ORNL/TM-2012/246

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

NEAMS Software Licensing, Release, and Distribution: Implications for FY2013 Work Package Planning

Preliminary Report (NEAMS Milestone M4MS-12OR0608113)

Version 1.0 (June 2012)

David E. Bernholdt

Oak Ridge National Laboratory

Version History

Version	Date	Changes
1.0	2012-06-30	Initial draft

Table of Contents

1 Executive Summary

The vision of the NEAMS program is to bring truly *predictive* modeling and simulation (M&S) capabilities to the nuclear engineering community in order to enable a new approach to the analysis of nuclear systems. NEAMS anticipates issuing in FY 2018 a full release of its computational "Fermi Toolkit" aimed at advanced reactor and fuel cycles. The NEAMS toolkit involves extensive software development activities, some of which have already been underway for several years, however, the Advanced Modeling and Simulation Office (AMSO), which sponsors the NEAMS program, has not yet issued any official guidance regarding software licensing, release, and distribution policies. This motivated an FY12 task in the Capability Transfer work package to develop and recommend an appropriate set of policies. The current preliminary report is intended to provide awareness of issues with implications for work package planning for FY13.

We anticipate a small amount of effort associated with putting into place formal licenses and contributor agreements for NEAMS software which doesn't already have them. We do not anticipate any additional effort or costs associated with software release procedures or schedules beyond those dictated by the quality expectations for the software. The largest potential costs we anticipate would be associated with the setup and maintenance of shared code repositories for development and early access to NEAMS software products. We also anticipate an opportunity, with modest associated costs, to work with the Radiation Safety Information Computational Center (RSICC) to clarify export control assessment policies for software under development.

2 Background and Approach

The vision of the NEAMS program is to bring truly *predictive* modeling and simulation (M&S) capabilities to the nuclear engineering community in order to enable a new approach to the analysis of nuclear systems. This vision leverages advances in high-performance computing, as well as computational science and engineering to change the relationship between experiment and simulation – as has already happened in many other fields of science and engineering. The goal is not to eliminate experiments, but rather to optimize how the measurements are used to gain scientific insight or solve problems of interest. In order to significantly influence the trajectory of nuclear M&S capabilities, NEAMS emphasizes increasing accuracy and fidelity, and broadening the range of applicability of methods. Uncertainty quantification is also considered extremely important to predictive capabilities. At the same time, there is an emphasis on ease of use and integration into current design and safety analysis processes, as well as ease of maintenance and future development of the software. The NEAMS predictive modeling approach is substantially different from current practice in the nuclear industry, which relies much more heavily on models parameterized by experiments. NEAMS anticipates issuing in FY 2018 a full release of its computational "Fermi Toolkit" aimed at advanced reactor and fuel cycles.

The NEAMS toolkit involves extensive software development activities, some of which have already been underway for several years. Further, the Fermi Toolkit will leverage a variety of existing software packages. To date, the federal managers of the NEAMS program, in the Advanced Modeling and Simulation Office (AMSO), have informally provided the following guidance on software licensing, release, and distribution:

- NEAMS software should be made available as widely as possible, consistent with requirements of export control, under open source licenses where possible, and
- NEAMS software should be distributed via the Radiation Safety Information Computational Center (RSICC), housed at Oak Ridge National Laboratory (ORNL).

However, AMSO has not issued any formal policies on these matters. Consequently, it has so far been up to the individual development teams to make their own decisions on these matters, leading to inconsistencies and possibly even impediments to sharing software across institutions for pre-release collaborative purposes.

The purpose of this task, which is part of the FY12 Capability Transfer work package, is to develop and recommend a set of policies on software licensing, release, and distribution, which, if accepted by AMSO management, can be formally adopted by the program, with the expectations that participants receiving NEAMS funding will conform to the best of their ability. This preliminary report is intended to provide awareness of issues with implications for work package planning for FY13. The final report, to be completed later in FY12, will provide a more comprehensive consideration of policy issues and provide appropriate recommendations.

3 Planning Implications of Software Licensing

Selecting and affixing a license to a software package is generally a one-time matter (though, of course licenses can be changed). As such, any new software packages and all existing packages which have not selected a license may wish to do so in FY13. Lead institutions for such software packages may wish to plan for appropriate time and effort to consult with their Technology Transfer office (or equivalent) for licensing procedures. Similarly, other institutions participating in development may wish to plan for consultations related completing a Contributor Agreement with the lead institution. However, with the assistance of appropriate formal guidance from the sponsors (AMSO), such matters should be fairly straightforward and should not require significant amounts of time. We estimate this time at a few tens of hours on the part of the software development team lead and their laboratory Technology Transfer staff.

4 Planning Implications of Software Release Schedules and Procedures

Release schedules and procedures may affect staffing requirements based on the frequency and intensity of effort required to make releases. For example, special pre-release testing regimes, documentation sprints, and other activities tied to the release cycle will make releases (appear to be) more expensive. However it is equally possible to structure the overall development process such that such activities are spread out, such as by continuous integration testing, and the discipline to update documentation with code changes rather than just at release time. Overall, the requirements for a formal release of a software package are more a reflection of the overall quality standards set for the software. Therefore, we consider the handling of release procedures to be part of the normal software development process, and without any special implications for the work package planning process.

The release schedule needs to balance the desire to get updates into the hands of users quickly and the costs of export control evaluation and of users obtaining new versions, which are distribution issues, discussed below. If there is a desire to maintain an overarching notion of a single "Fermi Toolkit" as a NEAMS software product, there will also be a need to coordinate releases of the constituent components, at least to some extent – especially for components that directly interact (i.e., coupled multiphysics models). This is not to say that absolute synchronization must be maintained across all components of the toolkit, but must be an understandable versioning model that allows users to understand and identify which components will and will not work together, and the ability to download and use the Toolkit without spending all of their time updating components. The development of a release plan that is mutually agreeable to the development teams contributing to the Toolkit would be expected to require a modest amount of time and effort to create. We estimate this at a few tens of hours on the part of the development team leads, backed by a modest amount of discussion within the individual teams.

5 Planning Implications of Export Control and Software Distribution

Given the nature of the NEAMS program, export control is an important consideration for all software products. We should expect all software products to go through export control review before they are released, and for packages covered by export control, each and every user must also be vetted. Technically, these reviews are required no matter what organization distributes the software, although in practice, some organizations take it more seriously than others. Further, export control reviews (of codes and users) are technically required for each and every release of a software package (because functionality, and therefore export control sensitivity, may change with each release).

The Radiation Safety Information Computational Center (RSICC), based at Oak Ridge National Laboratory (ORNL) is the one full-service organization, across the DOE complex, for the distribution of export controlled nuclear-related software. RSICC already receives some funding from the NEAMS program for their basic operations, helping to allow them to distribute software to educational institutions without charge (generally, a cost-recovery fee is applied to RSICC software requests, based on the user's funding sources). RSICC can handle the routine distribution of NEAMS software on a reasonable release schedule without additional cost to the program.

However it is important to recognize that RSICC is setup to distribute discrete releases of software. Within the NEAMS program, and probably for some users participating in testing programs, it would be more natural to share access to a code repository in order to be able to obtain continual access to pre-release software. While RSICC does not currently provide such code repositories, they would be willing to explore the possibility, or NEAMS can establish and operate their own code repositories and obtain relevant export control information from RSICC (assuming they are handling distribution of the discrete

releases of the software). While it is not strictly required that the NEAMS program establish a single code repository for development purposes, it would reduce operational costs, and facilitate coordination with RSICC regarding export control reviews. Regardless of the hosting site, the costs of such a repository would include an initial outlay for the server[1] and setup, plus recurring costs for system maintenance and support of the repository (including access control, two-factor authentication tokens, etc.).

One point to note is that the idea of a shared development repository presents a challenging issue for export control. Technically, every single software release should be reviewed for export control, and every user vetted for every release (because of the possibility of changes in capabilities, thereby affecting export control concerns). In a code repository, this would equate to every check-in. While this is clearly unreasonable and impractical, from discussions with RSICC, there are no defined and agreed alternative procedures to cover such cases. If NEAMS decides to distribute its software via RSICC, they would like to take the opportunity, working with us, to try to define criteria and processes that would provide a well-defined, streamlined, but still appropriately accountable process for evaluating when development activities have altered the export control considerations for a package, and thus should trigger a fresh evaluation, while allowing continued development and access below this threshold. Such guidelines would provide widespread benefits to the developers, distributors, and users of export controlled software. It is hard to quantify the level of effort that would be required, but it would require some time on the part of one or more representatives of the NEAMS program, in occasional consultation with NEAMS developers, working with RSICC staff and interested parties at DOE.

6 Implications of NEAMS Restructuring

Restructuring of the NEAMS program around reactors and fuels "product lines" is not expected to have any direct impact on software licensing, release, and distribution policies because it affects only the management structure for the work, not the nature of the software products that are to be produced.

7 Implications of the NEAC Subcommittee Review of the NEAMS Program

At the request of Alex Larzelere, a Nuclear Energy Advisory Committee (NEAC) subcommittee was commissioned to review the NEAMS program in FY2012. The review subcommittee has not yet completed its final report, but according to an email by Dan Funk[2] headed "NEAC Subcommittee's Preliminary Thoughts/Themes After Review of NEAMS", it appears that their concerns and recommendations are likely to be at a much higher level than we are concerned with in this task. However, as two of their concerns relate to stronger user involvement and a stronger, more compelling value proposition for the NEAMS program, it is possible that there will be some secondary impact on NEAMS software policies.

[1] A single server, reasonably provisioned, should be sufficient to meet the loads expected in the NEAMS program. However additional hardware may be desired to provide fail-over capabilities in the event of problems with the main server. Of course the development of a fail-over setup entails additional setup and operational costs, so the need for redundancy should be considered carefully.

[2] Email from Dan Funk to Trevor Cook, Alex Larzelere, James Peltz, and Rob Versluis, dated 24 May 2012, forwarded to the NEAMS PMT by Rob Versluis on 4 June 2012.