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Development Plan for NEAMS Neutronics Module

Nuclear Engineering Division

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1 Introduction

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) program of U.S. DOE [1] has focused funds on developing tools to model and simulate nuclear reactor technology. The NEAMS Project aims at developing a simulation toolkit, the "NEAMS ToolKit," which will enable predictive virtual tests and experiments by taking advantage of improvements in computing technology over the past several decades. The NEAMS ToolKit will generate insights by exploring reactor system behavior in regimes that are too difficult, too risky, or even impossible to achieve exclusively in a laboratory setting. Over the next 5-10 years, the project will develop a continuously maturing NEAMS ToolKit that will simulate the conditions necessary to understand the performance, safety, reliability, and economics of advanced fuels and reactor designs. The explosive growth in computing speed and memory capacity has enabled the reduction or elimination of empirical or ad hoc approximations upon which traditional codes have had to rely. By accurately simulating the underlying physical mechanisms, the NEAMS ToolKit will move from merely describing or reproducing previously observed behavior to predicting both observed and unobserved behavior in regimes that reach beyond the traditional test base.

Where required, the NEAMS ToolKit will have the ability to address fully coupled behavior. Under many conditions, the competition between different phenomena is weak or unimportant and can be treated by simulating a single phenomenon in isolation. In other instances, the full coupling of multiple phenomena will be essential for accurately predicting the outcome of an event. For example, rapid transients are likely to require this full coupling of phenomena to accurately predict outcomes. The NEAMS ToolKit will be developed to accommodate the full spectrum of needs, from isolated to fully coupled phenomena.

As one of the major components of the NEAMS ToolKit, the NEAMS neutronics module is a complete toolkit for the analysis of reactor physics phenomena. The module is built using the PROTEUS package and provides three-dimensional neutron transport, cross section generation, reactor kinetics, and depletion. This report discusses goals and objectives, functional requirements, and tasks of the NEAMS neutronics module as well as budgets and schedules to accomplish the tasks.

2 Goals and Objectives

The existing dynamics modeling approach of the primary system of a reactor core is relatively low fidelity. Taking a conventional sodium fast reactor as an example, the core model typically involves a simple energy balance relation for thermal fluids (sub-channel) combined with point kinetics models in neutronics and very simple thermal mechanics models to handle deformations of the entire core. Similar simple models (with correlations) are used to model the plenum region, heat exchangers, pumps, and coolant pool where the plenum region is of particular importance due to the mixing (thermal stress induced failures). The primary drawback of this modeling approach is a lack of generality (use on a wide range of reactor systems) and substantial questions about accuracy for any given design that does not have comparable measurement data (mostly in fuels performance, fluid dynamics, and neutronics). In the case of the plenum region, this modeling methodology is yet to be accurate and does not produce a meaningful prediction of the behavior.

Focusing on the NEAMS concept, we have a desire to replace or augment the existing modeling approaches in order to reduce the requirements on building experiments before building the desired reactor plant. In the fluid dynamics area, one of the augmentation ideas is to use high fidelity modeling to tailor correlations to specific features of a reactor design that do not fit within existing measured data. Existing tools will be used, and new tools will be developed as necessary. In neutronics, improvements in existing fidelity (I) would involve replacing existing point kinetics models with a more rigorous dynamics model with better cross section interpolation. However, one might also find a need for higher fidelity modeling (II) on design constraining accident scenarios. Figure 2.1 outlines the major requirements needed to augment such an existing code (I) or build a fully heterogeneous modeling capability (II) and also alludes to the concept that we can construct a hybrid model which combines aspects of the two approaches (III).

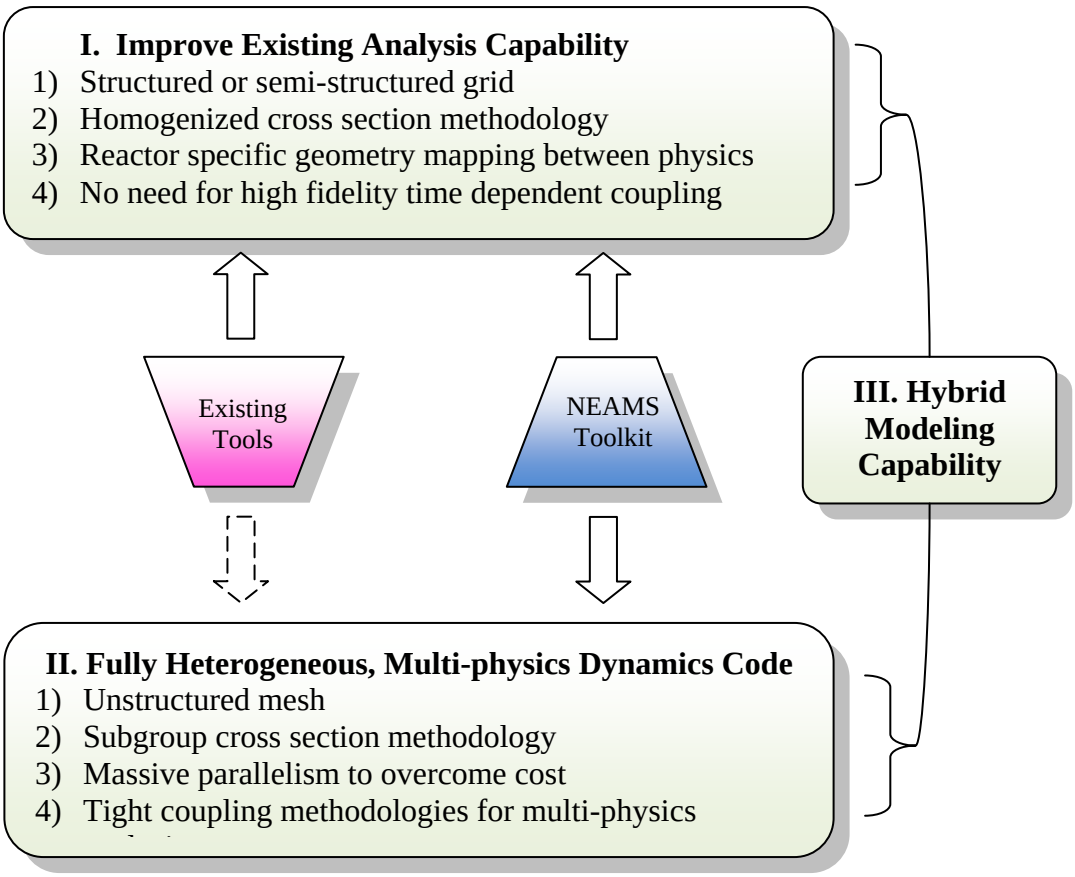

Figure 2.1 NEAMS Targeted Neutronics Generic Modeling Requirements

From Figure 2.1, we have clearly identified the role of existing tools which primarily are focused on homogenized cross section methodologies with relative few tools focused on heterogeneous modeling. We have also outlined the goals for the NEAMS Toolkit which will include many of those tools but will also have to augment some of them or create new tools to get the desired capability in a high fidelity modeling approach (II). In this regard, the NEAMS

work should focus on a hybrid approach which is capable of handling both the homogenized and heterogeneous modeling goals.

The existing tool packages with detailed historical usage and verification and validation include: ARC [2-4], SCALE [5], and ERANOS [6]. There are additional tools which could be considered specific component replacements in any of those packages such as PARTISN [7], PENTRAN [8], and ATTILA [9], the latter of which is focused more on a high fidelity modeling (II) although it has been reported to be too expensive for NEAMS work. In addition, there are the more recent developments including: MOOSE [10], PDT [11], DeCART [12], MPACT [13], and PROTEUS-SN [14-15]. In most cases these tools are available but have little verification or validation history like the more established packages or individual tools. In the case of PROTEUS-SN, significant funds have been invested by NEAMS to accomplish the stated hybrid approach outlined in Figure 2.1, but it still needs efforts to have the functionalities that are required for practical reactor design and analysis.

Of all these potential neutronics components of the NEAMS toolkit, the first goal is to have a cross section methodology that is flexible and usable on a wide range of reactor types. The second goal is to have a fuel cycle analysis capability that is appropriate for the reactor system of interest which includes solutions to the neutron and gamma transport equations along with the Bateman (depletion) equations. The final goal is to use the NEAMS toolkit to generate the typical kinetics parameters used in existing safety analysis tools in addition to a dynamics capable, kinetics functionality which can be alternatively combined with other components of the NEAMS toolkit for coupled simulation and more detailed analysis.

3 Functional Requirements

The NEAMS neutronics tool PROTEUS provides a complete neutronics analysis capability including three-dimensional transport solvers, cross section processing, and reactor kinetics. A depletion capability should be part of the NEAMS neutronics tool in the near future as well. The capabilities of the FY2018 release of the NEAMS neutronics tools will include four major modules: high fidelity cross section module, whole-core cross section module, high fidelity transport module, and near-term kinetics module.

High Fidelity Cross Section Module: The high-fidelity cross section module, based on the extended MC^2-3 methodology for a whole-core heterogeneous geometry, provides tools for generation of rigorously accurate multigroup cross section libraries for fast reactor analyses.

Whole-core Cross Section Module: The whole-core cross section module [16] provides the tools needed to generate cross section libraries applicable for various reactor types including light water reactor (LWR), high temperature reactor (HTR), and sodium fast reactor (SFR). This method provides a lower computational cost alternative to the use of the high-fidelity cross section module while retaining reasonable accuracy. This module can be applied to SFR analysis, but the MC^2-3 based cross section module can be used for higher fidelity needs.

High Fidelity Transport Module: The high-fidelity transport module, based on PROTEUS, provides tools for analysis of neutron transport phenomena within the reactor core. The module is, in essence multi-scale, because traditional homogenization approaches may be utilized to reduce computational cost – at the expense of accuracy. The module will

eventually offer a variety of transport solver options, but development efforts will focus on an unstructured finite element mesh based, second-order discrete ordinates method for the FY2015 early user release of the reactor product line (RPL). The module will be able to make use of both the high fidelity and whole-core cross section modules. At the end of FY2015, capabilities and computational expense associated with this module will be assessed and a decision will be made whether to implement kinetics and depletion capabilities based on this module. The current development plan assumes that a positive decision will be made and this scenario will be the outcome. If this is not the case, the module will continue to support cross section generation for the lower order methods.

Near-Term Kinetics Module: The near term kinetics module, based on the existing nodal diffusion method code DIF3D-K/VARIANT [17], provides functionality needed to complete near term transient reactor analyses while longer term development efforts, based on a transient capability of PROTEUS, are being executed. Development efforts related to this module are limited to integration of the existing code with the NEAMS Integrated Framework, but may be expanded if required by the outcome of the FY2015 assessment of the high-fidelity transport module.

4 Tasks to Meet Functional Requirements

The first step in meeting the functional requirements is to identify the reactor type(s) of interest for NEAMS which at this point include: SFR, HTR, and LWR, although there is a reduced focus on LWRs due to their focus in CASL [18]. With that selection, we can identify the tasks:

1) Identify what type of analysis work is to be done by users and what type of accuracy should be achieved by the NEAMS ToolKit.
2) Assess all existing, available packages and components of the NEAMS ToolKit that can potentially meet the functional needs of the targeted users of the NEAMS ToolKit.
3) [Optional] Devise a limited scope development plan on inclusion of an integrated package or existing tool identified in step 2 that covers all potential modifications to make it appropriate for the NEAMS ToolKit analysis work.
4) [Optional] If no tool exists to meet step 1, a limited scope development plan should be written to identify the appropriate tool that needs to be built for NEAMS work. That plan should be peer reviewed before any funds are dispersed to ensure that the end product is viable to satisfy step 1. It should be followed by a wider scope development plan within the given funding.

For the most part, this will preclude the use of commercial products like ATTILA, but this decision can be deferred until a full assessment is made in FY2015, noting the recent direction of NEAMS funds to use the commercial STAR-CCM+ [19] fluid dynamics code. In summary, a generic user of neutronics codes requires a very wide scope which NEAMS may lack sufficient funds to achieve by itself. However, for a targeted analysis purpose, NEAMS funds can be used to properly identify the appropriate tool for each analysis project along with any necessary augmentation or development.

5 Planned Demonstration Problems

The NEAMS ToolKit will be applied each year to selected demonstration problems, where the physics and length/time scales of the problems increase in complexity in successive years. These planned demonstrations lead up to the assessment of the performance of a sodium cooled fast reactor and its fuel during several transient calculations of interest. The planned demonstration problems are shown in Table 5.1, and it should be clear that neutronics is going to play a role.

Although development of the physics codes other than the neutronics code responsible for these demonstration problems is not in the scope of the NEAMS neutronics development plan, the success of simulating the demonstration problems depends on the successful development of the NEAMS neutronics tool. These demonstrations problems will be carried out in parallel with the development and extension of the NEAMS neutronics tool capabilities.

Table 5.1 Planned Demonstration Problems for the NEAMS ToolKit

Year	Demonstration Problem
FY13	Full-scale pin-resolved assembly with neutronics, thermal hydraulics and structural mechanics (no deformation)
	Multiple pin-resolved assemblies with neutronics, thermal hydraulics and structural mechanics (no deformation)
FY14	Multi-scale full core with neutronics, thermal hydraulics and structural mechanics with selected assemblies pin-resolved (no deformation)
FY15	Early-user release of Reactor Product Line
	Multi-scale full core with neutronics, thermal hydraulics and structural mechanics with selected assemblies pin-resolved (with deformation)
FY16	Multi-scale full plant steady state with detailed core simulation
	Fuel assembly simulation coordinated with Fuels Product Line
FY17	Multi-scale full plant transient with detailed core simulation
	Fuel assembly simulation coordinated with Fuels Product Line
FY18	Version 1.0 release of Reactor Product Line
	Fuel assembly simulation coupled to Fuels Product Line

6 Budget and Schedule

For a long while, NEAMS has focused on modeling sodium fast reactor technology with the most recent focus placed on the Experimental Breeder Reactor II (EBR-II). In this regard, the focus on fast spectrum reactor analysis work is expected to continue. As shown in Table 5.1, NEAMS will invest significant efforts for the next five years on demonstrating multi-scale multi-physics simulations using the NEAMS ToolKit. Table 6.1 shows the breakdown in planned funding for the next five fiscal years for the neutronics work which will be done in parallel with the demonstration problems outlined in Table 5.1.

In the preceding NEAMS work, the focus was primarily placed on developing a multi-physics capable dynamics tool as none of the existing tools were capable of treating a whole core heterogeneous reactor at the high fidelity level that NEAMS is targeting. As a consequence, NEAMS invested significant funds into the development of MC^2-3 [2] for cross section generation and PROTEUS-SN [15] for neutron transport calculations. In Table 6.2,

the PROTEUS related funds are expected to continue into 1.6 FTE next fiscal year, but this is for the integration effort of SHARP framework. Funds with 1.6 FTE for FY15 and FY16 and 0.8 FTE for FY17 and FY18 will be invested to support the NEAMS demonstration. There is only a little direct funding plan to focus on building a dynamics tool that targets coupling on fully heterogeneous reactor systems as outlined in Table 5.1. Therefore, it is somewhat uncertain whether the current funding plan will involve any improvement of transport methods envisioned in PROTEUS-MOC [20] or the advanced first-order S_N approach [21]. At the end of FY2015, capabilities and computational expense associated with PROTEUS-SN will be assessed and a decision will be made whether to implement high-fidelity kinetics and depletion capabilities and/or to improve transport methods.

The MC^2-3 work specifically targets the generation of equivalent coarse group cross sections for use in homogeneous or heterogeneous fast reactor modeling applications. The funding observed in Table 6.2 includes any augmentations or modifications necessary to support the ongoing work of NEAMS on fast reactor modeling. At this time, there is no other code equivalent to MC^2-3, and the minor amount of funding can be diverted to the whole-core cross section work in the coming years depending upon whether the reactor focus of NEAMS changes beyond sodium fast reactors.

The cross section work listed in Table 6.2 is intended to extend the NEAMS ToolKit capabilities beyond the demonstrated fast reactor work of PROTEUS-SN and into the thermal reactor regime. It was also anticipated that some of the problems related to the fast spectrum system could be eliminated, but the primary goal of the cross section work was to fix the outstanding issues associated with heterogeneous modeling by allowing the cross section methodology to be specifically tailored to the reactor type of interest without being constrained by the implementation into any specific code. In fact, it is a wider scope research project which starts with a limited focus on the subgroup methodology (i.e. thermal spectrum) and generalizes it to the resonance integral table methodology for broader applications. Within NEAMS, we must minimize and quantify the errors that result from the cross section methodology, and thus the funding on this task reflects part of what is required to accomplish that goal.

The depletion module is new work and is related to the development of a fuel cycle analysis code to increase the user base of the NEAMS ToolKit. While the stated funding is not close to what is required to develop a product capable of handling all proposed fuel cycle models in the community, it may be viable to attach the ORIGEN-based depletion into the NEAMS neutronics module and to update interfaces in PROTEUS for the depletion module.

The final aspect of work to be done in neutronics is verification and validation. Clearly none of the NEAMS products will have any users if there is insufficient verification and validation. The final task in Table 6.2 is intended to support the NEAMS ToolKit work. It should be clear that this funding will initially consider fast spectrum systems and potentially be widened to other reactor types. The funding shown in the table is the minimal required to achieve reasonable accuracy for the neutronics portion of the NEAMS ToolKit, although we note that the NEAMS ToolKit will have to rely considerably on existing packages. A coherent set of milestones is summarized in Table 6.1.

It is important to note that the actual functionality and application range of the neutronics ToolKit delivered in this set of milestones will become more clear with time as the

FY14 work and subsequent funding will dictate what components are required to accomplish the set of tasks in Table 5.1.

Table 6.1 Milestones for NEAMS Neutronics Development Efforts

Year	Due	Milestone
FY14	9/30/14

Table 6.2. NEAMS Neutronics Work Plan

(Unit: FTE)

Title	2014	2015	2016	2017	2018	*Total*
Transient 3D Neutronics Tools						
High Fidelity Transport Module						
Initial PROTEUS Transport Solvers						
Initial Integration with MC^2-3 Cross-Section Module						
Initial Integration with SHARP Framework	1.6 [a)]					*1.6*
Annual Updates to Support NEAMS Demonstrations		1.6	1.6	0.8	0.8	*4.8*
Subgroup Cross-Section Method						
Initial Subgroup Method Code Library						
Initial Subgroup Method Cross-Section Data Library						
Initial Integration with PROTEUS Components	0.8					*0.8*
Annual Updates to Support NEAMS Demonstrations		0.8	0.8			*1.6*
MC^2-3 Cross-Section Module Maintenance to support NEAMS	0.2	0.2	0.2	0.2	0.2	*1.0*
Reactor Kinetics Module						
Near-Term Kinetics Module						
PROTEUS Kinetics Capability	0.2					*0.2*
Annual Updates to Support NEAMS Demonstrations		0.2	0.2	0.2	0.2	*0.8*
Depletion Module [b)]						
Evaluation of Options for Integration of ORIGEN-based Depletion Capability	0.4					*0.4*
Initial Integration of ORIGEN with PROTEUS		0.4	0.4			*0.8*
Validation (Including Assessment Reports)						
Neutronics Validation Exercises	0.5	0.25	0.25	0.5	0.25	*1.75*
Annual Assessment Report	0.08	0.08	0.08	0.08	0.08	*0.4*
Total	***3.78***	***3.58***	***3.53***	***1.78***	***1.58***	***14.15***

a) Integration of PROTEUS with SHARP Framework will be led by the NEAMS Framework team
b) Integration of ORIGEN-based depletion capability will be led by the ORNL Neutronics team

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