NEAMS (NEAC) Program Review
Final Report

Introduction

At the outset of FY2012, Dr. Pete Lyons (through NEAC Chairman William Martin) chartered a subcommittee of the DOE Nuclear Energy Advisory Committee (NEAC) to conduct a program review of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, and to provide recommendations to the Assistant Secretary for Nuclear Energy through the NEAC channel. The recommendations would address the "efficacy of the prioritization and activities comprising NEAMS". The Statement of Work included: the basic strategy for NEAMS, the management and execution of NEAMS, the code development portfolio, and the scope of crosscutting/enabling work that supports code development. The chartering document is included with this Report as **Attachment A**.

A NEAC Subcommittee was formed of eleven members and chaired by Dr. Raymond Juzaitis. A full listing of Subcommittee members is included as **Attachment B**. Membership included participation from national laboratories, academia, government, and industry.

The first meeting of this sub-committee was held on December 14, 2011, at DOE Headquarters/Forrestal Building. All members of the Subcommittee were in attendance at the inaugural day-long session. A second (two-day) meeting was held in late May of 2012. The agendas for the two meetings are attached to this Report for reference purposes (**Attachment C**). The overall scope of the initial meeting in December 2011 covered the vision, strategy, and overall management structure of NEAMS. Technical approach and technical direction of the code development portfolio were reviewed in May 2012.

Observations Following Meeting #1

The original NEAMS program vision was observed as being broad-based and expansive, addressing modeling/simulation challenges in all major technical program elements of the DOE's Office of Nuclear Energy. The program was patterned after similar successful modeling & simulation efforts in the Nuclear Weapons Program (ASC) and the DOE Office of Science (ASCR). The committee resonated with the overall program goal of upgrading the national capability to model and to predictively simulate key systems that constitute the civilian nuclear energy enterprise: fuel-cycle and waste systems, as well as nuclear reactor systems. However, the Committee was generally concerned with the lack of balance between the grand program vision and the budgeted/appropriated resources needed to execute against it. Expectations had not been readjusted to the budget realities as they were becoming evident in FY12. The active efforts seemed to be too diffuse for the level of funding and amount of expertise captured by the NEAMS program umbrella. Concerns were raised that this vision-resource disconnect would ultimately be problematic for attracting needed technical talent; would inevitably result in frustration among the program leaders; and would possibly lead to program credibility issues wherein the expectations of the "grand vision" could not be met. Although the transformational effect of advanced modeling and simulation on NE programs was an unassailable aspiration, the leadership of the overall program will need to decide how much "transformation" can be afforded given other programmatic and budgetary drivers.

The Committee observed too much duplication between NEAMS and CASL (Center for Advanced Simulation of Light Water Reactors). Although at the high level, the distinctions between the shorter-term innovation hub (CASL objectives) and the longer-term NEAMS objectives were well articulated, the anecdotal descriptions of technical activities and accomplishments in the two Advanced Modeling and Simulation Office (AMSO) program elements belied the stated distinctions, and indicated significant overlap. The respective "visions" for NEAMS and CASL were found to require more harmonization, or perhaps differentiation if mutual exclusion was to be the program intent.

Federal management and reporting complexity appeared to be somewhat overwhelming for a $23M program (FY2012) and declining. The Committee noted too many participating organizations and principal investigators (PIs), as well as too many tasks. The programmatic environment in which NEAMS operates was observed to be very mercurial, with frequent changes in program priority and little stability in funding levels. In this difficult environment, overall program management appeared to reflect a "level-of-effort" resource allocation process, with work across all functions annually tailored to fit within available funding for that year. As such, there did not appear to be a sense of urgency permeating the program. Milestones were not indicative of a hierarchically ordered set of deliverables designed to create a coherent structure, compelling and defensible against externally-imposed budget cuts. The Committee suggested the adoption of a strategic and coherent set of product-based milestones that would derive from compelling priorities of the NE program in the next two to five years. Work could then be shaped to meet national needs. Such a hierarchical structure of nested product-based program deliverables would naturally admit a more coherent environment for program management and execution, providing natural interfaces for the roles and responsibilities of federal and laboratory program managers. This would also institutionalize proper resource loading and accountability, offering a more compelling defense against budget reductions.

The user community was found to be too ambiguously characterized and appeared to overly represent the National Laboratories themselves. End-user requirements had not been established, although stakeholders' needs were solicited via a meeting in February 2012 with national laboratory and DOE personnel, and subsequently (independently) from industry personnel. If resultant capabilities were to demand regular use of massively-parallel supercomputers, this could be problematic for the contemporary industrial/regulatory user community which does not embody such a hardware environment. The presentations referred to "industry partners", but it was noted that no industry partners had been identified that actually represented the commercial nuclear sector.

Program Changes Between First and Second Meetings

By the time the NEAMS Program Review Subcommittee reconvened in May 2012, major changes had taken place in the Advanced Modeling and Simulation Office (AMSO). The program had made some progress coming to grips with a much reduced level of resources; in fact, NEAMS resources had been slashed from $26M (FY10) to a projected $10M in FY13. Given higher-than-originally-appropriated actual expenditures in FY12, the reduction was more like a drop from $35M to $10M in one year. A realization was being socialized that the NE mission could simply not afford the transformational scope for Modeling and Simulation (M&S) such as that demonstrated earlier in the Nuclear Weapons ASC program. The NEAMS program accommodated these changes by downsizing from four original Integrated Performance and Safety Codes (IPSC) that addressed: fuels, reactors, safe separations, and waste forms; and from the four cross-cutting "Common Methods and Tools" (CMT): verification & validation/uncertainty quantification, fundamental methods and models, enabling computing technologies, and capability transfer. The organizing principle for the program now was focused along the lines of a comprehensive set of predictive modeling and simulation tools known as the "Fermi Toolkit". The key feature of this "toolkit" would be its versatility and adaptability to address any number of potential advanced fuel-reactor systems.

The management structure was also somewhat more streamlined from the one to which the Subcommittee had been introduced in December 2011. The more modestly scoped program was presented to the NEAMS Subcommittee in May of 2012. Whereas the CASL HUB ("Center for Advanced Simulation of Light-Water Reactors") was focused on meeting the simulation needs of the Light-Water Reactor community (especially PWR systems), the Fermi Toolkit would address the simulation needs of proposed "Advanced" fuel-reactor systems, in particular those that involve single-phase coolants (e.g., liquid metal or molten salt). Research would perhaps be more aligned to the needs of small startup companies currently pursuing advanced reactor technologies.

The FERMI TOOLKIT

The "Fermi Toolkit" presented to the subcommittee in May 2012 revolved around two basic product lines: fuels and reactors. The proposed toolkit addresses a significant shift in computing paradigm, based on modularity and flexibility that would be achieved through modern computing tools and techniques. The tools comprising the toolkit could be used both as "stand-alone" programs or strongly coupled tools to address those technical issues that require such coupling. Together, the tools would enable researchers, designers, and analysts to apply the dominant fundamental laws governing performance and safety of nuclear power systems from "pellet to plant"! Modular toolsets would address the following six areas: materials science, neutronics, structural mechanics, fluid dynamics, thermal mechanics, and supporting computational tools. Although the first version of the Fermi Toolkit was planned to appear in FY13, the full set of capabilities promised by this effort would be developed over a period of 5 years. Complementary experimental efforts that could conceivably be used for validation of the toolkit would not be covered by these resources. The committee also did not hear a clear vision about how the Fermi Toolkit would be distinguished or integrated with CASL, nor how these tools would be utilized throughout the overall DOE NE program to assist in evaluating fuel cycle options.

Fuels Product Line: Marmot and Bison

Marmot comprises the meso-scale microstructure evolution code, supported by separate atomistic, mesh, and visualization tools. The application focus would be on nuclear fuel design and analysis, enabling the acceleration of design through qualification of new fuels. Starting with the modeling of oxide fuels behavior, capabilities will be extended to additional fuel forms and compositions. Microstructure-resolved simulations will also enable the prediction of microstructure evolution under irradiation, something that current capabilities model by employing crude empirical burn-up calibrations.

Bison is the paired engineering-scale fuel performance tool and allows for the interfacing with reactor codes at the fuel assembly scale. The finite-element-based code solves the fully-coupled thermomechanics and species diffusion equations in 2D and 3D. A multi-scale modeling framework involves upscaling from lower-length-scale atomistic modeling through the continuum scale. Bison can address performance issues with LWR oxide, TRISO, and metal fuels. Prediction will focus on fuel pin failure and support for quantifying failure probability. The discrete-pellet simulations allow for the high-fidelity modeling of fuel/cladding interactions and fission gas release resulting from fuel failure. The necessary coupling is supported by the *Moose* (“Multi-physics Object-Oriented Simulation Environment”) framework which supports the coupled use of Marmot and Bison. Much of the effort that was briefed involved the imperative to replace currently-employed empirical formulations with higher-fidelity lower-scale models.

Legacy fuel simulation codes are currently based on empirical formulations that require specific time-consuming validation for each fuel behavior/phenomenology modeled. The new tool kit offers the opportunity for a much more efficient implementation process (consistent with NRC V&V requirements) by making the overall “code” more broadly applicable for a greater range of fuel types and conditions that would not have to be re-benchmarked for each new change. A more predictive approach promises significant gains in studying problems such as: fuel centerline temperature prediction, fission gas release, pellet-cladding mechanical interaction. Coupling to lower scales involves the use of “up-scaling” methods to capture the physics revealed by atomistic simulations by employing a “state-variable” approach in the modeling paradigm at the mesoscale level. MARMOT employs such a multiphysics phase field approach to model microstructure evolution (allows modeling of microstructure as a function of continuous variables). Phenomena represented include: intragranular bubble growth and intergranular fracture due to thermal expansion, fission gas release, fuel restructuring and relocation.

Lower length-scale modeling and methods development provides the ultimate foundation for predictive ability. Molecular dynamics simulations, dislocation dynamics models, and crystal plasticity models can inform the tools employed by fuels/reactor systems designers and provide a foundation for high-fidelity modeling of thermodynamic and kinetic properties under irradiation. However, the potentially large volume of work (in particular when also engaging the university community through NEUP, as well as engaging efforts at numerous national laboratories) does not seem to be prioritized or organized via programmatic direction that addresses needs of the end-user community. Justification in a resource-constrained environment demands compelling arguments that would demonstrably couple this effort to "value-added" merits expressed at the application level. Resolving explicitly identified physics deficiencies in the engineering-scale codes that limit the range-of-applicability of such codes in regimes of importance to end-applications would help significantly in this regard. (Ultimately, in the context of the total AMSO effort, this would also inform overall nuclear fuel/reactor system development by promising to reduce development time, regulatory effort and cost, ultimately bus-bar cost of electricity. The committee did not see this type of flow-down focusing effect for guiding the basic R&D effort.)

Reactor Product Line: SHARP and RELAP7

The ultimate objective of the "Reactor Product Line" derived from the Fermi Toolkit is to simulate reactor performance and safety from the plant scale, down to the detailed flow around a fuel spacer grid, and radiation transport and heat transfer resolved at the pin scale. The Fermi Toolkit allows for the flexible integration of modular toolsets for representation of key physical phenomena. This capability provides a foundation for the development of many "customized user environments"—the equivalent of what might have previously been called "codes" in the "Fortran Age".

The SHARP capability addresses the challenge of multi-physics, multi-scale simulation to enable the predictive modeling of a full reactor core in 3D. The multi-resolution capability in this type of performance and safety modeling requires a hierarchical simulation approach that bridges from direct numerical fluid simulation (DNS), through large eddy simulations (LES), Reynolds-averaged Navier-Stokes (RANS) based CFD, ultimately up to subchannel or lumped-parameter models used at the system scale. SHARP employs a Nek5000 fluids module to span the scales between DNS and RANS. Nek5000 is a high-fidelity spectral element CFD code with a substantial pedigree derived from open-source development. The spectral methods theoretically allow for exponential convergence. Other physics modules in the SHARP suite include:

neutronics (with focus on full-core representation in 3D, including embedded cross-section processing tools, and enabling reactor kinetics, depletion, and burn-up analyses); ***core thermal mechanics*** (providing accurate pin-resolved temperature distributions with scaling qualities good enough to represent a full pin-resolved core); and ***core structural mechanics*** (providing accurate assembly-resolved stress distributions and predictions of assembly scale distortions). The modularity and flexibility of SHARP is facilitated by an object-oriented software framework that allows for incorporation of distinct components along functional lines, with the SHARP application assembled from individual components. This framework is called MOAB (Mesh-Oriented datABase). MOAB allows for the representation of both structured and unstructured mesh models, including both geometry representation and data representation. This is critically important for the multi-physics modeling inherent in SHARP. The MOAB capability results from leveraging of investments made by DOE's Office of Science (ASCR).

The near-term "grand-challenge" focus application for SHARP involves the modeling of Sodium-Cooled Fast Reactors; specifically, the passive safety response features of such reactors in a loss-of-flow transient. This first challenge is one that is not addressed by current state-of-the-art codes, builds on significant prior accomplishments (e.g., LDRD, GNEP), and is favored by a significant volume of relevant available experimental validation data (EBR-II, FFTF, ETEC, and separate effects tests).

The RELAP7 element of the Reactor Product Line represents a modern 0D/1D reactor system/safety analysis application (i.e., full-plant, reduced-dimension simulations employing parameterized behavior of all system components). RELAP7 is an evolutionary extension of current-generation RELAP5 capability, re-factored for an object-oriented MOOSE-based simulation environment (see "Fuels Product Line" discussion). RELAP7 will address several of the limitations of RELAP5 (e.g., long transient modeling of weak driving sources, C++ computer software programming, advanced numerical methods, and well-posed modeling of 2-phase flow) and is projected to meet all NQA-1 requirements. The RELAP7 development effort is first focused on demonstrating success against the challenges posed by system-level modeling of a BWR transient associated with full-station blackout scenarios. As such, it represents capability needed to perform modern, relevant safety analysis.

The Reactor Product Line has successfully demonstrated advanced capability on a number of "integrated simulations". These include: SFR structural mechanics associated with a LOF transient; sensitivity studies of control-rod hole models in VHTR reactor designs; velocity, fuel temperature, and power distributions in VHTR, LWR quarter-core calculations, and BWR fuel assembly calculations. Results were presented to the committee.

Plans are being established to more closely integrate SHARP and RELAP7 with the Fuels Product Line.

Committee Observations and Recommendations

Having considered the briefings presented to us over the two sessions, as well as reflecting on discussions with program management and perspectives shared among ourselves, the NEAC/NEAMS Review Subcommittee provides the following set of observations and recommendations:

Observations

1. We completely understand the budget pressures that NEAMS is currently experiencing. We acknowledge the steps that have already been taken to downsize the program to a scope that more reasonably matches the resources that reflect the program's prioritization within the NE portfolio. However, we also continue to wholeheartedly support the role of advanced modeling and simulation in support of the broader NE mission, including its potentially transformational role in both fuel/waste management and reactor development/analysis sectors. We note that the funding for NEAMS pales in comparison to other national modeling and simulation programs. The goals of the NEAMS product ("Fermi Toolkit") is still as ambitious, if not more, than an NNSA/ASC burn code effort, as well as CASL which is funded at $25M/year. Overall, the NEAMS stated scope and associated budget still do not appear to be consistent.
2. The technical approach presented to us, particularly the introduction of the "Fermi Toolkit" paradigm, makes a great deal of sense. The "toolkit" provides a more flexible, collaborative, and affordable computational environment that is quite attractive to a new generation of users. The five attributes characterizing the environment (predictive, modular, trustworthy, useful, and broadly adaptive to a changing environment) are well founded. Emphasis on multi-physics and multi-scale modeling is future-oriented and aligned with the objectives of predictive capability.
3. We applaud the systematic leveraging of existing work and previous R&D investments in building out the Fermi Toolkit. The emphasis on attacking a diverse set of complex nuclear engineering problems (for relatively low funding levels) is noteworthy and compelling.
4. Emphasis on verification and validation was integrated into many of the presentations. However, despite the ubiquitous references to V&V, we did not see the NE R&D programs making a strong commitment to identify and integrate specific experimental efforts that would be aligned with (if not managed by) the NEAMS program. We see this as a deficiency in program direction, not in technical approach. The relevant experimental program for this effort seemed to be more opportunistic than planned. This will potentially create an "Achilles heel" for any strategic emphasis on scheduled/targeted predictive capability, and eventual application by end users. The DOE should seriously look to past, present, and future domestic and international programs to obtain the data needed to benchmark, i.e., V&V, the Fermi Toolbox, given the likely U.S. budgetary constraints in obtaining new data.
5. We saw a much more tractable organizational structure for program management than at our first meeting; however, the role of the National Technical Director (NTD) appeared

somewhat confusing given the NEAMS organization chart that shows this position in more of an advisory role than a “direction” role. The NEAMS program requires a strong, empowered technical director, who would galvanize a strong technical leadership team. (Some of our members participating on the CASL Advisory Board recommend strongly that NEAMS look at the leadership model in CASL, which is purportedly an excellent model.) Integration of key potential users into the development process from the very outset of the enterprise would also help to focus the program. (The CASL program not only has an industry council, but has TVA and Westinghouse engineers integrated into the project teams that are planning and executing the projects. This has been a significant help.)

6. The reactor-based effort appeared to be more coordinated than the fuels work. The latter effort appears to lack prioritization and application focus, especially in the area of lower-length-scale modeling.
7. The identified program milestones seem to be more associated with “code releases” than representative of technical advancement in predictive capability.
8. Concern exists that the movement from RELAP5 to RELAP7 may need a greater degree of socialization with the NRC and the industrial stakeholder community. RELAP7 would be a welcome capability to the nuclear industry if it gets proper V&V and NRC approval. In the near term, it could be valuable in designing and licensing SMRs.

Recommendations

1. The NEAMS program could greatly benefit from a stronger and more compelling requirements definition process. Our subcommittee strongly suggests a formal “Users Group”, which draws on the involvement of industry, regulatory, laboratory, and academic communities. (e.g., CASL has both an Industry Council and a Science Council). This would help in moving technical goals from an aspirational basis to a more defensible and sustainable programmatic basis.
2. The program needs to adopt a more formal and rigorous requirements “flow-down” process which coherently integrates the numerous elements of the program and rationalizes the prioritization of these elements to support compelling high-level milestones that meet urgent user predictive capability needs tied to reactor or fuel development timelines. A resulting “project plan” would institutionalize these objectives through disciplined and coordinated planning of scope, schedule, and cost.
3. If the NE program is committed to leveraging the full potential of predictive simulation for the nuclear power enterprise, it must move to integrate computational efforts with the requisite experimental activities that will support the validation of the computational tools. Program milestones should implicitly require successful simultaneous execution of both computational and experimental efforts. Integration in AMSO of all NE efforts that would support modeling and simulation would also be prudent. Finally, the modeling and

simulation budget should ultimately be sized to meet the scope and timelines requested by the user base.

4. The fuel performance modeling package (MOOSE-BISON-MARMOT) would be extremely valuable as new fuel types are pursued as part of the “accident tolerant fuel” program, since designs will likely move away from the well-known UO_2 pellets with Zirconium alloy cladding designs. This would require an intensive V&V program to obtain NRC approval to use the methodology for operating reactor fuel application. In addition, in concert with future program directions in the wake of the Blue Ribbon Commission Report, analysis of fuel performance in long term storage would be another excellent opportunity to exercise new predictive simulation capability.
5. We recommend more thought and progress in clearly stating a compelling “business case” for the NEAMS program, to support the aspirational goal of attaining predictive capability with broader and more practical socio-economic value. The missing value proposition potentially tied to quantified reduction of the cost and schedule of reactor development programs, reduction in regulatory burden, or even reduction in the busbar cost of electricity would go a long way to protecting program funding in an uncertain budgetary environment. It would also bolster support among the other elements of the NE program.

The committee wishes to thank all of the briefers and program management personnel for the significant effort that was made in preparing and hosting our two review sessions in Washington, DC.