithms, automated variance reduction techniques for Monte Carlo methods, and hybrid techniques. Prof. Haghighat presented a list of real-world problems (including a large BWR simulation) that have been simulated using the PENTRAN (Parallel Environment Neutral-particle TRANsport) 3-D parallel transport code system, and a new version of MCNP, A^3MCNP (Automated Adjoint Accelerated MCNP), with automated variance reduction based on the deterministic importance function. He showed that the new hybrid and parallel processing methods have been very effective in reducing the computation time for simulating detailed real-world problems from days to hours on PC clusters with 10's of processors. Prof. Haghighat's group is currently also working on new hybrid techniques (such as those implemented in Georgia Tech's COMET code) with the aim or reducing computation times for some problems from hours down to minutes or even seconds. Finally, Prof. Haghighat, in concurrence with many other presenters, emphasized that in order to develop efficient parallel/hybrid algorithms, problem physics must be accounted for and the algorithms must reflect the physics correctly while using its features to identify parallelization opportunities.

The next-to-last presentation of the Nuclear Engineering Applications Group, by Professor Adams, was a call to realism and focused on the difficulty of implementing solution methods (for any problem) on massively parallel machines and on the requirement for effective multi-disciplinary groups that cover the science, algorithm development and parallel implementation on the platform at hand. Finally, Professor Adams did relate some of his experiences with implementing a parallel neutron transport

code on a very large number of processors (~1000) while pursuing the goal of implementation on massively parallel computers.

The final presentation for this group was by Professor Hawari of North Carolina State University. He discussed the methods he recently developed for the computation of thermal scattering kernels in graphite. His new developments were for perfect graphite as well as for realistic graphite that includes models of radiation damage. He pointed out that the computation of the damage configuration, i.e., the structure of the imperfect crystal, must be obtained using molecular dynamic (MD) simulations. For realistic applications with sufficiently large supercells to represent all the defect structures with their proper relative frequencies, these MD simulations will require extremely massive parallel computing capacities. The same finding applies to the codes downstream from the MD simulation. Many in the audience, including Professor Yip and Dr. Wolf, agreed that the problem identified by Professor Hawari is important and that the approach to it that he initiated is relevant, feasible, and worthy of access to Leadership-Class computing facilities.

Conclusions for Nuclear Engineering Applications

Exploration of access to high end computing for nuclear engineering and nuclear physics applications was an important goal for the workshop. The presentations by the nuclear engineering and nuclear physics group covered a wide range of applications of multiprocessor computing. While code comparable to NWchem, with a wide range of applications is not available, the scientists and engineers working in this area are making use of parallel computing on systems that range from only a few to as many as 1000 processors while work is continuing to extend the methods to increasingly larger numbers of processors.

Some nuclear engineering applications, which were deliberately not presented at the workshop, such as Monte Carlo simulations, for example, are trivially parallel and a distributed computing (grid computing) approach could be used for them. Although these applications could be run on large DOE computers, they are not challenging problems for high end computers, and DOE may restrict the application of its most powerful computers for these ‘embarrassingly parallel’ problems in the future.

In contrast, other reactor physics and engineering applications that were presented at the workshop, such as deterministic whole-reactor neutron transport modeling or scattering kernel computation, are challenging to implement in parallel. Yet many early successes have been achieved. Examples of successes were discussed in three presentations at the workshop. The three presentations, from the University of Florida, Texas A&M University and the Georgia Institute of Technology described independent and *different* approaches to achieving parallel implementation of the solution of the gamma and neutron transport equations. In all the presentations the limiting factor to massively parallel implementation was identified as the lack of access to suitable computers. Therefore, whereas the trivially parallel applications such as Monte Carlo can be run on existing large DOE distributed computing machines, the deterministic transport

applications will eventually require access to leadership class computing in order to take full advantage of the algorithmic advances that have recently been achieved and that are expected in the near future. It is also recognized that through ACSI the NNSA laboratories have developed linear and nonlinear transport equation solvers that perform well on massively parallel computers. Depending upon availability, this ready capability may serve as a starting point for utilization and future development by the reactor physics and nuclear engineering community.

In addition to the deterministic neutron and gamma transport methods, other applications are of direct importance to nuclear engineering. These include the preparation of nuclear data as they apply in the *realistic* material setting within reactors. One such application is the preparation of thermal neutron scattering data. These data are necessary in the modeling of the thermalization of neutrons, an essential step in their participation in the continuation of the chain reaction that constitutes the fundamental underlying phenomenon of an operating nuclear reactor. The computation of the thermal scattering data combines advanced material modeling and scattering cross section computation. This area of science is in essence an interface between nuclear engineering and material science. Long neglected as unimportant in light water reactors, it is now emerging as an important and fundamental area of required understanding for the safety mechanisms in gas-cooled graphite-moderated reactors. One presentation at the workshop shared some recent advances and showed that the main impediment to modeling increasingly realistic systems is the unavailability of massively parallel computing capability. Whereas the methods and (simple) models currently used are implemented on a cluster of about 500 processors, the move to realistic models with a fully realistic, high-fidelity, treatment of the material microstructure will immediately require tens of thousands of processors, and in the near future millions of processors.

During the discussion of the nuclear engineering applications, it was recognized that the optimization of reactor designs and the propagation of errors from data down to the predictions from the various codes are important goals and that their implementation will also require access to massively parallel computing. The employment of mathematical optimization often utilizes sensitivity coefficients to facilitate the search for the family of near optimum solutions, implying that optimization and sensitivity/uncertainty analysis share a common mathematical basis. The computational burden of evaluating sensitivity coefficients, whether via a forward perturbation approach or through an adjoint approach, is recognized to have the potential of being several orders of magnitude higher than just solving the original forward problem. Fortunately, both approaches are amendable to massively parallel implementation.

Summary of Path Forward

The path forward defined at the workshop consists of three components.

I. The computational chemistry and computational materials groups will collaborate on a ‘computational materials chemistry’ proposal, initially to focus on the

behavior of nuclear fuels. Because of time constraints (The Innovative and Novel Computational Impact on Theory and Experiment -INCITE - solicitation appeared today, Sunday February 26, and the submission deadline is Friday July 15 [2]. The National Energy Research Scientific Computing Center - NERSC - call for proposals for fiscal year 2007 allocations is expected to open on June 15 [3]) the people involved in this collaboration believe that an additional workshop to support this activity would not be helpful.

II. The computational chemistry group will prepare a proposal focused on the separation of the components of 'spent' fuel. Because of the time constraints mentioned above, they do not believe that a second workshop would be useful.

III. The nuclear engineering/reactor physics group and the computational fluid dynamics groups are not ready to submit a proposal in time for the upcoming INCITE and NERSC calls. They would like a second workshop to lay the groundwork for a Scientific Discovery Through Advanced Computing (SCIDAC) proposal to develop software for the simulation of nuclear reactors on high-end computers and the development of a 'Virtual Reactor Center' supported by the DOE Office of Nuclear Energy. The National Science Foundation Directorate for Computer and Information Science and Engineering might also support these projects. We plan to conduct the follow-up workshop in 4-6 months. At this workshop, participation by some members of the computational materials group may be appropriate.

[1] http://www.emsl.pnl.gov/docs/nwchem/nwchem.html

[2] http://hpc.science.doe.gov/allocations/incite/

[3] http://www.nersc.gov/nusers/accounts/allocations/ercap/