NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

INITIAL EXPERIENCES WITH THE NEAMS EARLY USER PROGRAM

 (NEAMS Milestone M3MS-12OR0608045)

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Version History

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1.0	2012-10-10	Initial version

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1 Executive Summary

In FY 2012, the NEAMS program initiated an Early User Program to get the modeling and simulation codes being developed by the program into the hands of "friendly" users outside the development team. The primary purpose of this activity was to provide the development teams with independent feedback as to the scientific and computational performance of the codes, their usability and other factors. It also serves to provide the stakeholders of the NEAMS program with visibility into the progress and capability of the codes prior to their anticipated first full official release in 2018. Seven teams were supported under the FY 2012 Early User program, working with the BISON/MOOSE and AMP fuel performance codes, and the Nek5000 computational fluid dynamics code for reactor modeling, primarily in validation studies. The program was considered successful and useful by the Product Line Leads, and worked largely as expected. However we have noted a number of areas in which the program could be adjusted and improved in the future. The most significant have to do with ensuring Early Users get training on the applications as early as possible, and finding ways to reduce some of the constraints imposed by the NEAMS financial schedule and the effects of Continuing Resolutions.

2 Introduction and Background

The Capability Transfer (CT) element of the NEAMS program is intended to facilitate dissemination of the products and results of the NEAMS program to a wider audience. Among the key products of the program are the new modeling and simulation capabilities being developed in the Fuels and Reactors Product Lines. Although the NEAMS program is focused on the DOE R&D community as its primary user base, there is a desire and expectation that, over time, the M&S capabilities being developed by NEAMS will become interesting and useful to the nuclear energy industry and academia. NEAMS anticipates issuing in FY 2018 a full release of its computational toolkit aimed at advanced reactor and fuel cycles.

However, for several reasons, it is not desirable to wait until the toolkit is ready for the first official release to put it into the hands of users. First, it is not realistic to expect the stakeholders in the NEAMS program to wait five years to see the fruits of the project. While there will certainly be scientific results in this period, the software itself, as noted above, is a key deliverable of the overall program. Putting development versions of the codes into the hands of a small and appropriately selected group of users gives the program a means to demonstrate the capabilities of the software as it matures. The thoughtful selection of these "early users" can also help raise awareness within the targeted user communities as to the capabilities and accomplishments of the NEAMS program. Second, it gives the software development team the opportunity to get feedback from users as to the scientific and computational performance of the codes, their usability, and other factors. While it is useful for software developers to "eat their own dog food" in using the codes for their scientific research, experience shows that it is also extremely useful to obtain feedback from users who are not intimately familiar with the code by having been part of the development team. Outsiders will approach the code differently than developers, who are familiar with its quirks and limitations, and therefore provide a more thorough test.

With these points in mind, the NEAMS program in FY 2012 initiated a formal Early User Program, overseen by the CT element of the program, with the cooperation of the Product Line Leads and their software development teams. This report summarizes the experience of this first year from a management perspective. (Reports from the Early Users of their technical work are also deliverables of the relevant work packages and available separately.)

3 The FY 2012 Early User Program Strategy

During planning for the Early User Program, we interacted with the Fuels and Reactors Product Line leads to identify appropriate target codes and users. The end result for FY2012 was a total of seven Early User teams at five different institutions, which, from a management perspective were funded by three different work packages (ANL and LANL were funded via memorandum purchase orders (MPOs) from INL).

Product Line	Target Code	Team Lead	Institution	Work Package
Fuels	AMP	Larry Ott	ORNL	MS-12OR060804
Fuels	AMP	Brian Ade	ORNL	MS-12OR060804
Fuels	BISON	Pavel Medvedev	INL	MS-12IN060812
Fuels	BISON	Abdellatif, M. Yacout	ANL	MS-12IN060812
Fuels	BISON	Pratap Sadasivan	LANL	MS-12IN060812

Reactors	Nek5000	Yassin Hassan	Texas A&M U	MS-12OR060804
Reactors	Nek5000	Richard W. Johnson	INL	MS-12IN060805

Each Early User team was allocated $50,000 for their activities. This level of funding was chosen arbitrarily, in advance as a compromise between providing a participant enough support to do a useful amount of work, while keeping it small enough that busy researchers could still incorporate it into their work without major perturbations (such as having to completely drop other activities). The level of effort to which this corresponds clearly depends on how the money was spent. In some cases, it was used by laboratory staff directly, in which case, as a rule of thumb, it would be expected to purchase 10-15% of a person's effort. When used to support postdocs or graduate students, it obviously goes significantly further, perhaps 30% or more. Additional funds were allocated to an ORNL staff member to serve as liaison to the Early Users and provide initial support.

Early User teams were asked to work with the Product Line leads and software development teams to develop a plan for their work. The Fuels teams focused primarily on validation studies based on well-established, internationally known experiments. The Reactors teams focused primarily on standard CFD test problems.

All Early User teams were requested to provide feedback to the development teams as appropriate during the course of their work, and at the end of the year to deliver a report summarizing both their activities, and their findings relating to the code itself. During the course of their work, the primary monitoring of the progress of the Early User teams was via their monthly reporting in the PICS:NE system. Year-end reports were scheduled to be delivered approximately one month before the end of the fiscal year in order to allow time for review by the Product Line Leads and iteration with the Early User teams to ensure the reports (combined with other feedback during the course of the work) provide useful feedback for the development teams. One of the final reports is pending at this time, due to inability to meet the schedule due to conflicting activities. Another report was late due to a discrepancy between the deadlines specified in the PICS:NE work package and those specified on the memorandum purchase order (MPO) statement of work. Reviews of reports by the Product Line Leads did not result in any changes to the reports. Finally, it is worth noting that Aaron Phillippee (ORNL and the University of Tennessee) used this work as the basis for his Master's thesis.

The Early User teams have provided the following reports of their technical work:

Product Line	Target Code	Author(s)	Institution	Title	Milestone
Fuels	AMP	Aaron Martin Phillippe	ORNL	A Validation Study of the AMP Nuclear Fuel Performance Code	MS-12OR0608047
Fuels	AMP	*Pending*	ORNL	*Pending*	MS-12OR0608048
Fuels	BISON	D. M. Perez	INL	Early User Experience with BISON Fuel Performance Code (INL/EXT-12-26947)	MS-12IN0608121
Fuels	BISON	Di Yun and Abdellatif, M. Yacout	ANL	Assessment of BISON multi-physics fuel performance simulations with IFA-513 assembly rod1 and rod6 (ANL/NE-12/40)	MS-12IN0608122
Fuels	BISON	Pratap	LANL	Early User Experience with BISON	MS-12IN0608123

		Sadasivan			
Reactors	Nek5000	Paul Ward	Texas A&M U	NEAMS Early User End-of-Year Report	MS-12OR0608046
Reactors	Nek5000	Richard W. Johnson	INL	Capability Transfer (CT) – INL – Early Use Support for Fuels and Reactors IPSCs, Work Package	MS-12IN0608052

4 Lessons Learned and Recommendations

Overall, the Product Line Leads felt that the Early User program was very beneficial to their software development activities (see Appendix A for detailed comments). This was particularly true in the Fuels area, where the users were carrying out validation studies while simultaneously giving the development teams insight into how they were using the code.

The value in the Reactors area was somewhat dampened by the fact that NEAMS Reactors program ended up heading in a different direction from that anticipated when the Early Users in that area were selected. While we hope that such changes in direction will be relatively rare, it is important to recognize that the Early User program cannot turn on a dime. The commitment between the NEAMS program and the Early Users was year-long, and it would have been inappropriate to cut it short. **If, in the future, more agility is needed, the year could be divided into two or more periods, potentially with different Early Users in each period.** However this would multiply the overhead of identifying, recruiting, and establishing Early Users. Further, we suspect would make it harder to find and recruit Early Users – especially in the national labs, most researcher look for year-long commitments, and may not be available mid-year to take on a new Early User task.

Not surprisingly, the selection of the Early Users is important to the program's success. **In particular, it is important to choose people with the right background to cover the area(s) of interest to the Product Line Leads,** *and with the appropriate level of experience.* Inexperienced researchers may provide important insights into the quality of documentation, the robustness of the code, and the expectations of such users, but they are unlikely to be able to critically assess the code, or provide deep insight into its capabilities.

Regardless of the Users' level of experience, the importance of training Early Users was evident in several experiences. On the Fuels side, the BISON/MOOSE training appeared to be very effective at helping Early Users learn how to use the code. On the other hand, it was challenging to schedule this training, and in this case it didn't take place until halfway through the year. Similarly, the Reactor Product Line Lead noted that their users did not receive adequate training "on a radically different simulation toolset than you've been accustomed to using" due in part to the mismatch between the availability of the Early User funding and their usual training schedule, which focuses more on student users. These users also required more individualized support effort from the development teams. A further advantage of carrying out organized training sessions is that the development teams are forced to develop and present training materials, which are needed in the long run in any case. **We recommend that training should be an explicit part of each Early User's assignment, and that it should take place as early as possible in the period of performance.** As noted above, there can be challenges to this due to established schedules and the timely availability of funds. It may be useful to try to decouple participation in a training class from the primary Early User task in order to provide more flexibility as to schedule and funding – the cost of attending a training class is relatively small, even if it is necessary to cover the participant's labor costs as well as travel. If training were schedule very early in the Early User's period of performance, or even prior to it, the costs might be covered by prior-year funds held in

reserve. If the participant's labor must be covered, the funding will need to be at the participant's institution, however if only travel needs to be covered, this can in principle be done by any lab with available funding.

The content of trainings is also important. Noteworthy in the BISON/MOOSE training was the discussion of how to build the required third-party libraries and software packages, as well as BISON/MOOSE itself. For some users, this may be equal in importance to the training in how to *use* the code.

The original vision for the Early User program was that CT would provide support staff, intended to be the first point of interaction for Early Users in order to triage issues and reduce the load on the development team in dealing with more routine issues from the Early Users. The secondary purpose of this activity was to develop some degree of experience and expertise with the software outside of the development teams, anticipating the desire of the NEAMS program to provide a "help desk" for users of their software as it is more widely distributed. This aspect of this year's program was less successful than hoped. Although we requested Early Users to keep CT support staff informed of what they were working on, and to work first through them when issues arose, in practice, these requests were ignored. **We recommend a discussion with the development teams and Product Line Leads to reassess this aspect of the program, and if it is to continue, to develop strategies to make it more effective.** For example, it may be useful to provide more structured engagement between the Early Users and the CT support staff via regularly scheduled teleconferences. Or for the development teams to actively try to redirect the users to the CT staff when appropriate. We anticipated that there would be more basic issues related to building and running the code than were evident in practice, and it may be that the kind of support Early Users really need involves deeper domain expertise, which would require a different approach than we used this year. However, even if it may not be so important right now, as NEAMS software products reach a larger and less experienced user base the need for more basic, general support would be expected to increase. And the need to develop and deliver this kind of support around NEAMS software products should be taken into account in planning future Early User programs.

One of the premises of the program this year was that asking for a modest time commitment (dictated by the $50,000 funding level) would be a good compromise between the ability of the Early Users to fit the work into their schedule, and their ability to accomplish something meaningful. We believe the results were mixed this year. While we did not have anyone refuse to participate due to their schedule being too full, we did have several cases where the work was not completed in the planned time frame. Additionally, while the guidance to the Early Users was to work out with the software developers a combination of activities that both provides value to the application development team and is interesting to the Early User, the outcomes were somewhat mixed. **We recommend that there be more detailed discussions with prospective Early Users to agree in advance on the statement of work, the schedule, and the level of effort.** The $50k amount still seems to be a good starting point for discussion, but it may also be useful to be more flexible in this.

The timeliness of the availability of funding for the Early Users has been previously alluded to as an issue. This can be particularly challenging when subcontracting is involved (i.e. to an academic or industrial Early User), and the fiscal year begins with a Continuing Resolution (CR). Lab financial officers will generally not allow a subcontract to be executed until there is sufficient budget authority (BA) to cover the financial commitment. Under a CR, it can take several months to build up sufficient BA. **It may be possible to mitigate issues due to delayed funding and subcontracts if they can be anticipated and taken into account in the plans made with the affected Early User team.** For example, as noted above, other funding mechanisms may be used to support training in advance of being able to execute a subcontract. Since the recipient of the funds has flexibility as to how to use them within a work package, **another mitigation strategy is to try to bundle tasks that require subcontracts with other tasks within the same work package, scheduling them so that the initial funding can be put towards the subcontract, and later funding towards the other tasks.**

Taking a step back, it may also be useful to consider trying to decouple the schedule of the Early User program from the federal fiscal year that has historically governed the NEAMS program. Obviously this requires the ability to do multi-year planning in both the technical and financial senses. While we recognize the challenge here, it is worth noting that the desire for multi-year planning has been articulated by numerous program participants in many other contexts as well. Further, there are other program sna d offices within DOE that operate in this way.

Finally, we note an issue of oversight related to the use of subcontracts and MPOs (the equivalent of subcontracts between labs). In one case this year, an MPO did not correctly reflect the milestones and deliverables in the governing PICS:NE work package. Since the CT Lead, who is ultimately responsible for the Early User program as a whole has no visibility into contracting that takes place at other institutions, this error did not come to our attention until a deliverable deadline was missed. **Consequently, we recommend that wherever possible, the use of subcontracts and MPOs should be limited to the CT lead institution in order to ensure better oversight.**

Appendix A Feedback from Product Line Leads

A.1 Steve Hayes, INL, Fuels Product Line Lead

"The BISON development team felt the BISON Early User program was predominantly very useful. This was especially the case for the early users at INL and ANL, who were knowledgeable fuels people and were able to develop and execute validation problems from the FRAPCON and FUMEX-III databases assigned to them by the BISON team. It was a win-win in that we got to see how a new user interacted with BISON, and at the end of the day our assessment database was expanded. The LANL postdoc assigned by Cetin as the early user at LANL was not knowledgeable about fuels, so his progress in developing validation problems was more limited, and his conclusions were often incorrect."

"In the future, we should make sure the users we recruit are fuels people to ensure maximum benefit from the funds spent."

A.2 David Pointer, ANL, Reactors Product Line Lead

"I think the program does have significant value, but may not have been as successful as it could have been in FY12. The early users provided very little feedback that actually led to improvements in the code in this first round, largely because the funds were not available until late in the year and it simply takes more time than was available to come up to speed on a radically different simulation toolset than you've been accustomed to using. The program was successful establishing users in the nuclear energy field outside the development team, but these users were selected in anticipation of a strong shift in NEAMS focus toward LWR technology and do not necessarily represent the DOE programs to which NEAMS is targeted following the April 2012 PI meeting."

"Since funds were not immediately available at the start of the fiscal year, the Early Users started using the code off cycle and missed the planned user training opportunities. As a consequence of providing individualized support, the effort involved in supporting the program was substantial. It remains to be seen whether the investment was worthwhile, but I am optimistic that we'll see some return on investment."

"I think we really need to work on the timing so that new early users can participate in group training opportunities that will typically be organized in the fall when new graduate students are starting to use the codes. The program would have also been more valuable if the early users had ties to the DOE program office from which we are now trying to solicit support."