25 August 2006

Dr. Dennis Spurgeon, Director
Office of Nuclear Engineering
&
Dr. Michael Strayer, Director
Office of Advanced Scientific Computing
U. S. Department of Energy
Washington, DC

Dear Dennis and Michael,

On behalf of a large group of contributing scientists, engineers, applied mathematicians, and computer scientists from the national laboratories of the Department of Energy and our partners abroad, as well as leading universities and industries, we are pleased to deliver a preliminary letter report on the Workshop for Simulation and Modeling for Advanced Nuclear Energy Systems, held in Washington, DC last week.

We find herein (and detail further in a forthcoming report) that favorable trends in computational capability, modeling and algorithmic advances, and scientific software infrastructure should allow nuclear scientists and engineers to accelerate dramatically progress towards closing the nuclear fuel cycle through the development of new fuels, power plants, separations facilities, and repositories, relative to the pace of progress without the infusion into this endeavor of advanced computational technologies. While some of the required technologies appear to be available “off the shelf,” others are in their infancy. In both cases, a significant investment in human and computational resources will be required to realize their potential in the Global Nuclear Energy Partnership program. This investment, however, should be dwarfed by the savings relative to a purely experimental program and should begin paying off much earlier – perhaps a decade or more.

We also find that the multiscale, multiphysics research challenges inherent in closing the nuclear fuel cycle are as fully worthy of the best efforts of the applied mathematics and computer science research communities as they are of the nuclear research and design communities, and will stimulate exciting work in new directions. Now is an especially opportune time to build groups to work in a multi-disciplinary way towards the goals of the Global Nuclear Energy Partnership.

Best regards,

Phillip J. Finck
Associate Laboratory Director for Applied Science and Technology
Argonne National Laboratory

David E. Keyes
Fu Foundation Professor of Applied Mathematics
Columbia University

Rick L. Stevens
Associate Laboratory Director for Computing and Life Sciences
Argonne National Laboratory

Simulation and Modeling for Advanced Nuclear Energy Systems

Preliminary Report on a Workshop held August 15–17, 2006

Executive Summary

A joint DOE NE/SC workshop was held August 15–17, 2006, in Washington, DC, to explore the simulation and modeling needs for developing advanced nuclear energy systems. The purpose of the workshop was to obtain community input on the role of computational science and high-performance computing in the DOE advanced fuel cycle initiative (AFCI) and the emerging global nuclear energy partnership (GNEP).

The open workshop was attended by over 140 participants, representing 20 American universities, 10 Department of Energy national laboratories, the nuclear and computer industries, and international collaborators (France and Japan). A core of workshop invitees ensured close coupling of the workshop discussions and activities to the science and engineering needs of the Office of Nuclear Energy (NE). Approximately two-thirds of the representatives at the workshop were drawn from the nuclear engineering and nuclear energy communities.

Effort was made to ensure that participants explored a full spectrum of research and development opportunities, in both the short term (1 to 5 years) and the long term (5 years and beyond), since the GNEP program unfolds over several decades. Special attention was paid to tie workshop findings and recommendations both to Office of Nuclear Energy needs and to current and expected future capabilities of the Office of Science (SC), and in particular, the Office of Advanced Scientific Computing Research (ASCR). This objective was facilitated by a series of plenary talks providing overviews of current and planned activities of these Offices.

Technical discussions focused on six major areas where simulation and modeling are clearly relevant to the GNEP program: reactor core, seismic/structural mechanics/ balance-of-plant, repositories, separations chemistry, materials and fuel design, and model validation, with the goal of defining opportunities for collaboration between the nuclear energy research community and the applied mathematics and computer science communities. This agenda was pursued first through breakout groups under the six areas above, organized by experts in the nuclear energy technologies for the mathematicians and computer scientists. Roles were then reversed and the nuclear scientists and engineers participated in sessions organized around the six categories of: mathematical and geometrical modeling, verification/validation and uncertainty quantification, scalable and multiscale algorithms, software tools and software engineering, data analysis and visualization, and computing facilities, data and networking.

Several crosscutting issues in the enabling technologies emerged as themes in more than one breakout group and are likely fertile for investment and collaboration. These include:

- Uncertainty quantification and error estimation in simulations

- Methods for systems that couple multiple models
- Movement away from empirical models toward physics-based and even first-principles models
- Methods for systems with multiple scales
- Algorithms and software that scale well on high-capability computational platforms
- Simulation workflow management, including data archiving and automated discovery

The following are tentative high-level findings of the workshop:

1. The existing code base available to the nuclear industry and its regulators is insufficiently predictive to guarantee attainment of the ambitious technology stretch goals of the Global Nuclear Energy Partnership.
2. A significant opportunity exists to apply advanced modeling and simulation and high-performance computing to improve designs of future reactors, reduce uncertainty in facilities development and construction costs, improve safety, and reduce development times of new fuel types needed to close the nuclear fuel cycle.
3. Significant research challenges remain in developing and scaling multiscale and multiphysics codes to the performance levels needed for fundamental studies, as well as engineering and design use. These research challenges are similar (but not identical) to those faced in other science and engineering domains; thus many techniques can be leveraged from other disciplines.
4. Accomplishing the development priorities of GNEP will require investment in existing nuclear energy codes and software tools to address short-term design and planning use, simultaneously with investments to start longer term projects aimed and future needs with long development times.
5. The United States has the needed expertise and is capable of deploying computational infrastructure to begin building a new generation of nuclear energy simulation codes that could shift paradigms in the development of new nuclear energy systems. To reap the benefits of an approach that uses computation to reduce the scope, cost, and time latency of required experimentation will, in turn, require a sustained software development activity and a corresponding buildup of human resources and large-scale faculties.
6. The creation of new physics-based high-fidelity simulation codes offers the possibility of accelerating the licensing process, if the regulatory process can be modified to incorporate first-principles simulations as a basis for risk analysis and design approvals.

Tentative high-level recommendations, subject to revision in the final report, include:

1. Establish a significant number of multidisciplinary development teams comprised of experts in applied mathematics, computer science, nuclear engineering, materials science, chemistry, and advanced software engineering to begin the development of next generation simulation codes based on models closer to “first principles,” aimed at deployment in the 5-to-10-year time frame. These teams should have the explicit goal of developing open source community codes that will be used for next-generation design of nuclear fuels, power plants, separations plants, and repositories.

The SciDAC and ASC experiences offer confidence that this can be achieved, as well as much software to be leveraged.

2. Establish and support teams of software engineering and parallel computing experts to work with the established nuclear engineering community on existing codes, to port these codes to modern platforms in the near term, to integrate them into modern engineering workflows, and to support near-term design and engineering.
3. Establish a scientifically demonstrated validation process that will provide sufficient assurance the predictive capabilities of simulations – first of components and ultimately of integrated systems – that stakeholders beyond the technical realm will be able to rely upon simulation to support capital investment and national and international policy making.
4. Create a long-term research program including a mix of university and laboratory research aimed at advancing the cross-cutting issues (e.g., new approaches to uncertainty quantification and error estimation, multiscale and scalable algorithms, and development and validation of coupled multiphysics codes). This work should be motivated by the actual research and development needs of the GNEP program and should be supported at a level that permits rapid acceleration.
5. Dedicate significant resources on DOE's large-scale facilities for proof-of-principle runs, development of new methods, and for the production use of existing and new tools by the US nuclear energy community and its international GNEP partners.
6. Develop a foundation (university programs and laboratory internships) for training the next generation of computationally oriented nuclear engineers and scientists in related disciplines needed to support the long-term redevelopment of nuclear energy in the US and the world.

Simulation Agenda of the Office of Nuclear Engineering for the GNEP Program

GNEP envisions the implementation of a novel set of nuclear technologies to enable long-term sustainability of the nuclear fission power option. GNEP will, in particular, extend long-term energy resources, drastically reduce the need for geologic repositories, and dramatically reduce the proliferation risk associated with the inevitable global expansion of nuclear energy.

To achieve these objectives, GNEP proposes replacing the current once-through nuclear fuel cycle with a nearly closed fuel cycle, relying on a combination of technologies:

- Commercial reactors, mostly light water reactors (LWRs), will continue to operate in their current mode, and as a result will produce significant quantities of spent nuclear fuel (SNF).
- The SNF, instead of being sent to geologic disposal, will be treated to separate its constitutive elements. Certain elements will be encased in novel waste forms to be disposed of, whereas the transuranic elements (TRU) will be transmuted (mostly via the fission process) in specialized fast reactors.
- Specifically, the TRUs will be sent to a fuel fabrication plant, where they will be incorporated in novel forms of fuel.
- The novel fuels will be irradiated in a fast neutron reactor, where a fraction of the TRUs will be destroyed. The irradiated fuel will be treated to separate its

constitutive elements. The remaining TRUs will be sent to the fuel fabrication plant, whereas other elements will be incorporated in specialized waste forms for disposal.

New nuclear technologies are generally extrapolated from existing technologies over a long gestation period, following which there is strong confidence that their implementation will be technically successful. Nevertheless, we have identified a number of challenges that might hinder the deployment of GNEP technologies. We have classified these challenges into three categories: technical feasibility issues (can the GNEP requirements be met?); cost issues (will GNEP be affordable?), and regulatory issues (can the GNEP technologies be licensed?). Our discussions have led us to conclude that along with well structured engineering and basic science programs, a robust modeling and simulation program will have major impacts in eliminating these challenges. Following are summaries, for each technology, of the major challenges and of the most important contributions expected from modeling and simulation.

LWR separations technologies: Key technical feasibility issues include the needs to reduce separations losses to a very low level, create waste forms that will last for extremely long periods, and track materials throughout the plant with high precision. Losses, and the concomitant need to clean up and recycle waste streams, contribute to increased costs. Finally, a licensing approach for separation plants needs to be established; this will likely impose additional requirements on the design approach.

Transmutation fuel fabrication and irradiation: Advanced fuels with significant quantities of minor actinides have not yet been demonstrated; this is the key feasibility issue for all of GNEP. The current approach to fuel development is very empirical, relying on sequential experimentation, with significant implications for schedule and cost. The scientific understanding of fuel irradiation behavior is very limited and creates additional constraints on the licensing process.

Fast Reactors: There are no significant feasibility issues for fast reactors; nevertheless, the cost of fast reactors is expected to be higher than that of thermal reactors, unless design margins can be reduced and simplified designs can be used. Furthermore, the licensing approach to the fast reactor might create additional costs.

Back-end separations: The issues here are similar to those described for the front-end separations plants.

Repositories: The key feasibility issue is that the small volume of waste forms leaving the GNEP fuel cycle must be stored robustly for the long term in repositories.

Modeling and simulation can have a major impact on resolving each of these challenges, as described below.

Separations plants and repositories: Accurate process models are needed both to guide the R&D process and to predict loss mechanisms. Such models are needed first for individual processes, but they also need to be coupled for a complete plant. Accurate waste form models are needed to predict waste behavior for a variety of scenarios, ranging from local handling and transportation to temporary storage and long-term geologic disposal.

Fuels: The development of predictive fuel behavior models (during fabrication and during irradiation) can have a major impact on the R&D process, shaving years off of a purely experimental approach. Both feasibility and rate of deployment are at stake.

Fast reactors: High-fidelity coupled neutronics, thermo-hydrodynamics, and structural models can reduce margins without compromising safety and confidence, and hence reduce cost and facilitate licensing demonstrations. Materials performance models and seismic analysis tools are also needed. Without the efficiency gains possible from predictive plant modeling, GNEP may be too costly to deploy.

Several crosscutting simulation needs are identified with bullets in the Executive Summary above. Two of these resonate most broadly and are not available “off the shelf” but require long-term research. A fundamental need is the development and implementation of a validation methodology for the suite of codes to be employed in a predictive sense in GNEP. Second, we need to develop means of coupling component models to produce whole system models. This is a process that demands both deep engineering insight into what interactions and scales must be represented and flexible and powerful software tools to capture and balance them.

Contributions to the GNEP Program from the Office of Science

The Office of Science holds simulation assets – scientific software tools, hardware platforms, and interdisciplinary research staff – without equal in the world. As the nation architects an internationally competitive next generation nuclear industry, its international strengths in large-scale simulation confer advantages that offset lack of recent experience in designing plants. Furthermore, the GNEP research agenda challenges the limits of our simulation capabilities in every direction, making it a worthy focus of simulation leaders. Opportunities for a mutually beneficial partnership abound.

Favorable trends in capability and cost of large-scale simulation are transforming other fields of science and engineering into substantially simulation-based activities. As measured by the Gordon Bell peak performance prize, sustained processing rates on science and engineering tasks formulated similarly to GNEP applications – as systems of particles, partial differential equations, etc. – have improved by five orders of magnitude over the seventeen years of prize history and should remain on this trajectory. Beneath the peak performance prize, the Gordon Bell special prize tracks steady progress for unstructured adaptive applications of billions of degrees of freedom on many thousands of processors. As measured by the Gordon Bell price performance prize on the same set of applications, acquisition cost per sustained processing capability has dropped by four orders of magnitude over the same period. Though simulations cannot replace experiments altogether, their vastly greater affordability creates an incentive to employ simulation to bypass experimentation wherever possible. Simulation has the potential both to focus experimental effort on the most important parametric regimes and to reduce the long lead times of experimentation in yielding understanding.

For simulation to achieve its potential, close collaboration will be required between tool developers in the Office of Science and users in the Office of Nuclear Energy. Both the challenges and the tools are too complex for a transfer of technology that is short of shared personnel. The promised return for this investment of the time of valuable personnel in learning new techniques and applications is a computational lever that will raise human productivity for scientific advancement and engineering design. DOE's ASC and SciDAC programs have amply demonstrated that large-scale simulation can enhance research and design programs in both expected and unexpected ways, the latter including re-examination of trusted models on the application side and breakthroughs driven by new challenges on the techniques side.

The GNEP research agenda for the Office of Science embraces two different and equally important directions: harnessing the growing capabilities of computation to improve the fidelity of complex geometry, multiscale, multirate, multi-physics models on one hand, and lowering the threshold of expertise required to employ "best practices" and scalable software on the other.

The simulation techniques required to support the GNEP program include CAD-to-mesh geometric adaptivity, solution-based adaptivity, mesh partitioning, discretizations of virtually all types (with attention to advanced high-order discretizations), optimal implicit solvers, stiff method-of-lines integrators, kinetic and particle methods, unconstrained and constrained optimization (for parameter identification, control, design, etc.), uncertainty quantification, sensitivity analysis (both statistics-based and derivatives-based), multiscale methods, homogenization, and reduced-order modeling.

Computational techniques underlying this agenda include: parallel programming models (MPI, multithreading, etc.), dynamic load balancing, language interoperability, componentization, high-performance I/O, performance monitoring/debugging, distributed data archiving, visualization, automated discovery tools/data mining, assimilation and fusion of experimental data with simulations, workflow description and codification.

GNEP represents a rare and ripe opportunity for developers of the enabling technologies in applied mathematics and computer science to demonstrate a paradigmatic shift that they have envisioned for years. Since the current code base for GNEP technologies, with some notable exceptions, was created for computing environments of much lower capabilities than what is now available, it will have to be substantially rewritten. This substantial task can be accomplished while preserving key code assets at low levels, like physical property data bases and software that evaluates constitutive properties (in its original language). However, the connective and control code and the majority of the means of interchange of data between code components will be written to take advantage of modern software practices and high-performance parallel architectures. Virtually all large-scale data structures in existing codes will have to be replaced with distributed versions. As the software infrastructure is rebuilt, due attention can be given to extensibility, reusability, object orientation, componentization, portability, performance portability and tuning, code self-description and self-monitoring, and the construction of multi-layered interfaces that enforce correct usage.

Transcending the monolithic software applications of earlier eras will potentially confer two benefits on the GNEP program beyond the immediate practical scientific and engineering advantages, in terms of debugging, correctness, efficiency, and so forth. With modularity, export control and intellectual property restrictions can be applied with fine granularity, enabling sharing of open standard modules without compromise of security or company propriety. In addition, for that subset of the GNEP research software infrastructure that is useful in the federal regulatory process (licensing/certification) streamlined approvals may be possible through reuse of approved standard components.