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Nuclear Energy Advanced Modeling and Simulation (NEAMS) Structural Mechanics Module Development Plan

R.M. Ferencz
Methods Development Group

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1 Introduction

Quoting from the NEAMS Project Plan of June 2013:

The NEAMS Project aims to develop a simulation toolkit, the "NEAMS ToolKit," which will enable predictive virtual tests and experiments. 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.

To be truly predictive, the NEAMS ToolKit must simulate the right mechanisms at the right spatial and temporal dimensions. While the performance and safety of a system is usually understood by directly observing continuum (engineering-scale) behavior, often it is governed by smaller-scale phenomena that must be understood and accurately described in the ToolKit. However, even with today's supercomputing power, simulation of large systems at a subcontinuum scale remains intractable. For this reason, the NEAMS ToolKit will approach simulation at multiple spatial and temporal scales. Considerable effort will be required to transfer the understanding obtained at the subcontinuum scale to the continuum-scale tools. Yet this is essential if the NEAMS ToolKit will be truly predictive.

2 Objectives, Requirements and Assumptions

The objective of the NEAMS ToolKit is to develop a "pellet-to-plant" simulation capability useful for predicting performance and safety for a broad range of nuclear reactor power systems. Development of the ToolKit is being undertaken in support of the on-going R&D programs in the U.S. Department of Energy (DOE)

Office of Nuclear Energy (DOE-NE), as outlined in the Nuclear Energy R&D Roadmap. The NEAMS ToolKit is organized under a Fuels Product Line (FPL) and a Reactors Product Line (RPL) and will be modular in design. The modeling approach and system integration architecture reflects the need to simulate a broad range of nuclear reactor power systems, however, the development and validation of the NEAMS ToolKit focuses initially on one advanced reactor concept and will incorporate additional designs as development proceeds.

The ToolKit must enable simulations that are:

- Multi-physics (coupled phenomenology),
- Multi-scale (concurrent coupling),
- Multi-resolution (hierarchical coupling).

Individual ToolKit components will be updated and released annually. They will initially function only as standalone tools, with functionality and coupling capability increasing over time. The initial release of the NEAMS ToolKit with the capability for coupled simulations using multiple ToolKit components is planned for the end of fiscal year (FY) 2018. A metallic-fueled, sodium-cooled fast reactor (SFR) nuclear reactor power system will be the target of the initial release (including an option for use of oxide fuel as well).

2.1 Functional Requirements

In the context of the ToolKit simulation goals, the structural mechanics module must provide the following high-level capabilities:

- Multi-physics
  - Access physics responses from thermal-hydraulics (T-H) (e.g., temperature) and neutronics (e.g., dose).
  - Compute deformation of the major structural components, e.g., assembly ducts, core restraints, etc.
  - Share deformation information with T-H and neutronics.
  - Perform these actions either off-line or within a coupled time-stepping, nonlinear iteration scheme
- Multi-scale
  - Share assembly-scale response quantities as needed for FPL to compute localized pin-scale response.
  - Access FPL material models for advanced response of structural components.
- Multi-resolution
  - Support a limited number of high-resolution assembly models within a largely homogenized core model.

- Share assembly-scale response quantities as needed for FPL to compute pin- and pellet- scale response.
- Access FPL material models for advanced response of structural components.

Data interchange between, and coordination with, other physics modules and product lines will be provided by the SHARP framework, illustrated conceptually in Figure 1.

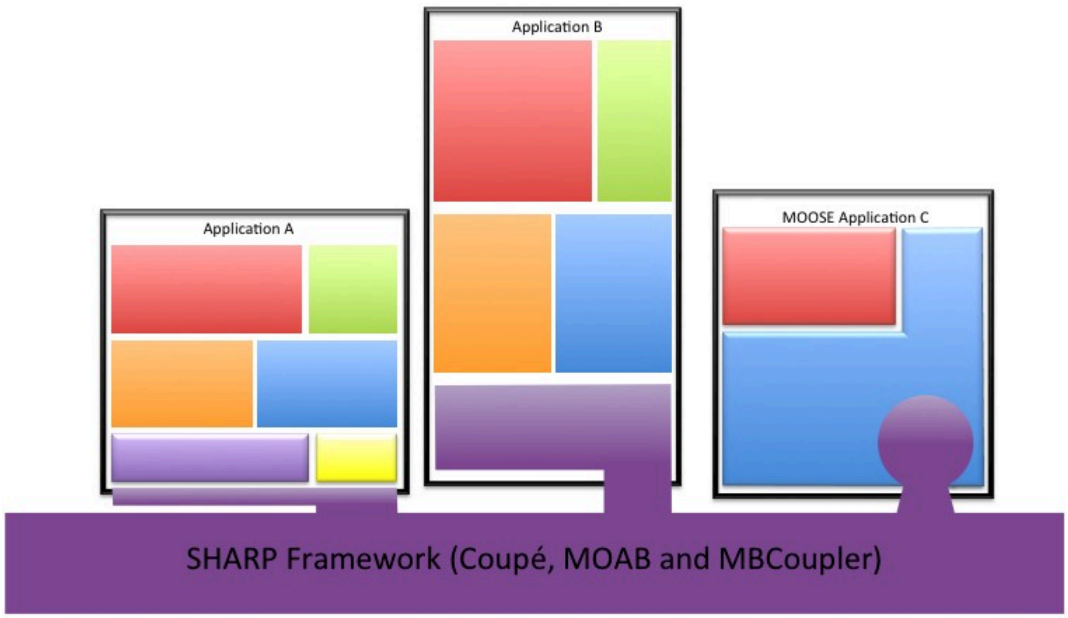

Figure 1. Notional illustration of three different modes of connectivity provided for integration of multi-physics simulations using the SHARP framework.

In Section 4 we will provide more specificity to these requirements as dictated by the demonstration objectives defined by the NEAMS Program Plan.

2.2 Resource Assumptions

The scope and schedule of NEAMS Structural Mechanics Module development, as described in this plan, are based on the budget assigned budget to WBS area 3.1 in the overall NEAMS Program Plan. This resource allocation is shown in Table 1 in Full Time Equivalents. The Program Plan assumes an FTE rate of $500K per year, which is slightly higher than actual FTE cost to allow for travel, material, supply, and publication costs which are all, but tangible, secondary costs for this project. For completeness, Table 1 also shows the coordinated effort level associated with structural validation exercises.

Table 1. Resource Assumptions for Structural Mechanics Module (FTEs)

WBS	Title	2013	2014	2015	2016	2017	2018	Total
3	Reactors Product Line							
3.1	NEAMS Structural Module							
3.1.1	Initial Integration of Diablo with SHARP Framework	0.6						0.6
3.1.3	Expanded Integration of Diablo with SHARP Framework		1					1
3.1.5	Integrated Multiphysics Simulations with Structural Deformation			1				1
3.1.7	Annual Updates Based on Demonstration Problem Needs				1	1	1	3
3.5	Validation (Including Assessment Reports)							
3.5.3	Structural Validation Exercises		0.5	0.25	0.25	0.5	0.25	1.75
3.5.3.1	Annual Assessment Report		0.08	0.08	0.08	0.08	0.08	0.4

A crucial assumption is that the Diablo code will retain support from the NNSA's Advanced Simulation and Computing (ASC) Program components executed at LLNL and/or other projects which can underwrite the development and support of modeling & simulation software.

3 NEAMS Structural Mechanics

The NEAMS structural modules provides structural mechanics and material performance analysis. The structural mechanics module, based on the code Diablo, supports continuum-scale analysis of structural performance of integrated structures, such as fuel assemblies, reactor vessels, and containment buildings. Diablo provides an implicit finite-element simulation capability for nonlinear solid mechanics on large-scale parallel computers. It also has capabilities for conduction heat transfer, and as the SHARP team's experience with multi-physics reactor simulation builds, it may be found useful to have the Nek5000 (thermal hydraulics) and Diablo codes partition or otherwise share the duties of solving for updates to the reactor temperature field. An initial structural mechanics capability will be available as part of the FY2015 early user version, and a fully enabled version will be part of the FY2018 release.

The Diablo integration with the RPL's SHARP framework is through a thin "veneer" of Application Programming Interfaces to exchange data and control logic.

In reference to Figure 1, this would be analogous to the "Application A". Spatial data, e.g., the mesh and physical fields discretized on that mesh, are passed through the iMesh interface supported by the MOAB library. The mapping of mesh-resident data between different meshes, tailored to different physics modules, will be performed by the MBCoupler. In the future, control logic such as time step coordination, will be facilitated through the Coupé module.

After the multi-physics capabilities of the RPL have been established for reactor-scale simulation, the Structural Mechanics Module will need to leverage (and enable) the capabilities of NEAMS Material Tool in concert with reactor-scale simulation. We envision that this will begin as multi-resolution simulations, where local environmental histories, e.g., temperature, are passed to the Material Tool for evaluation of pin-scale response. Building on that capability will lead to multi-scale modeling, where the Material Tool is called in real-time to provide constitutive response to at least select portions of the Structural Mechanics module. Development of the material performance analysis capability will be initiated in FY2018 with expected delivery at the end of FY2019.

4 Development Plan

This development plan is driven by a sequence of multi-physics simulation demonstrations sketched within the Program Plan. We reprise the sequence in Table 2. We include annotations noting that both FY13 demonstrations were successful. These included the calculation of structural deformations at LLNL using temperature fields read from MOAB databases produced at ANL as coupled thermal hydraulics / neutronics simulation proceeded. From this foundation we will work to first provide deformation fields back to thermal hydraulics and neutronics which will provide a static update of the geometrical configuration. In turn, this will lead to having the structural mechanics operational under Coupé and participating in the nonlinear iterations within each time step.

Table 2. Planned Reactor Product Line (RPL) demonstrations, FY2013-18

Year	Planned Demonstration
FY2013	Full-scale pin-resolved assembly with neutronics, thermal hydraulics, and structural mechanics (no deformation feedback) ***Completed*** *– See report ANL/NE-13/9* Multiple pin-resolved assemblies with neutronics, thermal hydraulics, and structural mechanics (no deformation feedback) ***Completed*** *– See report ANL/NE-13/21*
FY2014	Multiscale full-core with neutronics, thermal hydraulics, and structural mechanics with selected pin-resolved assemblies (no deformation feedback)

FY2015	Early-user release of the RPL Multiscale full-core with neutronics, thermal hydraulics, and structural mechanics with selected pin-resolved assemblies (with deformation feedback)
FY2016	Multiscale full-plant steady state with detailed core simulation Fuel assembly simulation coordinated with FPL
FY2017	Multiscale full-plant transient with detailed core simulation Fuel assembly simulation coordinated with FPL
FY2018	Version 1.0 release of the RPL Fuel assembly simulation coupled to the FPL

5 Work Breakdown Structure

Here we expand upon the WBS provided in the Program Plan by detailing the next lower level of structural mechanics development tasks. These tasks will need to balanced, i.e., scoped appropriately, to harmoniously co-exist with the efforts associated with the yearly demonstration activities.

Table 3. WBS for implementation of the NEAM Structural Mechanics Module

WBS	Description	Delivery Year
3	Reactors Product Line	
3.1	Transient 3D Structural Model (Greater Than Assembly Scale)	
3.1.1	Initial Integration of Diablo with SHARP Framework	
3.1.1.1	Complete static MOAB database reader/writer function integration	FY13
3.1.1.2	Exercise MBCoupler as stand-alone utility and begin integration	FY13
3.1.1.3	State-of-practice material models for slow deformation: creep and swelling	FY14
3.1.3	Expand integration of Diablo to enable integrated transient analysis	
3.1.3.1	Complete initial MBCoupler integration	FY14
3.1.3.2	Initial integration with Coupé for coordinated multi-physics time stepping	FY14
3.1.3.3	Developer coordination and early adopter support	FY14,15
3.1.5	Integrated Multi-physics Simulations with Structural Deformation	
3.1.5.1	Collaborate on deformation feedback re: time stepping and mesh smoothing	FY15
3.1.5.2	Integrate option to utilize memory-resident mesh transfers	FY15
3.1.5.3	Feature addition to support FY16 demonstration, e.g., FPL coordination.	FY15
3.1.5.4	Feature addition to support FY17 demonstration, e.g., full-plant support	FY16

3.1.5.5	Collaboration and updates to support NiCE deployment	FY15-17
3.1.5.6	Design for multi-scale collaboration with FPL Material Tools	FY16
3.1.5.7	Implementation of multi-scale collaboration with FPL Material Tools	FY17
3.1.5.8	Collaboration and updates to support NiCE deployment	FY15-17
3.1.5.9	Preparation for FY18 general release	FY17
3.1.7	Annual Updates Based on Demonstration Problem Needs	

6 Milestones

As compiled in Appendix A, the Program Plan defines a handful of milestones for Structural Mechanics (and other modules) on a recurring basis across FYs 14–18. At the envisioned funding level for development, this number of milestones should provide enough metrics for project management. We therefore do not propose any additional milestones at this time, while also expecting that the existing milestones will necessarily be refined or redirected as dictated by project experience to accumulated and unfolding budgetary realities.

7 Risks and Mitigations

The following risks are identified as the basis for future conversation with project partners. At this time they are presented without any relative rank order.

1. The Diablo code has a limited number of finite element formulations, selected based upon decades of experience with the nonlinear, large-deformations structural problems typical at LLNL. These formulations may prove inadequate, or more likely, represent non-optimal computational performance for the needs of Reactor Product Line.

Mitigation: Monitor the experience with successive RPL demonstration problems and as necessary prioritize available development effort to remediate any unacceptable bottlenecks.

2. Introducing structural deformations into the RPL multi-physics simulations will degrade or destabilize the existing algorithmic options utilized by SHARP.

Mitigation: It is almost a certainty with multi-physics simulations that there will be surprises along the way. Adequate time must be allocated for the demonstration simulations, and as an adjunct to these, representative “model problems” must be identified and exercised so algorithmic exploration can take place in a context of limited computational expense.

3. Balance of Plant modeling may require functionalities and features not currently available in, or planned for, Diablo. For example, depending on the modeling objectives, features such as "pipe elements" and "pipe snubbers" could be important for representing primary and secondary loops without using excessive numbers of more fundamental element types.

Mitigation: Requirements such as these will need to be explored through interactions with targeted users and fellow RPL developers, and refined as we move outward from our current concentration on reactor core modeling.

8 References

D. Pointer *et al.*, "Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program Plan, June 2013.

T. Tautges, *et al.*, "SHARP Single-Assembly Multiphysics Demonstration Simulations", Argonne National Laboratory, ANL/NE-13/9, March 31, 2013.

E. Merzari, *et al.*, "SHARP Multi-Assembly Multiphysics Demonstration Simulations", Argonne National Laboratory, ANL/NE-13/21, September 30, 2013.

I.D. Parsons, J.M. Solberg, R.M. Ferencz, M.A. Havstad, N.E. Hodge, and A.P. Wemhoff. "Diablo User Manual", Lawrence Livermore National Laboratory, UCRL-SM-234927, September 2007.

Appendix A: Selected NEAMS Milestone Dictionary

The following table captures the subset of the NEAMS Toolkit milestones requiring participation and/or integration of the Structural Mechanics Module. These entries were distilled from the NEAMS Program Plan of June 2013. Notional dates are assigned in that document's GANTT chart,

WBS	Milestone / Deliverable	Description
3.1.2	NEAMS Structural (Structural Analysis Module)	Initial version of Diablo with integrated SHARP framework components.
3.1.4	NEAMS Structural (Structural Analysis Module)	Release NEAMS Structural module for development and demonstration team use.
3.1.6	NEAMS Structural (Structural Analysis Module)	Release updated NEAMS Structural module for development and demonstration team use.
3.1.7.1	NEAMS Structural (Annual Update)	Release update of NEAMS Structural module which enables use of NEAMS Integrated framework as part of early user release of the RPL.
3.1.7.2	NEAMS Structural (Annual Update)	Release update of NEAMS Structural module with improvements based on user experience.
3.1.7.3	NEAMS Structural (Annual Update)	Release update of NEAMS Structural module with improvements based on user experience.
3.1.7.4	NEAMS Structural (Annual Update)	Release update of NEAMS Structural module with improvements based on user experience as part of full NEAMS ToolKit release.
3.5.3.1.1	Structural Annual Assessment Report	Issue assessment report for the NEAMS Structural module components for validation comparisons with experiments selected during the FY2014 planning process.
3.5.3.1.2	Structural Annual Assessment Report	Issue assessment report for the NEAMS Structural module components for validation comparisons with experiments selected during the FY2015 planning process.
3.5.3.1.3	Structural Annual Assessment Report	Issue assessment report for the NEAMS Structural module components for validation comparisons with experiments selected during the FY2016 planning process.
3.5.3.1.4	Structural Annual Assessment Report	Issue assessment report for the NEAMS Structural module components for validation comparisons with experiments selected during the FY2017 planning process.
3.5.3.1.5	Structural Annual Assessment Report	Issue assessment report for the NEAMS Structural module components for validation comparisons with experiments selected during the FY2018 planning process.
3.6.1	Demonstrations (RPL only)	Execute and document demonstrations of steady- and pseudo-steady-state integrated multiphysics simulations using NEAMS Neutronics, NEAMS Thermal Hydraulics, and NEAMS Structural for a full-scale SFR fuel assembly (no mesh deformation).
3.6.2	Demonstrations (RPL only)	Execute and document demonstrations of steady- and pseudo-steady-state integrated multiphysics simulations using NEAMS Neutronics, NEAMS Thermal Hydraulics, and NEAMS Structural for a full SFR core (no structural deformation).

3.6.3	Demonstrations (RPL only)	Execute and document demonstrations of steady- and pseudo-steady-state integrated multiphysics simulations using NEAMS Neutronics, NEAMS Thermal Hydraulics, and NEAMS Structural for a full SFR core (with structural deformation).
3.6.4	Demonstrations (RPL only)	Execute and document demonstrations of steady- and pseudo-steady-state integrated multiphysics simulations using NEAMS Neutronics, NEAMS Thermal Hydraulics, and NEAMS Structural for a full SFR plant with detailed core representation.
3.6.5	Demonstrations (RPL only)	Execute and document demonstrations of transient integrated multiphysics simulations using NEAMS Neutronics, NEAMS Thermal Hydraulics, and NEAMS Structural for a full SFR plant with detailed core representation.
3.6.6	Demonstrations (RPL only)	Define demonstration and tutorial problems to support FY2018 release of NEAMS ToolKit.
3.7	Reactor Tools Documentation	
3.7.1	Development and Original Roll-Out	Develop and deliver user documentation for the NEAMS Neutronics, Thermal Hydraulics and Structural modules
3.7.2	Original Theory Manuals and User Manuals (Reactors)	Issue theory and user manuals for NEAMS Structural, NEAMS Thermal Hydraulic, and NEAMS Neutronics modules for completing steady state and quasi-steady state simulations of reactor core performance in either single physics or integrated multiphysics modes.
3.7.3.1	Updated Theory Manuals and User Manuals (Reactors)	Issue theory and user manuals for NEAMS Structural, NEAMS Thermal Hydraulic, and NEAMS Neutronics modules for completing steady-state and quasi-steady-state simulations of reactor core performance in either single physics or integrated multiphysics modes. Annual updates include new or refined models developed by users, adjustments to existing models based on continued assessments vs. experimental databases, and/or bug fixes.
3.7.3.2	Updated Theory Manuals and User Manuals (Reactors)	Issue theory and user manuals for NEAMS Structural, NEAMS Thermal Hydraulic, and NEAMS Neutronics modules for completing steady-state, quasi-steady state, and transient simulations of reactor core performance in either single physics or integrated multiphysics modes. Annual updates include new or refined models developed by users, adjustments to existing models based on continued assessments vs. experimental databases, and/or bug fixes.
3.7.3.3	Updated Theory Manuals and User Manuals (Reactors)	Issue theory and user manuals for NEAMS Structural, NEAMS Thermal Hydraulic, and NEAMS Neutronics modules for completing steady-state, quasi-steady-state, and transient simulations of reactor core performance in either single physics or integrated multiphysics modes. Annual updates include new or refined models developed by users, adjustments to existing models based on continued assessments vs. experimental databases, and/or bug fixes.
3.8.2	User Training (RPL only)	Develop tutorials for all RPL components and integrated multiphysics simulations. Perform training workshops for RPL components that are ready for outside users (high-fidelity CFD, MCC3 cross-section generation, near-term reactor kinetics, structural mechanics, and meshing).

3.8.3	User Training (RPL only)	Develop tutorials for all RPL components and integrated multiphysics simulations. Perform training workshops for FY2015 "friendly user" RPL release.
3.8.4	User Training (RPL only)	Develop tutorials for all RPL components and integrated multiphysics simulations. Perform training workshops for FY2016 RPL update.
3.8.5	User Training (RPL only)	Develop tutorials for all RPL components and integrated multiphysics simulations. Perform training workshops for FY2017 RPL update.