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Innovations in Multi-Physics Methods Development, Validation, and Uncertainty Quantification

Maria Avramova *, **Agustin Abarca, Jason Hou** and **Kostadin Ivanov**

2107 Burlington Engineering Lab, North Carolina State University, 2500 Stinson Drive, Raleigh, NC 27695, USA; aabarca@ncsu.edu (A.A.); jhou8@ncsu.edu (J.H.); knivanov@ncsu.edu (K.I.)
* Correspondence: mnavramo@ncsu.edu

Abstract: This paper provides a review of current and upcoming innovations in development, validation, and uncertainty quantification of nuclear reactor multi-physics simulation methods. Multi-physics modelling and simulations (M&S) provide more accurate and realistic predictions of the nuclear reactors behavior including local safety parameters. Multi-physics M&S tools can be subdivided in two groups: traditional multi-physics M&S on assembly/channel spatial scale (currently used in industry and regulation), and novel high-fidelity multi-physics M&S on pin (sub-pin)/sub-channel spatial scale. The current trends in reactor design and safety analysis are towards further development, verification, and validation of multi-physics multi-scale M&S combined with uncertainty quantification and propagation. Approaches currently applied for validation of the traditional multi-physics M&S are summarized and illustrated using established Nuclear Energy Agency/Organization for Economic Cooperation and Development (NEA/OECD) multi-physics benchmarks. Novel high-fidelity multi-physics M&S allow for insights crucial to resolve industry challenge and high impact problems previously impossible with the traditional tools. Challenges in validation of novel multi-physics M&S are discussed along with the needs for developing validation benchmarks based on experimental data. Due to their complexity, the novel multi-physics codes are still computationally expensive for routine applications. This fact motivates the use of high-fidelity novel models and codes to inform the low-fidelity traditional models and codes, leading to improved traditional multi-physics M&S. The uncertainty quantification and propagation across different scales (multi-scale) and multi-physics phenomena are demonstrated using the OECD/NEA Light Water Reactor Uncertainty Analysis in Modelling benchmark framework. Finally, the increasing role of data science and analytics techniques in development and validation of multi-physics M&S is summarized.

Keywords: multi-physics methods; modeling and simulation; validation; uncertainty quantification

1. Introduction

The nuclear industry has always prioritized the safe, reliable and economically attractive operation of the nuclear power reactor fleet. Given these priorities, the development, validation, and application of multi-physics predictive modeling capabilities for both normal and accident conditions have evolved from the so-called best-estimate calculations to the first principle high-fidelity multi-physics simulations. This paper provides a review of the current and upcoming innovations in the development, validation, and uncertainty quantification of reactor multi-physics simulation methods.

There are many interactions between different physics phenomena at various scales in different components of the nuclear power plants (NPPs). Especially important are the multi-physics interactions in the nuclear reactor cores. In the past, these different interactions were treated either as boundary conditions (i.e., each physics calculation was performed independently and the impact of other physics phenomena was considered through boundary conditions), or using very simplistic models for some of the

physics phenomena. The multi-physics modelling and simulations (M&S) describe the non-linear multi-physics phenomena by simultaneous treatment of feedback effects of different physics; and provide more accurate and realistic predictions of a nuclear reactor behavior including local safety parameters.

Multi-physics simulation tools can be subdivided in two categories—traditional and novel [1]. The traditional multi-physics M&S, currently used in industry and regulation, are on an assembly/channel spatial scale. Coupling reactor core to the system and coupling system to the containment also belong to traditional multi-physics simulations. The novel high-fidelity multi-physics M&S are on a pin (sub-pin)/sub-channel spatial scale. These include the high-resolution coupling of several physics such as neutronics (reactor physics), thermal-hydraulics, fuel performance, structural mechanics, and chemistry. The current trends in reactor design and safety analysis are towards further development, verification, and validation of multi-physics multi-scale M&S combined with uncertainty quantification and propagation.

Traditional multi-physics calculation schemes are currently used in industry and regulation for routine calculations. As an example of traditional multi-physics M&S capability and its applications, the multi-physics platform developed at North Carolina (NC) State University is introduced in Section 2 of this paper [2]. Approaches currently applied for validation of the traditional multi-physics M&S are also summarized in the same section and illustrated using the established Organization for Economic Cooperation and Development (OECD)/Nuclear Energy Agency (NEA) multi-physics benchmarks [3,4].

Novel high-fidelity multi-physics M&S allow for insights crucial to resolve industry challenge and high impact problems previously impossible with the traditional tools. As an example, the US Department of Energy (DOE) Consortium for Advanced Simulation of Light Water Reactors (LWRs) (CASL) Virtual Environment Reactor Analysis (VERA) system is used in Section 3. In the same section, the challenges in validation of novel multi-physics M&S are discussed along with the needs for developing validation benchmarks based on high-resolution experimental data.

Due to their complexity, the novel multi-physics codes are still computationally expensive for routine applications. This fact motivates the use of high-fidelity novel models and codes to inform the low-fidelity traditional models and codes (high-to-low or Hi2Lo) leading to improved traditional multi-physics M&S. Examples are provided in Section 4.

The uncertainty quantification and propagation across different scales (multi-scale), and multi-physics phenomena is demonstrated in Section 5 using the OECD/NEA Light Water Reactor Uncertainty Analysis in Modelling (LWR UAM) benchmark framework.

Finally, the increasing role of the data science and analytics techniques in the development and validation of multi-physics M&S is summarized and discussed in the conclusion section of this paper.

2. Traditional Multi-Physics Simulation Methods

The main tools utilized in the design and safety analyses of NPPs are computer codes that simulate physical processes. The current trends in the nuclear power generation and regulation are to perform design and safety evaluations using "best-estimate" codes, which are based on traditional multi-physics M&S and allow for realistic modelling of nuclear and thermal-hydraulic processes in the reactor core and the entire plant, including control and protection functions. Best-estimate implies that such codes use sets of data, correlations, and methods designed to represent the phenomena of interest using the best available techniques. The best-estimate results should be supplemented with uncertainty and sensitivity analysis. Significant progress was achieved by developing coupled codes in which full three-dimensional (3D) reactor core models were incorporated into thermal-hydraulic system codes. Such coupling is required in order to perform best-estimate calculations of the interactions between the core behavior and the thermal-hydraulic behavior of the plant dynamics. The development and application of these advanced coupled codes were supported by the continuous growth of computing capabilities and were accompanied

by international activities on the comprehensive validation and uncertainty quantification. The traditional multi-physics tools have been used in two different ways in current licensing practices depending on the country and the associated regulatory framework: best-estimate bounding, and best-estimate plus uncertainty approaches.

The traditional multi-physics simulation methods have reached maturity and have several common features. The 3D core neutronics model is based on a few-group coarse-mesh diffusion approach using nodal nuclear data (library of parameterized nodal equivalent parameters). The spatial neutronics/thermal-hydraulic coupling is performed on an assembly/channel level. Simplified lumped fuel rod models are utilized as part of the system or sub-channel thermal-hydraulic codes. The temporal neutronics/thermal-hydraulic coupling is performed in an operator-splitting approach using nested loop iteration (fixed point iterations) for steady-state simulations and a sequential parameter exchange (explicit coupling) at each time step for transient simulations. The evaluation of safety related parameters on a pin/sub-channel level for the hot assembly/channel is performed via pin-power reconstruction combined with sub-channel calculations using boundary conditions provided by the coupled core model. The traditional multi-physics simulation tools are computationally efficient and extensively verified and validated. However, these tools utilize approximations for evaluations of local safety parameters on a pin/sub-channel level such as pin-power reconstruction in neutronics, spacer grid modelling in thermal-hydraulics, and gap conductance in fuel rod heat transfer.

As an example of traditional multi-physics M&S, a multi-physics platform developed at NC State University [2] and its applications are presented in this paper. The platform is based on the US Nuclear Regulatory Commission (NRC) codes TRACE, PARCS, and FRAP-CON/FRAPTRAN combined with CTF/CTFFuel. CTF/CTFFuel is a state-of-the-art sub-channel/heat transfer simulation code jointly developed by NC State University and Oak Ridge National Laboratory (ORNL). The SCALE package is used for cross-section generation and nuclear data uncertainty propagation. The whole-core PARCS assembly-wise and pin-wise (in two options—using pin-power reconstruction and direct simplified third-order spherical harmonic, SP_3, pin-by-pin calculations) M&S are coupled with CTF/CTFFuel on both assembly- and pin-levels. Additionally, a methodology was developed to generate the Discontinuity Factors (DFs) necessary for the 2nd flux moment in the SP_3 core calculations in addition to 0th moment DFs using generalized equivalence theory (GET) in assembly Method Of Characteristics (MOC) based lattice calculations (such as the ones performed by POLARIC/SCALE). Semi-implicit coupling between CTF (core) and TRACE (system) was designed for coupled core-to-system thermal-hydraulic M&S. The calculation sequence POLARIS-SAMPLER-GenPMAX is utilized for lattice calculation, cross-section generation, and uncertainty quantification. The coupled simulations and data transfer are managed by a control module. The data exchange between different codes was done via Message Passing Interface (MPI). A methodology was developed for uncertainty quantification and propagation through the multi-physics multi-scale simulation platform using DAKOTA. This platform, illustrated in Figures 1 and 2, improves the local safety margins estimates for real-size reactor core modeling white being computationally efficient. Figures 3 and 4 show results for the OECD/NRC Boiling Water Reactor (BWR) Turbine Trip Benchmark [5]. The initial steady state prior the turbine test at 80.9% of the core rated mass flow and 61.6% of the core rated total power is simulated. CTF/CTFFuel-PARCS coupled code was used to quantify the accuracy of the temperature feedback prediction in multi-physics simulations. The impact of two different levels of fidelity in the fuel physics was studied: (1) using the traditional lumped simplified fuel rod model in CTF, which uses a constant gap conductance modeling and default thermal fuel conductivity correlations (only as function of fuel temperature) in CTF; and (2) using the improved fuel performance models in CTFFuel. The CTFFuel model is shown in Figure 3. Figure 4 depicts the differences in Doppler (fuel) temperature predictions for different fuel types presented in BWR cores. The impact of the coupled calculation on the predictions of core multiplication factor and axial and radial power distributions are summarized in Table 1.
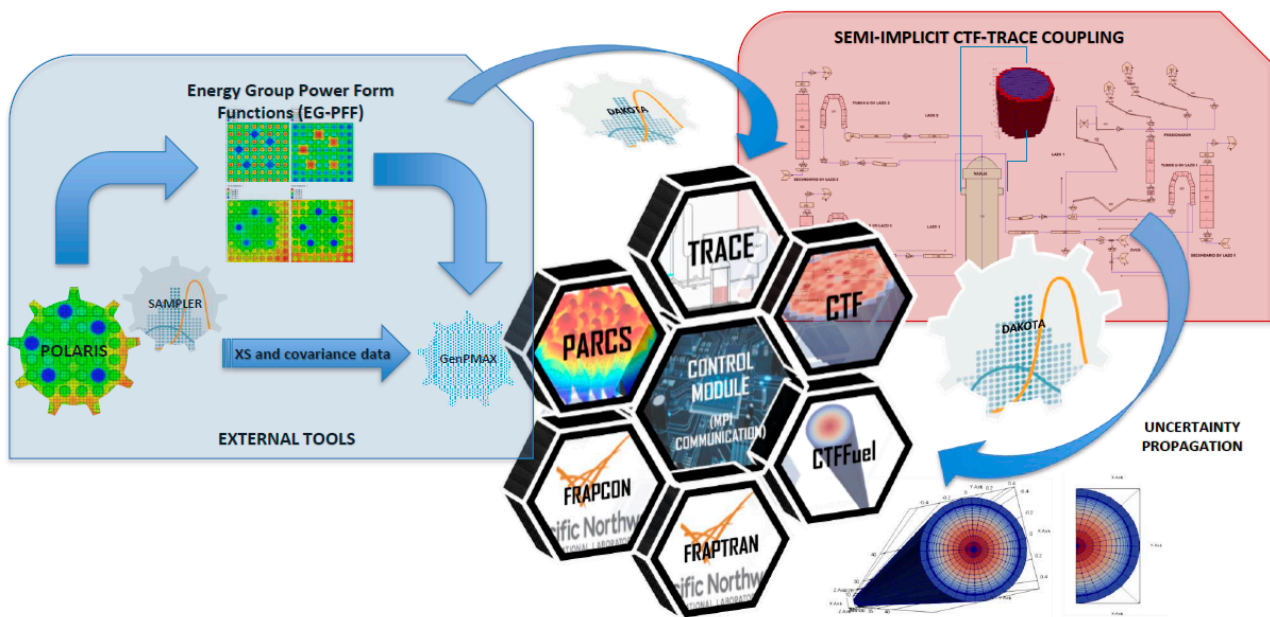
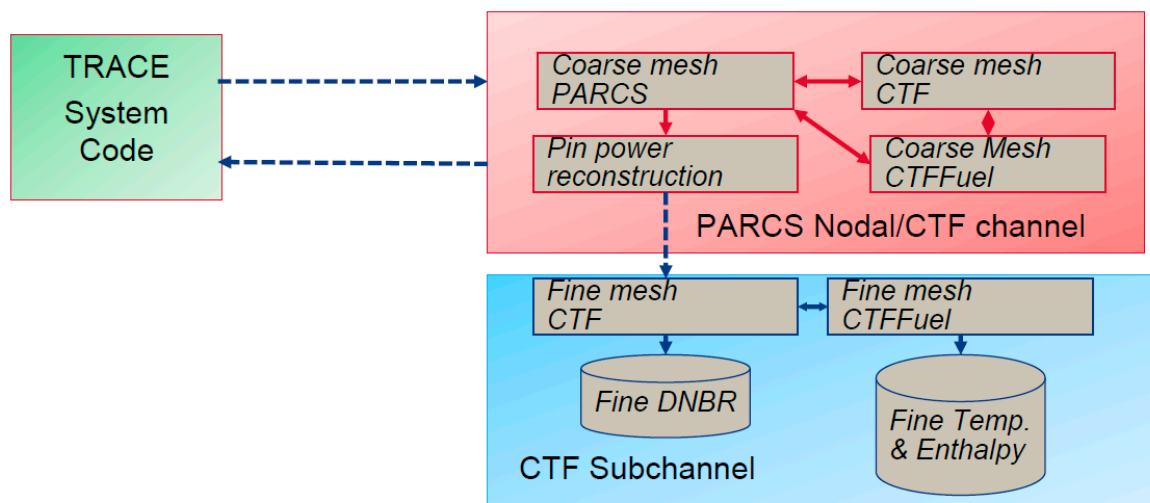**Figure 1.** Overview and data flow of the multi-physics platform.

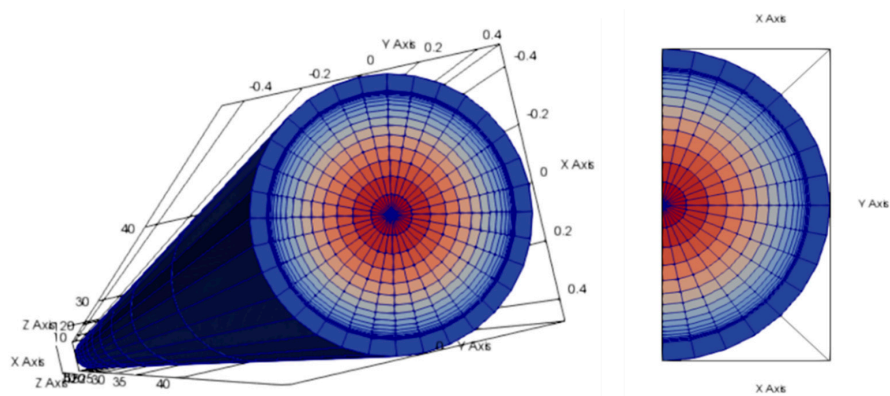**Figure 2.** Multi-scale coupling in the multi-physics platform.

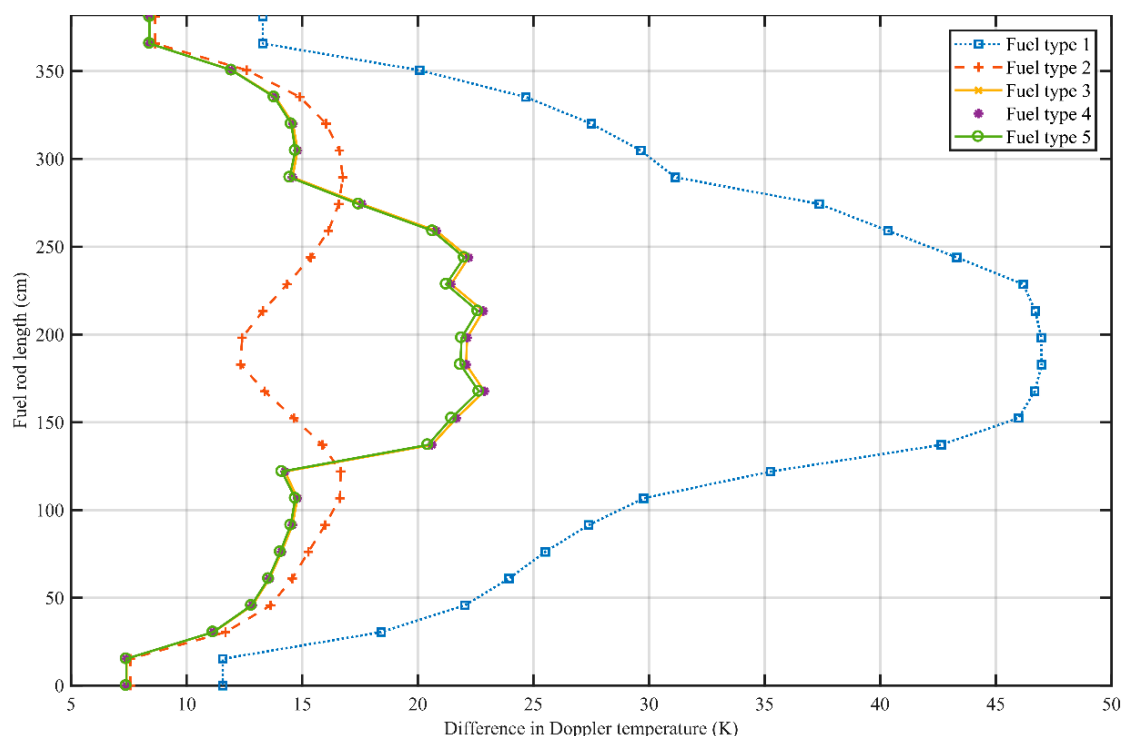**Figure 3.** CTFFuel model.

Figure 4. Differences in Doppler (fuel feedback) temperature predictions for different fuel types.

Table 1. Differences in predictions of core multiplication factor and power distribution.

Code	Effective Multiplication Factor, k_{eff}	Absolute Difference k_{eff} (pcm)	RMS Difference Axial Profile (%)	RMS Difference Radial Profile (%)
CTF/PARCS	1.007760	—	—	—
CTF-CTFFuel/PARCS	1.007272	48.8	0.1291	0.4036

A multi-level validation methodology for traditional multi-physics calculations, which allow for a consistent and comprehensive validation process, was developed and tested for different steady-states and transient cases using appropriate benchmarks established by NEA/OECD. These benchmarks permit testing of neutronics/thermal-hydraulics coupling and verifying the capability of the coupled traditional multi-physics codes to analyze complex transients with coupled core/plant interactions [6,7]. These benchmarks provide a validation basis for the current generation of coupled best-estimate codes.

3. Novel Multi-Physics Simulation Methods

Novel multi-physics M&S means more tightly coupled and more physics-based modelling with higher accuracy. Such approaches include physics-based materials models of the fuel system, reactor vessel and internals, improved constitutive relations of coolant and corrosion chemistry, and scalable, robust, modern methodologies for 3D full-core thermal hydraulics and pin-resolved radiation transport. The motivation behind development and application of novel multi-physics tools is to develop capabilities to predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modelling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics (*source: CASL*). The ultimate goal is to address essential industrial issues for achieving power uprates, lifetime extension, and higher fuel burn-up while ensuring that fuel performance and safety limits are met for the existing reactors and to improve and optimize the design and safety of the new reactors. The novel multi-physics simulations have demonstrated value added over

traditional multi-physics calculations for application to important nuclear industry issues associated with design, operational and safety challenges of current and next to be build nuclear reactors.

There is a need to extend the modeling capability of current "best-estimate" coupled codes for design and safety assessment in such a way that the prediction of the fuel rod response is based on first principles high-fidelity modelling of local parameters. Subsequently, the current developments have been towards performing whole-core high-fidelity multi-physics calculations on pin/sub-channel level and even on sub-pin (pin-resolved) level in order to understand and predict key aspects of fuel and cladding performance. Such capabilities allow for determining radial, axial and azimuthal flux distribution, energy deposition, coolant and fuel temperature distributions for different pin cells/sub-channels (fuel rod with surrounding coolant) at different core locations. High-fidelity multi-physics tools have been developed as part of several large projects—the NURESAFE and McSAFE programs in Europe (supported by the European Commission) and the US DOE sponsored Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program and CASL, which are being currently merged in one Joint Modeling and Simulation Program.

The novel multi-physics high-fidelity simulation methods have the following common features. For deterministic neutronics methods, two-group diffusion neutronics solvers are replaced with multi-group transport solutions. Continuous energy Monte Carlo codes are coupled with thermal-hydraulic solvers for reference coupled solutions. The thermal-hydraulic solvers are based on sub-channel, porous media or Computational Fluid Dynamics (CFD) solutions. Spatially the coupling is done on pin/sub-channel scale and even on sub-pin heterogeneity scale, which requires the implementation of improved and flexible coupling methodologies. Such refined coupled simulations can be performed in direct and embedded manner (utilizing multi-level coupling schemes). High-performance computing is efficiently utilized by using modern and user-friendly simulation platforms and parallel computing. Examples of such platforms are: MOOSE (finite element framework for the development of tightly coupled multi-physics solvers), SALOME (platform for simulation code integration in the field of reactor safety); and VERA. Fully implicit time-integration methods for simultaneous solution of the coupled non-linear system are implemented.

In the novel applications, uncertainty analysis is being integrated in high-fidelity, multi-physics calculations or, in other words, uncertainty and sensitivity analysis methods are considered as an integral part in the development of multi-physics methods. The uncertainty methodologies for novel applications include consistent propagation of large number of uncertainties and sensitivities through different physics phenomena coupled with non-linear feedback effects on a refined local scale.

To summarize, the scope of novel multi-physics applications is to provide first principle, accurate, high-fidelity predictions of local parameters, and reference and insightful design and safety simulations of local multi-physics phenomena, supplemented by comprehensive and consistent uncertainty propagation. An example of a novel high-fidelity M&S capability is the VERA system developed by CASL and now maintained and further developed by the VERA Users' Group to address LWR challenge problems. VERA (as illustrated in Figure 5) may be considered the most advanced 3D Pressurized Water Reactor (PWR) reactor simulator in the world. Currently, under a US DOE sponsored industry funding opportunity project, VERA is being further developed and applied to whole-core pin-by-pin simulation of BWRs.
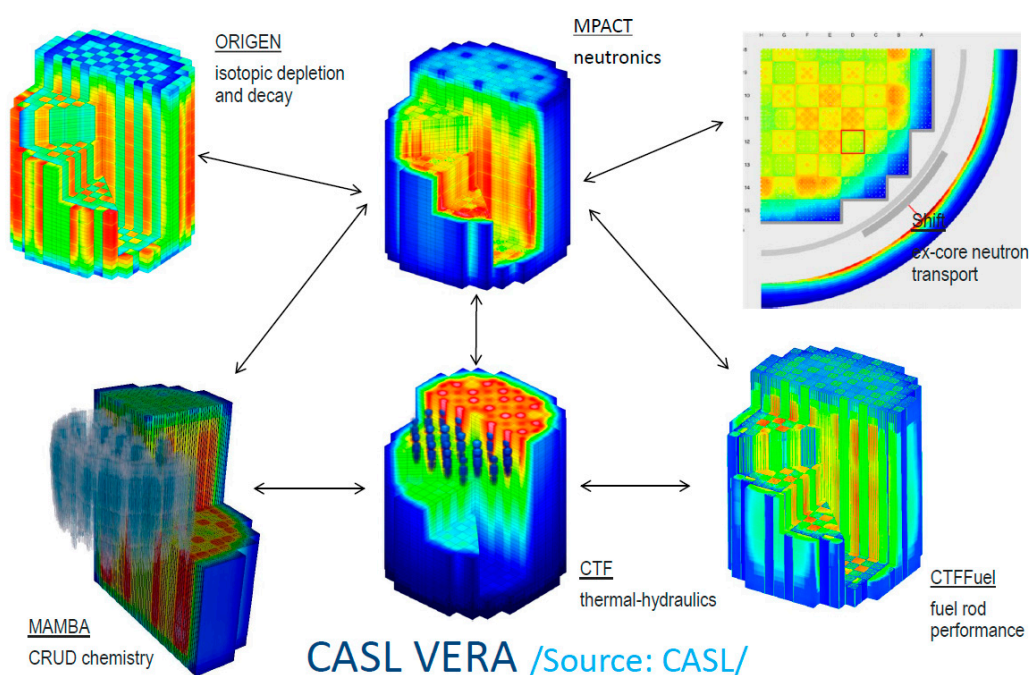
Figure 5. CASL VERA code system/Source: CASL/.

NC State University in cooperation with ORNL develops and maintains CTF and CTFFuel within the CTF Users' Group for standalone applications and coupling with other codes and within the VERA Users' Group for multi-physics applications. CTF provides whole-core two-phase sub-channel thermal-hydraulics solutions with the following features: two-fluid three-field representation of the two-phase flow; cross flow between channels; solution extends outside of active fuel; modeling of spacer grid pressure loses and blockages as well as intra-grid form losses; CFD-informed turbulence modeling; transient analyses; and an efficient parallel solution. In summary, CTF provides the best available sub-channel methods to the scale of an entire reactor core. CTFFuel provides a fast, robust fuel temperature capability to VERA for whole-core depletion and transients. CTFFuel has the following features: burnup-dependent thermal conductivity, clad creep, relocation, and pellet swelling models; fast intra-pin burnup and temperature coupling; functional for steady-state and transient conditions; consistent temperature feedback for multiple fuel types; and implemented as an extendable interface.

While there are some existing procedures and guidelines for traditional multi-physics verification and validation, there is a need for implementing verification and validation protocols for novel methods. The development of validation benchmarks for novel methods should also utilize sequence (series) of progression validation experiments. It is challenging to apply a consistent hierarchical validation of novel multi-physics simulation methods—it is difficult to find data to validate interaction parameters using publicly available experimental data sources: for single physics validation as well as for two-physics validation where the non-linear interactions are modeled. Another data gap in validation of high-fidelity multi-physics calculations is the lack of high-quality high-resolution simultaneously measured data of feedback parameters. In order to validate such models, high-quality experimental data on such refined local scale are needed. The measurements must be done on pin (or sub-pin) level using state-of-the-art experimental methods. The progression benchmark experiments need to be designed to provide adequate data resolution in time and space, adequate measurement of boundary conditions, and adequate characterization of uncertainty.

The new OECD/NEA verification benchmark for novel multi-physics simulation methods is the C5G7-TD (Deterministic Time-Dependent Neutron Transport Benchmark without Spatial Homogenization) benchmark [8,9]. A new set of validation OECD/NEA

benchmarks have been initiated by the Expert Group on Multi-Physics Validation data, Benchmarking and Validation (EGMPEBV) at the NEA/OECD to address the current validation needs. These benchmarks have the following common features: utilization of high-quality experimental data; refined local scale modelling in addition to global predictions; more detailed comparisons and analysis; and including uncertainty and sensitivity analysis of modelling predictions. The benchmarks include the Multi-Physics Pellet Clad Mechanical Interaction Validation (MPCMIV) Benchmark; the Rostov-2 VVER-1000 Benchmark; and the TVA Watts Bar Unit 1 (WB-1) Multi-Physics Multi-Cycle Benchmark. The WB-1 measured data consists of both types of measured data—integral parameters and local distributions. Figures 6 and 7 illustrate the different types of benchmark measured data for WB-1 Cycle depletion for Exercise 3—Physical Reactor Depletion for Cycle 1 [10].
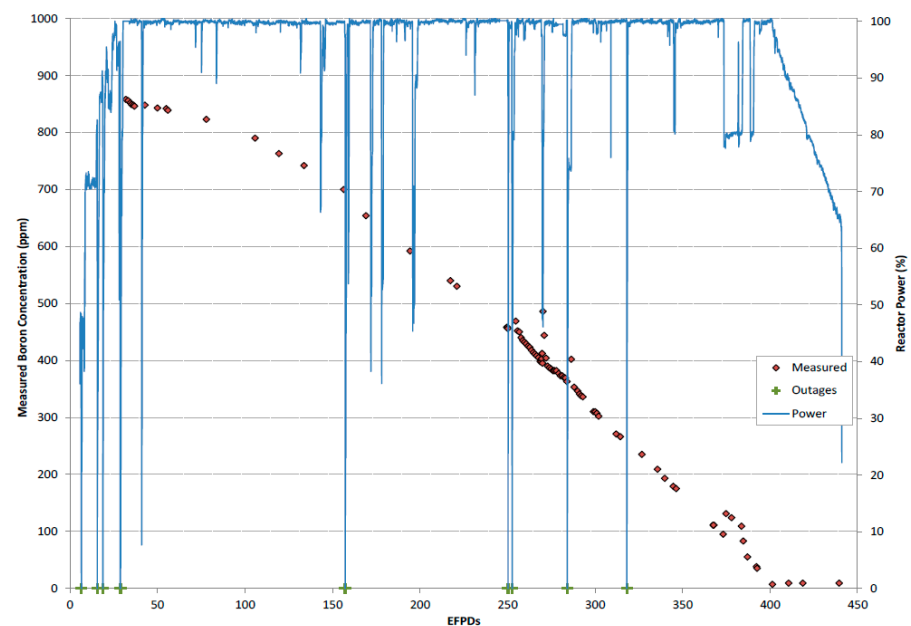

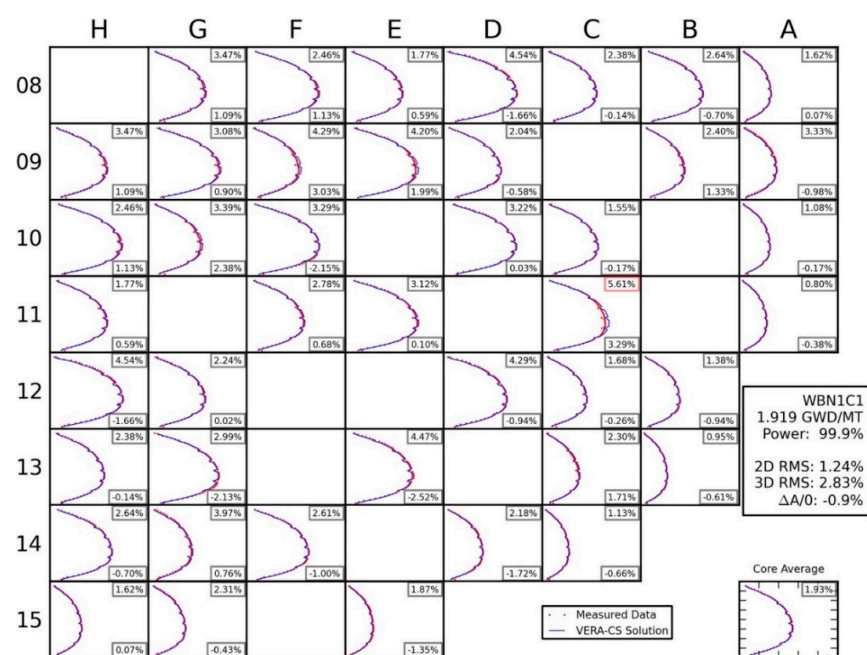**Figure 6.** Critical boron concentration as function of burnup for Cycle 1 [10].

Figure 7. Example of 3-D flux map at a point in Cycle 1 depletion [10].

4. Improved Multi-Physics Multi-Scale M&S

In many applications, several simulators of a physical process are available to describe the same system each with different levels of fidelity. In these cases, a higher fidelity model is thought to better represent the physical process than a lower fidelity model, but also takes more computational time and memory to execute. Therefore, combining relatively cheap lower fidelity model calculations with more costly high-fidelity simulations (known as the high-to-low, Hi2Lo, information scheme) to emulate the high-fidelity model prediction accuracy has been a significant problem of interest. The Hi2Lo approach is currently being adopted in nuclear reactor research and industry. The focus is on the use of validated high-fidelity simulation codes to inform, improve and calibrate low-fidelity codes to facilitate multi-physics coupling, design, performance analysis, and risk assessment.

Due to their complexity, the high-fidelity calculations are computationally expensive, and may take in the orders of hours to days to complete. This motivates the use of low-fidelity models, which are less comprehensive but provide numerical efficiency required for practical applications in design and safety evaluations. The low-fidelity codes have parameters or inputs that must be informed or calibrated using experimental data or simulations from validated high-fidelity codes. High-fidelity models can be used to predict physical behavior in regimes or on scales where physical data is not available. Several methods have been proposed to address the integration of high-fidelity and low-fidelity codes to predict quantities of interests in an efficient manner. Examples are the improved modelling of spacer grid effects in sub-channel thermal-hydraulics M&S [11] and the calibration methodology developed for gap conductance modeling in fuel rod heat transfer of a core thermal-hydraulics model by leveraging a high-fidelity fuel performance code [12].

The simultaneous implementation of Hi2Lo to different physics models within the coupled multi-physics M&S can be performed more efficiently using a common platform. An on-going project at NC State University, funded by the US DOE Nuclear Energy University Program, is focused on demonstrating the utilization of high-fidelity NEAMS tools (PROTEUS, Nek5000, and BISON) to inform the improved use of conventional tools (DIF3D, CTF, and CTFFuel) for single- and multi-physics calculations within the NEAMS Workbench platform on the NEA/OECD C5G7-TD benchmark [13]. High-fidelity models (MOC in neutronics, CFD in thermal-hydraulics, and fuel performance codes in fuel rod modelling) are then used to evaluate the improved traditional multi-physics M&S.

5. Uncertainty Quantification in Multi-Physics M&S

The uncertainty quantification and propagation in multi-physics simulations require development of methodologies that can treat large, highly dimensional data sets, allow for combinations of different input sources of uncertainties, and account for non-linear feedback effects. When this is combined with uncertainty propagation through multi-scale and Hi2Lo model information processes for individual physics models, there is a need to make the overall uncertainty quantification and propagation procedure also more efficient by using for example surrogate models or reduced order modelling techniques (for reducing the computational complexity of mathematical models in numerical simulations), etc.

A comprehensive OECD/NEA LWR UAM benchmark framework was recently established for uncertainty propagation through multi-physics, multi-scale calculations in order to compare different uncertainty analysis methods [14]. The benchmark framework is designed to propagate most significant uncertainties through the traditional multi-physics calculations. Within the benchmark off-line single-physics multi-scale M&S is used to inform (improve) the single physics models within the traditional multi-physics coupling. Uncertainties propagated in these single-physics Hi2Lo multi-scale model information schemes form the input uncertainties in traditional multi-physics calculations. Figure 8 illustrates the approach.
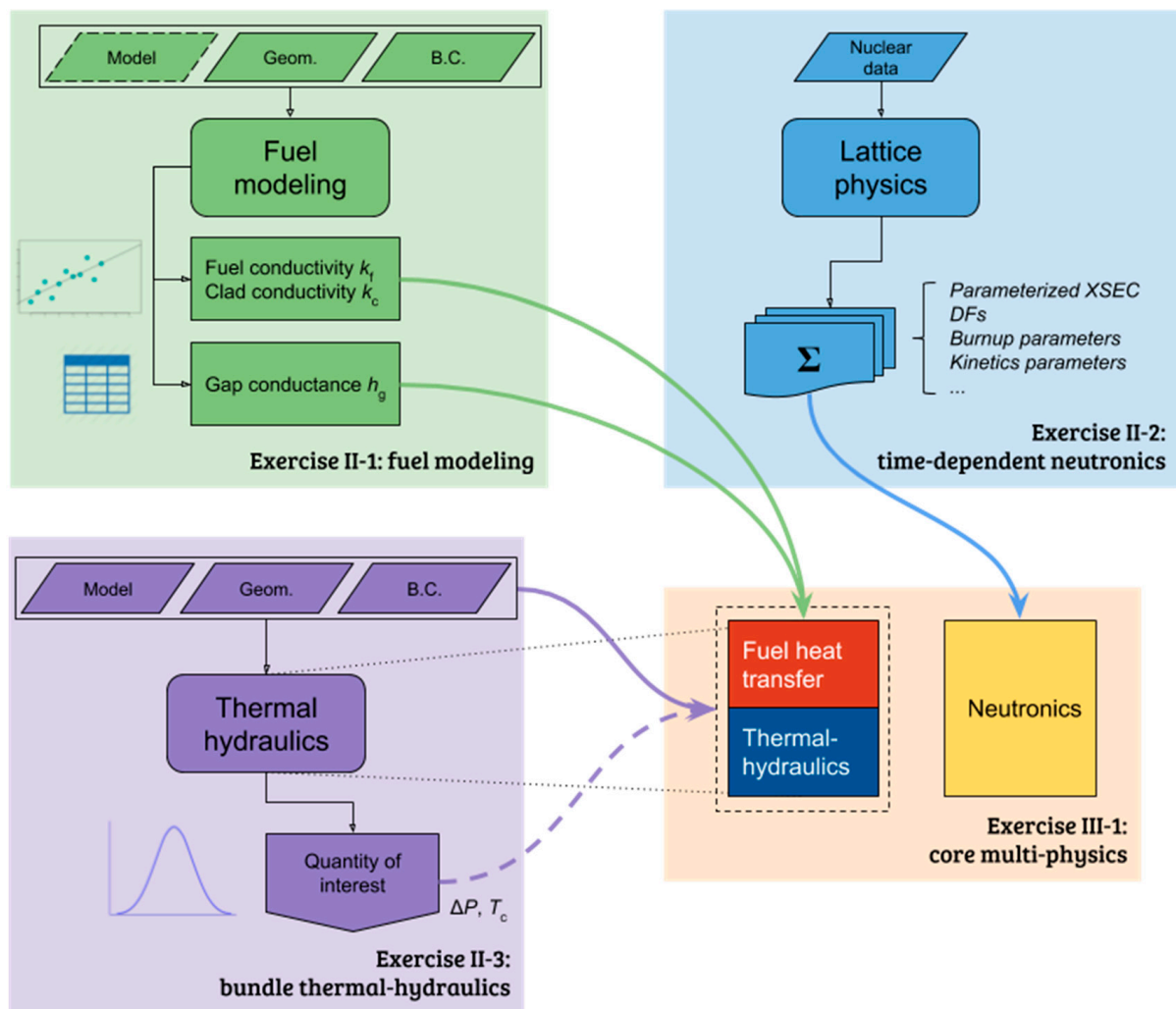
Figure 8. OECD/NEA LWR UAM benchmark multi-physics with uncertainties framework.

Uncertainty propagation methodology (shown in Figure 9) has been developed at NC State University based on a stochastic sampling method by taking into account the uncertainties of the three physics M&S (neutronics, thermal-hydraulics, and fuel physics) in the simulation of PWRs that can be incorporated in the conventional LWR simulation approach.
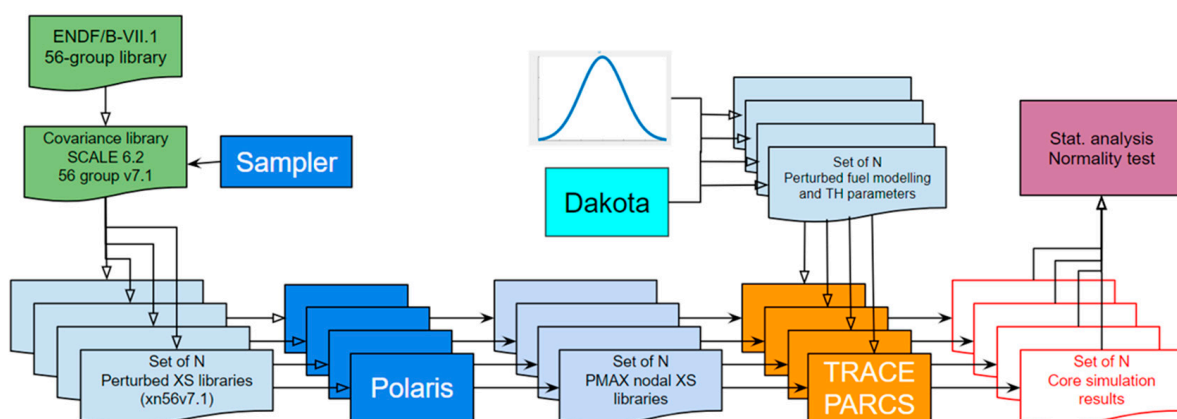

Figure 9. Statistical multi-physics uncertainty propagation methodology.

More specifically, the Three Mile Island Unit 1 (TMI-1) related exercises from the LWR-UAM benchmark were modeled using the coupled TRACE/PARCS code system in 3D core representation [15]. The input uncertainties of the neutronics simulation include few-group cross sections and kinetics parameters generated using the SAMPLER/POLARIS sequence of SCALE 6.2.1. DAKOTA was used to sample input parameters of the coupled code system and to perform the uncertainty analysis. Two types of simulations were conducted: steady-state calculation at hot full power condition and transient scenario initiated by the spatially asymmetric Rod Ejection Accident (REA). Quantities of interest for the steady-state calculation, including core multiplication factor and power peaking factors, were calculated with associated uncertainties. For transient calculations, best-estimate plus uncertainty results of the time evolution of core reactivity, core power, and peak fuel temperature were generated and analyzed. Selected results for the beginning of cycle TMI-1 REA—time evolutions of total core power and core peak fuel temperature are shown in Figures 10 and 11. The drawback of the utilized independent input uncertainty propagation is investigated and obtained results indicate the importance of investigating the correlation between input parameters from different physics domains. It is suggested constructing the correlations among selected input parameters and propagating them consistently in the core calculation.
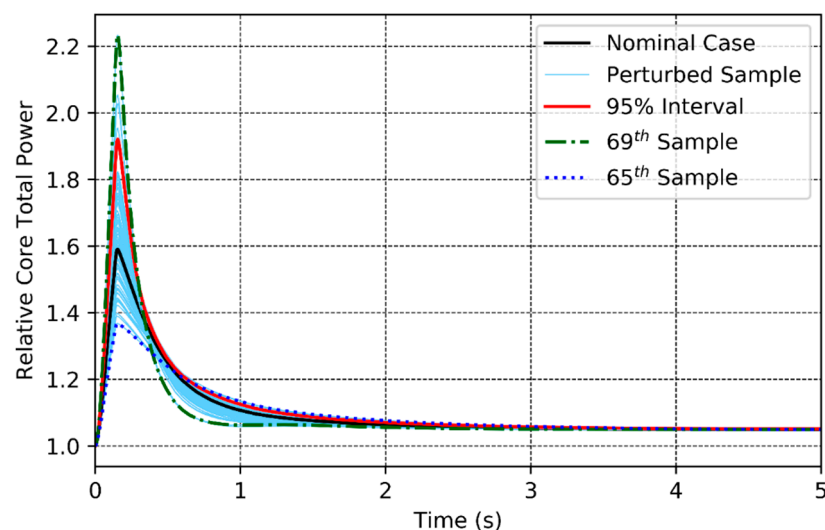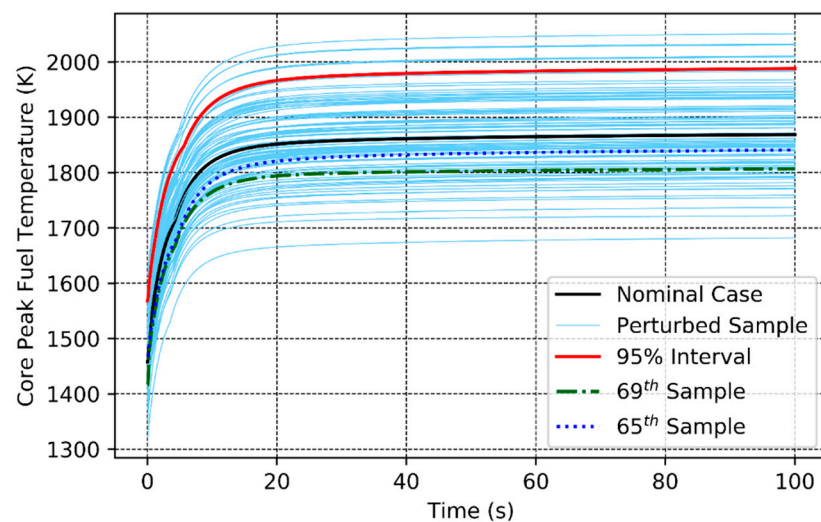

Figure 10. Total power evolution.

Figure 11. Core peak fuel temperature evolution.

6. Conclusions

The traditional multi-physics calculations are being used in industry and regulation for routine design and safety evaluations. In parallel, the currently on-going projects worldwide in the area of advanced modelling and simulation aim at delivering to the corresponding stakeholders an advanced and reliable software capacity, usable for the design and safety analysis needs of present and future nuclear reactors. These novel multi-physics simulations are based on state-of-the-art simulation platforms, which include advanced core physics, two-phase thermal-hydraulics, and fuel modelling as well as multi-scale and multi-physics features together with sensitivity and uncertainty tools. While there are some existing procedures and guidelines for traditional multi-physics validation, there is a need for implementing validation processes for novel methods.

Data science and analytics techniques have been utilized in different applications in nuclear science and engineering. There is a unique opportunity to integrate a modern data technology platform in advanced modeling and simulation including verification, validation and uncertainty quantification. Collection, qualification, and management of data are instrumental for the data-driven modeling. The growing interest and potential application of data-driven modeling creates a new domain in verification and validation of codes that involve machine-learning-based data-driven models. The current tendency is to utilize physics-informed data-driven frameworks for model development and validation.

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