U.S. DOE NEAMS Program and SHARP Multi-Physics Toolkit for High-Fidelity SFR Core Design and Analysis

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Abstract. Under the U.S. DOE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, 3-D, high-fidelity multi-physics simulation capabilities are being developed to address the needs of designers and analysts in studying advanced reactor systems with a particular focus on sodium-cooled fast reactors (SFRs). Simulation-based High-fidelity Advanced Reactor Prototyping (SHARP) is a tool-kit developed under the Reactors Product Line of NEAMS, and it consists of pin-by-pin neutronics, thermal-hydraulics, and structural mechanics analysis modules, as well as the capabilities to integrate these modules for multi-physics calculations. Physics modules currently include the PROTEUS neutronics code with associated cross section generation and evaluation components, the Nek5000 computational fluid dynamics (CFD) code for thermal-hydraulics, and the DIABLO implicit finite element analysis code for structural mechanics. Each module can be utilized as a standalone code component or as part of an integrated analysis. The Reactor Product Line also supports the development of the advanced reactor Systems Analysis Module (SAM), the multigroup cross section generation module MC^2-3, and the perturbation and sensitivity analysis module PERSENT. The development philosophy for the modules is to incorporate as much fundamental physics as possible in order to extend functionality to general reactor types, rather than developing tools for a limited set of specific reactor analysis applications.

Key Words: High-fidelity modelling, reactor core simulation, multi-physics calculations.

1. Introduction

The Nuclear Energy Advanced Modelling and Simulation (NEAMS) Program was established in 2009 to develop a high-fidelity simulation tool kit using modern computational techniques and innovative methods and solvers to support design of advanced nuclear reactor concepts. Building on an earlier effort with a similar high-fidelity modelling and simulation focus on LWRs [1], the broad NEAMS program objective has been to develop a predictive "pellet-to-plant" simulation capability for nuclear reactor systems. The objective has been to develop the tools in a general, mission agile way to support a broad base of reactor technologies, but applications have focused on analysis of sodium-cooled fast reactor (SFR) technologies for which significant international experience and of high-quality data exists for V&V.

The NEAMS program is organized along three modular product lines: The Fuels Product Line (FPL), the Reactors Product Line (RPL), and the Integration Product Line (IPL). The FPL and RPL consists of various physics modules to simulate the key phenomena and, when possible, they employ mechanistic descriptions to replace empiricism embedded in more conventional tools. The IPL focus is to integrate these modules to predict behaviours dominated by the often-competing phenomena and factors.

The RPL adopts a multiscale approach as well as multi-physics integration to connect the separate phenomena governing the reactor core behaviour through a hierarchal coupling that allows the coarse one-dimensional plant-level system models to be informed by high-fidelity, three-dimensional thermo-fluid-structural-dynamics calculations. Use of high-performance computing methods and increased modularity allows the high-fidelity simulations feasible on leadership class computing platforms. To accommodate a more diverse user base, however, a range of reduced-order models/methods are also being pursued to operate on the spectrum of more common computer platforms, from desktop or small cluster computers, available in the academia and industry. Portability is provided by built-in options for resolution and scale, by either reduced-order physics models or managed functionality for multiple platforms. V&V studies using numerical benchmarks or comparisons with experimental data are being prepared for each release to build confidence in their reliability.

2. Role of High-Fidelity Modeling and Simulations in Advanced Reactor Design

The ability to reliably simulate plant operating conditions and transient response is an essential component of advanced reactor R&D. Traditionally system analysis codes are commonly used to support concept development and licensing efforts for advanced reactors. The fast-running system simulation codes such as SAS4A/SASSYS-1 in the U.S. [2] can be used on desktop workstations. In a systems analysis, the major physics of the entire plant and integral effects are captured but with significant uncertainties: The geometry is only coarsely modelled (with one-dimensional coolant flow in reactor code and typically zero-dimensional control volumes with perfect-mixing in plena), and correlations with known (but limited) range of applicability are relied on to characterize the heat transfer between the fuel pins and coolant. Since the differences in various advanced reactor concepts (geometry and physics) can be significant, the implementation needs to be optimized for specific concepts: SFRs, HTGRs/FHRs, and MSRs each require their own specialized system analysis tools.

For bounding case studies in which peak temperatures are needed, the system analysis codes are often sufficient. While the results predicted with the system tools would be approximate, they still represent the major physics and integral effects with sufficient conservatism. For SFRs, as-irradiated fuel performance (constituent redistribution, fission gas migration and release, fuel-cladding mechanical and chemical interactions), the reactivity feedback mechanisms that contribute to inherent safety (e.g., Doppler, coolant density and void, fuel/structure density, fuel axial, core radial, and control-rod driveline expansions), natural circulation decay heat removal, sodium boiling, in-pin and ex-pin molten fuel motion with reactivity implications are examples that can be reliably obtained with system analysis codes with embedded sufficient conservatism.

In a conventional high-fidelity analysis, typically only the separate-effect physics (such as the neutronics or thermal-hydraulics) are simulated but with significantly reduced uncertainties: The geometric details are captured and the flow field is resolved in 3-D (including the ability to resolve the viscous and thermal boundary layers near the heated surfaces), largely eliminating the need for correlations. Since the separate effect physics modules are typically applicable to a wide range of neutron spectrum as well as variety of coolants and structural materials, high-fidelity tools can be used for multiple advanced reactor concepts. The NEAMS program aims to extend these high-fidelity capabilities to capture the integral effects through multi-physics simulations.

Higher fidelity is needed when the system codes provide limited information on parameters that have a significant effect on safety or have large uncertainty. High-fidelity can also be key for specific component design to evaluate detailed flow and temperature distributions, for example in a wire-wrapped SFR fuel assembly. Specific examples where high-fidelity modelling and simulation is key include the mixing and thermal-stratification in large volumes (e.g., upper plena, cold pool), thermal-striping of different temperature jets leading to thermal fatigue induced failures in upper core structures, thermal stresses on reactors vessel due to temperature gradients, high temperature, or its rate-of-change, flow-induced vibrations, and bypass flow between hot and cold pools.

The concept-optimized system analysis tools can best be used to improve the technical readiness level of an advanced reactor concept, whereas high-fidelity approaches can be of greater use for mature concepts to support their commercial deployment. For design optimizations and sensitivity studies, system codes coupled with appropriate sub-grid physics or higher-fidelity tools can provide the best information needed for an advanced concept.

3. NEAMS Reactor Product Line

The NEAMS program aims to take advantage of the advances in computing power and algorithms for solving complex systems of equations to enable high-fidelity simulations inclusive of multi-physics effects. The goal is to use advanced simulation tools to improve accuracy of advanced reactor core modelling, allowing reduced conservatism and improved safety assurance. Another goal is also to understand and reduce the uncertainty in conventional computational models.

To achieve these goals, the NEAMS program strategy has been to develop a flexible, mission-agile toolbox for construction of advanced reactor models. A multi-scale strategy has been adopted to enable application to problems relevant to industry using a wide range of computing platforms by utilizing a modular architecture to enable component-wise or integrated use. Development of these capabilities has been a multi-faceted effort:

- Teaming up with other (complementary) R&D programs (such as the U.S. DOE-NE's Advanced Reactor Technologies Program) to obtain functional requirements, identify relevant experiments for validation, and in some cases, taking advantage of complementary efforts to accelerate model development and validation,
- Continuing to benefit from computational technology improvements and modelling work funded by non-NE programs, such as the Office of Science and NNSA, e.g., in the areas of fluid behaviour and materials modelling,
- Enjoying continued access to high-performance computing resources, including leadership-class computers at the U.S. national laboratories.

Development team and collaborations include:

- DOE National Laboratories: Most of the advanced modelling and simulation expertise and technical leadership needed for NEAMS reside at the U.S. National Laboratories. The labs also provide a bridge to stakeholders in DOE-NE R&D programs and the nuclear industry. NEAMS leverages DOE and NNSA investments in expertise and leadership-class computing facilities.
- Universities: NEAMS has access to academic expertise through the Nuclear Energy University Program (NEUP) and occasional subcontracts with programs with specific capabilities. Their contributions include cost-effective acceleration of capability development and access to high-quality validation data. Up to date, collaborations have been established with several university teams (all U.S.-based).

- Industry: Although the DOE-NE R&D programs are the primary stakeholders in the near term, the NEAMS leadership has been reaching out to the nuclear industry and Nuclear Regulatory Agency to participate in the enhancement of the NEAMS Toolkit to address their specific needs.
- International Collaborations: NEAMS participates in several international collaborations to accelerate development of specific modules and obtain relevant validation data. Benchmarking and validation collaborations have been established with three countries (Japan, France, S. Korea) as well as the European Community.

4. SHARP Toolkit

RPL supports development of high-fidelity computational methods to simulate key phenomena involved in core design and analysis by applying modern, high-performance computing techniques. It targets to facilitate core/component design and optimization through separate effect analyses as well as to model integral phenomena mechanistically through tightly coupled physics solvers. By achieving these goals, RPL also allows a better understanding of the limitations of, and reduces the uncertainty in, conventional computational codes and methods such as those used in system simulations.

Following multi-year, multi-laboratory efforts for development of coupled neutronics, computational fluid dynamics (CFD), and computational structural mechanics (CSM) analysis capabilities, the NEAMS Reactor Product Line released the Simulation-based High-fidelity Advanced Reactor Prototyping (SHARP) multi-physics toolkit in March 2016.

SHARP is a “framework” to achieve tightly-coupled solutions using three physics modules: Heterogeneous deterministic neutron transport in exact geometries, 3-D thermal-fluid analysis, and 3-D finite element structural mechanics analysis. It is comprised of several physical modeling tools and capability to integrate these tools for multi-physics analyses:

- PROTEUS/MC2-3/PERSENT for neutronics
- Nek5000 for CFD and thermal-hydraulics
- Diablo for structural mechanics
- SIGMA interface for multi-physics coupling.

4.1 SHARP Neutronics: PROTEUS/MC2-3/PERSENT

The neutronics module, PROTEUS, developed exclusively under the NEAMS program is a high-fidelity finite-element neutron transport code with matching level of fidelity cross-section generation capabilities of MC^2-3 code. PROTEUS is based on using deterministic neutron transport solutions on an unstructured grid for complex geometries. It allows solutions on deformed SFR core configurations with moving grid analysis capabilities to assess the dynamic impact of core radial expansion during the transients without scram function. Designed for massively parallel supercomputing platforms, PROTEUS has excellent parallel computing capabilities with scalability to hundreds of thousands of processors (it was a finalist for Gordon Bell prize in 2009). PROTEUS has been applied to a variety of nuclear reactors, including SFRs [3] [4] [5] [6], LWRs [7] [8], ATR [9], and TREAT [10].

PROTEUS itself is a toolkit that encompasses a set of transport solvers:

- PROTEUS-SN: It is a massively parallel solver on a fully unstructured finite element mesh based on 2nd-order discrete-ordinates formulation of the even-parity form of the neutron transport equation. In can handle $>10^{12}$ degrees of freedom and includes an adiabatic quasi-static kinetics formulation.

- PROTEUS-MOCFE: It is a fully three-dimensional Method of Characteristics (MOC) solver for unstructured finite element meshes. As such, it is practical for two-dimensional, or small three-dimensional problems due to high memory requirements.
- PROTEUS-MOCEX: This solver combines the two-dimensional MOC method for an unstructured mesh with discontinuous Galerkin finite element method in axial direction as a more computationally efficient alternative to the PROTEUS-MOCFE solver for axially-extruded geometries. It is a more promising approach avoiding the limitations of more conventional 2D+1D MOC approaches.

The SHARP neutronics toolkit also includes a suite of cross section generation, evaluation and sensitivity analysis capabilities:

- MC^2-3: Generates multigroup cross section library using NJOY for thermal and fast spectrum, accounting for 3-D transport effects using subgroup or resonance table method based on two-dimensional method of characteristics based neutron transport solver for both rectangular and hexagonal geometries with discontinuous Galerkin finite element method in axial direction. It has been validated for the ZPR/ZPPR fuel drawers and BFS fuel with wrapper, and has been extended to the thermal energy range [11], widely adapted by the DOE-NE ART program and licensed to industry to support commercial SFR design efforts.
- Cross-section API (CSAPI): Allows transport solvers to generate self-shielded multi-group cross-sections on-the-fly, accounting for the effects of heterogeneous geometry as well as temperature and composition variations. Developed as a functional module, it is adaptable to other transport codes with fixed source solver.
- PERSENT: Performs perturbation and sensitivity analyses based on hybrid finite element method by computing the space-energy breakdown of proposed perturbations of material constituents and linear cross section sensitivity coefficients for uncertainty quantification.
- Other cross section generation/evaluation tools includes Genesis as a cross section library generation code, GenISOTXS that can read Serpent and OpenMC Monte Carlo code outputs to generate ISOTXS, and BuildBOT for nightly regression tests.

4.2 SHARP Thermal Hydraulics: SAM and Nek5000

The SHARP toolkit thermal-hydraulics analysis capabilities include a new System Analysis Module (SAM) [12] and Computational Fluid Dynamics (CFD) code, Nek5000 [13]:

- System Analysis Module (SAM): It is a practical plant-level system analysis tool for advanced reactors with single-phase flow and heat transfer. The targeted concepts include SFR, LFR, MSR, and the FHR. Built-on the MOOSE framework [14], it takes advantage of advances in modern software environments and design, numerical methods, and physical models to build a flexible multi-physics framework for multi-scale integration with other high-fidelity tools. It employs high-order spatial and time discretization schemes for improved accuracy and enhanced code performance, as well as component-based structure for user friendliness. Its SFR system simulation capabilities have been demonstrated through benchmark analysis of EBR-II shutdown heat removal and inherent safety demonstration tests [15]. And it has been integrated with SAS4A/SASSYS-1 SFR system and safety analysis code system [16] and commercial software for coupled system+ CFD simulations [17]. Ongoing efforts focus on development of reduced-order multi-dimensional mixing and heat transfer modeling capabilities for thermal-stratification and mixing in large enclosures.

- Nek5000: A CFD code that leverages the spectral element method to achieve rapid spatial convergence, and high scalability up to 10^6 cores [18]. Nek5000 was honored by a R&D 100 Award in 2016 [19], and a Gordon Bell Prize in 1999. It has incompressible and weakly-compressible flow [20] modeling capabilities with Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) capabilities, as well as Reynolds-Averaged Navier-Stokes (RANS) [21] formulations for turbulence modeling. Extensive verification and validation exercises have been performed for advanced reactor applications [22]. Development of two-phase boiling models is underway [23], with the goal of being able to predict critical heat flux in BWRs

Working with partners at Areva, TerraPower and Texas A&M University, Nek5000 is being used to support analysis as part of experimental and computational campaign to evaluate the influence of irradiation-induced fuel pin deformation on thermal performance of wire-wrapped SFR fuel bundles [24]. An important outcome of this exercise will be experimental validation of CFD codes, including Nek5000, for supporting SFR fuel assembly design and safety analysis. So far, preliminary large eddy simulations have been performed on the appropriate geometry at with Reynolds numbers as high as 10,000, as shown in FIG. 1.

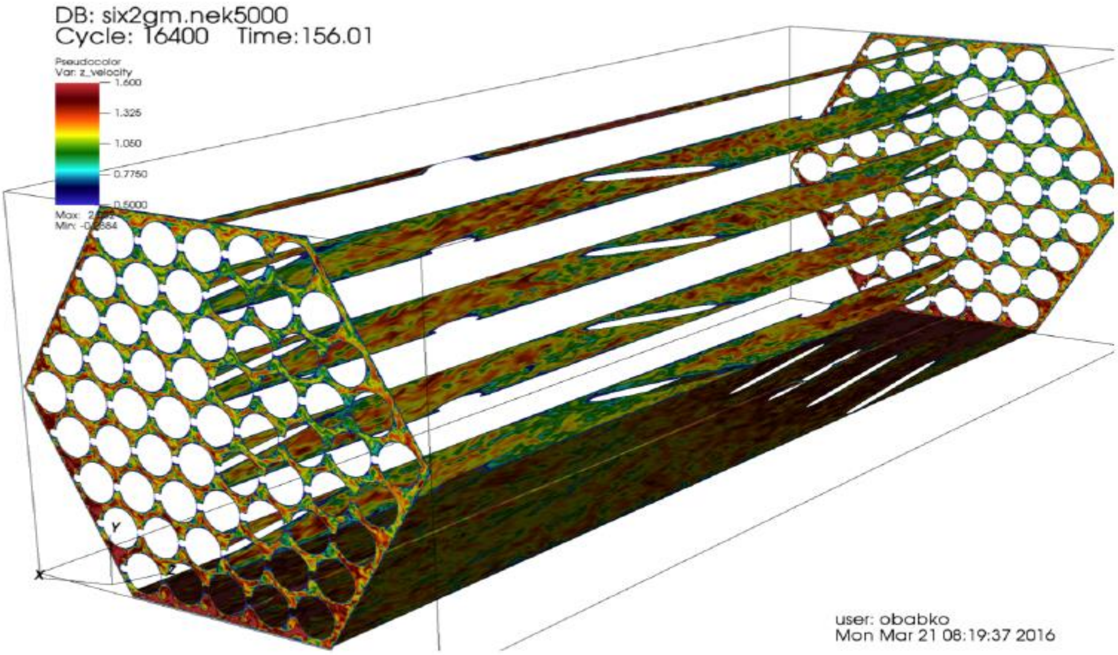

FIG. 1. Nek5000 predictions of instantaneous axial velocity at Re=10,000 in an SFR fuel bundle [24]

4.3 SHARP Structural Analysis: DIABLO

The Diablo code being developed at Lawrence Livermore National Laboratory uses implicit, Lagrangian finite-element methods for the simulation of solid mechanics and multi-physics events over moderate to long time frames [25]. A primary focus is nonlinear structural mechanics and heat transfer. The code provides a venue for applying parallel computation to discretization technologies developed and user-tested in the legacy serial-processor codes NIKE3D and TOPAZ3D. Diablo includes state-of-the-art algorithms for the simulation of “contact”, i.e. the interaction between unbonded material interfaces. Their experience with contact motivates the use of low-order spatial discretizations, such as eight-node hexahedra for continua and four-node quadrilaterals for shells. Appropriate formulations are employed to accommodate nearly incompressible material models, such as for metal plasticity and rubber elasticity. Global algorithms include second-order and quasi-steady time integration and a number of approaches for nonlinear iteration: full Newton, modified-Newton, multiple quasi-Newton updates, and line search. Linear solvers are utilized from multiple libraries. The Diablo User Manual is available in the SHARP distribution package.

4.4 SHARP Multi-Physics Integration: SIGMA

The SHARP framework employs a "bottom-up" approach that seeks to minimize the intrusion into existing physics modules to perform the coupling. This is performed by leveraging infrastructure capabilities provided by Scalable Interfaces for Geometry and Mesh-based Applications (SIGMA) [26]. The SIGMA package consists of several software components such as the Common Geometry Module (CGM) to generate ACIS and OCC geometry models; MeshKit to generate optimal quality meshes on complex geometries with smoothing, copying, moving, rotating, extruding functions and various extensions to use external packages like Cubit, Tetgen, and Netgen; the Mesh-Oriented datABase (MOAB) to represent and evaluate mesh data as scalable arrays based on ITAPS (Interoperable Technologies for Advanced Petascale Simulations) iMesh interface for access and storage; and CouPE for coupled physics global nonlinear solvers based on PETSc for multi-physics solutions. For multi-physics simulations, SIGMA supports reading mesh and associated data, propagating solution variables back onto each domain's mesh, while simulations are performed in parallel.

As mentioned previously, one of the target SFR demonstration problems has been to develop a mechanistic capability to predict the neutronics impact on SFR core deformation. In the initial exercise, only the influence of thermal, rather than fluence, gradients are considered. Predicting the SFR behavior includes at least three physics: the deformation is predicted by Diablo, the thermal field is predicted by Nek5000, and the neutron flux and reactivity changes are predicted by PROTEUS (see FIG. 2) For this demonstration, the internal fuel pin, cladding, and coolant within each assembly were homogenized in the PROTEUS model, but the duct walls were represented explicitly. Similarly, Nek5000 employed a porous media representation of the flow within each fuel assembly, while it predicts the temperature along the duct wall. Using this information, Diablo predicts the multidimensional thermal strain assocaiated with these thermal gradients. The neutronics simulations are repeated on the deformed geometry provided by Diablo. For this steady-state exercise at the hot core condition, these SHARP iterations were repeated several times to achieve a converged k_{eff}.

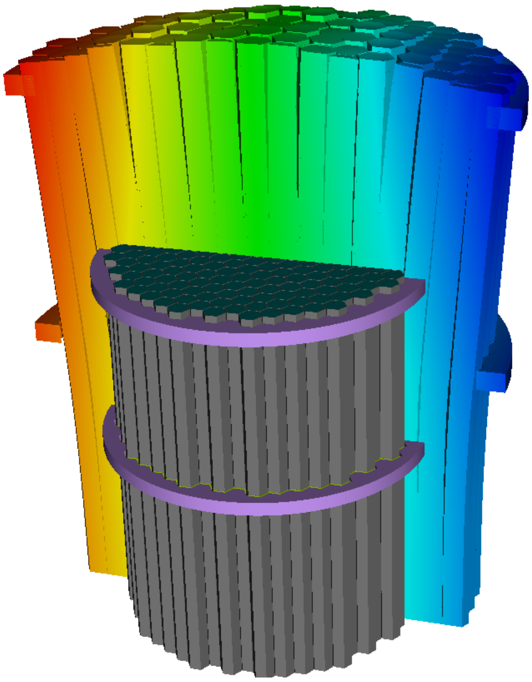

FIG. 2. Predicted deformation of SFR fuel assemblies in SHARP

5. Summary and Future Plans

SHARP leverages state-of-the-art single-physics tools to solve multi-physics nuclear reactor problems in a manner closer to first-principles. It aims to provide insight into core/component design that can't be easily measured or accounted for with conventional tools or methods.

After release of SHARP in March 2016, focus has shifted to assessment and V&V of its component and multi-physics analyses capabilities. A systematic approach is pursued for greater DOE-NE ART program engagement with joint modeling and experiment design to set the foundation for future work based on assessed strengths and shortcomings for the SHARP toolkit.

The development and integration of models to predict steady-state and transient behaviour of a pin-resolved, three-dimensional SFR core has been an early focal point of the NEAMS RPL. The turbulent flow analysis capabilities are currently being demonstrated for a wire-wrapped SFR fuel assembly as part of a DOE-NE ART program funded and industry-led collaboration between Areva, TerraPower and Argonne, involving comparisons of Nek5000 predictions with data from 61-pin wire-wrapped for SFR fuel assembly tests conducted at Texas A&M University and Areva. Other applications of SHARP to SFR challenge problems include Advanced Fast Reactor, AFR-100, hot-channel/pin factor analysis and coupled system-CFD analyses to support U.S. bilateral collaborations with Japan, France, China.

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